Supporting Information

Nickel-Catalyzed Decarboxylative Cross-Coupling of Indole-3-acetic Acids with Aryl Bromides by Convergent Paired Electrolysis

Zhen-Hua Wang, Lei Wei, Ke-Jin Jiao, Cong Ma, and Tian-Sheng Mei*

State Key Laboratory of Organometallic Chemistry, Center for Excellence in Molecular Synthesis, Shanghai Institute of Organic Chemistry, Chinese Academy of Science, 345 Lingling Lu, Shanghai 200032, China

*E-mail: mei7900@sioc.ac.cn

Table of Contents

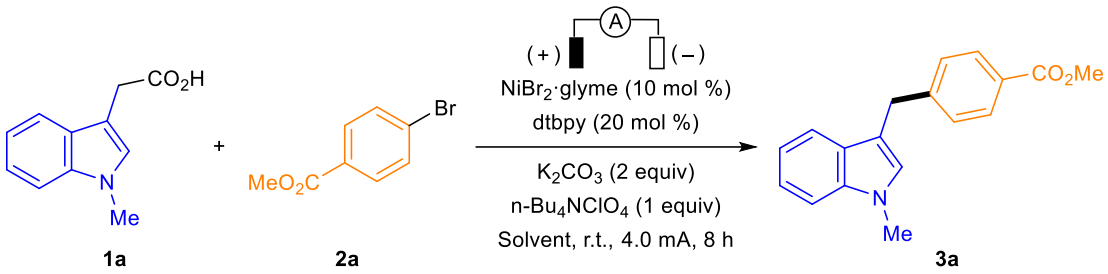
1. General Information

Commercially available materials were used without further purification. Column chromatography was performed using either 100-200 Mesh or 300-400 Mesh silica gel. Visualization of spots on TLC plate was accomplished with UV light (254 nm) and staining over I_2 chamber.

All commercial reagents were purchased from TCI, Alfa-aesar, Adamas-beta, J&K, Bide chemistry and Energy Chemical of the highest purity grade. They were used without further purification unless specified. Nickel(II) bromide ethylene, glycol dimethyl ether was purchased from Strem chemicals and was used as received. DMA (99.8%, SuperDry) was purchased from J&K and was used without further purification. ^{1}H NMR and ^{13}C NMR spectra were recorded on Agilent AV 400, Bruker 400, Varian Inova 400 (400 MHz and 100 MHz, respectively). ^{19}F NMR spectra were recorded on Agilent AV 400, Varian Inova 400 (376 MHz) instrument. The peaks were internally referenced to TMS (0.00 ppm) or residual undeuterated solvent signal. The following abbreviations were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, and br = broad. Infrared spectra were obtained on a Bio-Rad FTS-185 instrument. High resolution mass spectra were recorded at the Center for Mass Spectrometry, Shanghai Institute of Organic Chemistry. Analytical and spectral data of all those known compounds are exactly matching with the reported values.

2. Optimization Details

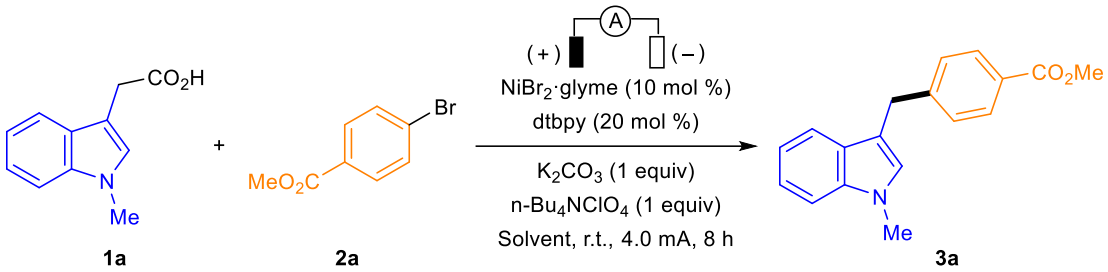
Table S1. Screening of solvent.[a]



Entry	Solvent	Yield (%)[b]
1	DMAc	30
2	DMF	18
3	MeCN	0
4	DMSO	0

[a] Reaction conditions: anode (Pt), cathode (Ni foam), **1a** (0.3 mmol, 1 equiv), **2a** (0.60 mmol, 2 equiv), $NiBr_2$ glyme (10 mol %), dtbpy (20 mol %), *n*-Bu_4NClO_4 (0.3 mmol, 1 equiv), K_2CO_3 (0.6 mmol, 2 equiv) in solvent (3 mL) at room temperature, 4 mA for 8 h. [b] Yields were determined by ^1H NMR using CH_2Br_2 as an internal standard.

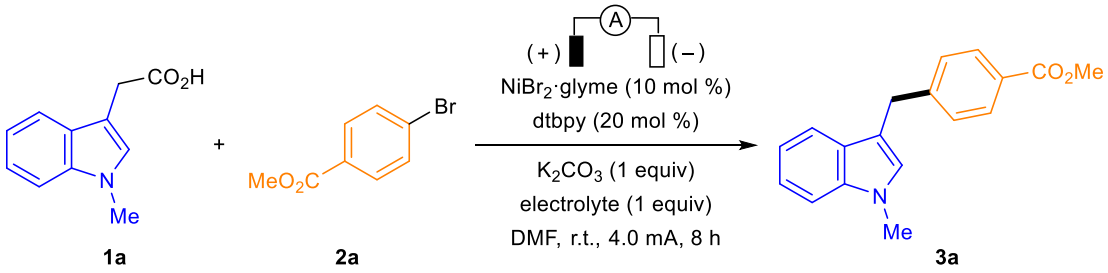
Table S2. Screening of anode.[a]



Entry	Anode	Solvent	Yield (%)[b]
1	Pt	DMAc	10
2	Pt	DMF	37
3	C	DMAc	16
4	C	DMF	15

[a] Reaction conditions: cathode (Ni foam), **1a** (0.3 mmol, 1 equiv), **2a** (0.60 mmol, 2 equiv), $NiBr_2$ glyme (10 mol %), dtbpy (20 mol %), *n*-Bu_4NClO_4 (0.3 mmol, 1 equiv), K_2CO_3 (0.3 mmol, 1 equiv) in solvent (3 mL) at room temperature, 4 mA for 8 h. [b] Yields were determined by ^1H NMR using CH_2Br_2 as an internal standard.

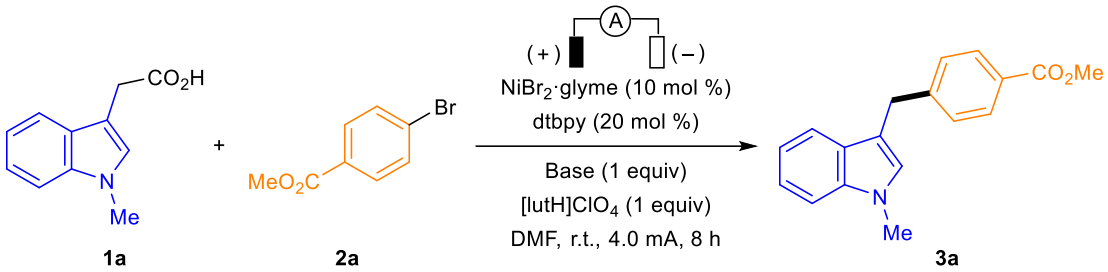
Table S3. Screening of electrolyte.[a]



Entry	Electrolyte	Yield (%)[b]
1	*n*-Bu_4NClO_4	37
2	*n*-Bu_4NBr	33
3	*n*-Bu_4NBF_4	52
4	[lutH]ClO_4	55

[a] Reaction conditions: anode (Pt), cathode (Ni foam), **1a** (0.3 mmol, 1 equiv), **2a** (0.60 mmol, 2 equiv), $NiBr_2$ glyme (10 mol %), dtbpy (20 mol %), electrolyte (0.3 mmol, 1 equiv), K_2CO_3 (0.3 mmol, 1 equiv) in solvent (3 mL) at room temperature, 4 mA for 8 h. [b] Yields were determined by ^1H NMR using CH_2Br_2 as an internal standard.

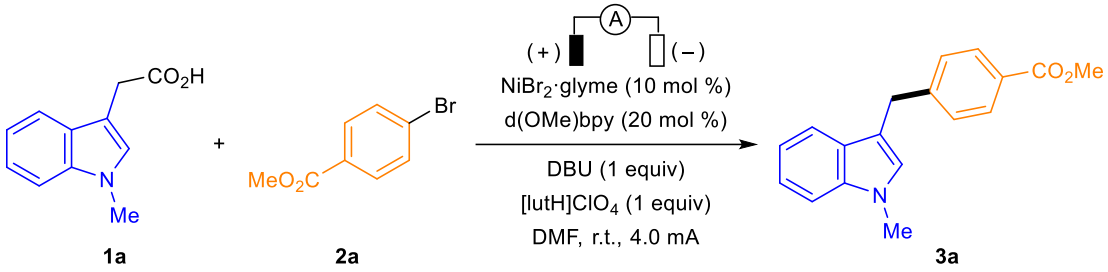
Table S4. Screening of base.[a]



Entry	Base	Yield (%)[b]
1	K_2CO_3	55
2	2,6-lutidine	14
3	2,4,6-collidine	15
4	(*t*-Bu)(*i*-Pr)NH	48
5	DBU	60
6	no base	0

[a] Reaction conditions: anode (Pt), cathode (Ni foam), **1a** (0.3 mmol, 1 equiv), **2a** (0.60 mmol, 2 equiv), $NiBr_2$ glyme (10 mol %), dtbpy (20 mol %), [lutH]ClO_4 (0.3 mmol, 1 equiv), base (0.3 mmol, 1 equiv) in DMF (3 mL) at room temperature, 4 mA for 8 h. [b] Yields were determined by ^{1}H NMR using CH_2Br_2 as an internal standard.

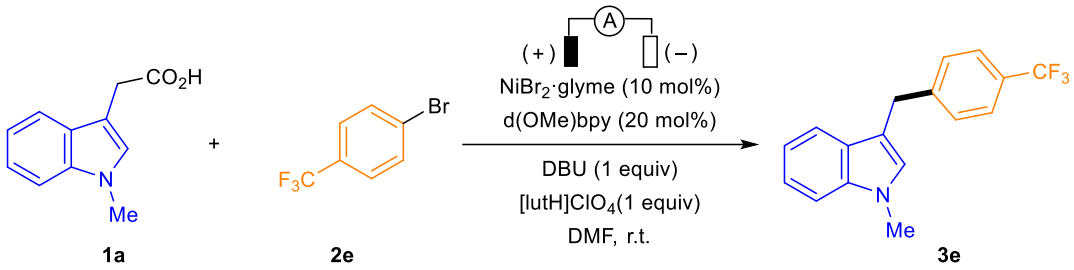
Table S5. Screening the reaction time.[a]



Entry	Time (h)	Yield (%)[b]
1	8	60
2	10	71[c]
3	12	53

[a] Reaction conditions: anode (Pt), cathode (Ni foam), **1a** (0.3 mmol, 1 equiv), **2a** (0.60 mmol, 2 equiv), $NiBr_2$ glyme (10 mol%), d(OMe)bpy (20 mol%), [lutH]ClO_4 (0.3 mmol, 1 equiv), DBU (0.3 mmol, 1 equiv) in DMF (3 mL) at room temperature, 4 mA. [b] Yields were determined by ^{1}H NMR using CH_2Br_2 as an internal standard. [c] Isolated yield.

3. On/Off experiment



The dried nickel foam electrode (2.0 × 3.0 cm^2), platinum electrode (1.0 × 1.0 cm^2) and 10 mL hydrogenation tube charged with a proper stir bar are moved into the glove box. To the hydrogenation tube was added **1a** (0.3 mmol, 1 equiv), **2e** (0.60 mmol, 2 equiv), $NiBr_2$ glyme (10 mol %), d(OMe)bpy (20 mol %), $[lutH]ClO_4$ (0.3 mmol, 1 equiv), DBU (0.3 mmol, 1 equiv), (trifluoromethoxy)benzene (0.3 mmol, 1 equiv) in DMF (3 mL). The tube was sealed with a septum equipped with anode (Pt), cathode (Ni foam), and the reaction mixture was electrolyzed under a constant current of 4.0 mA at room temperature. Periodically, an aliquot (~ 0.1 mL) was removed from the mixture and analyzed by ^{19}F-NMR (Figure S1).

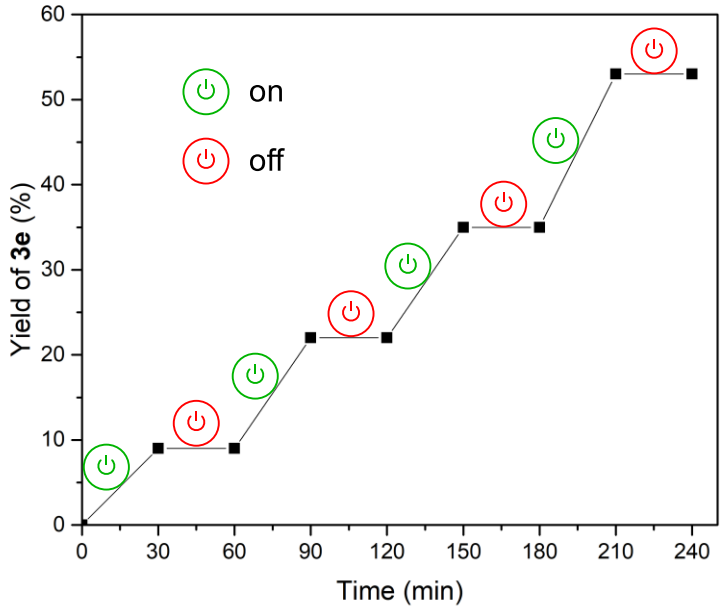


Figure S1. On/Off experiment.

4. Cyclic Voltammetry

Cyclic voltammograms were recorded with a CHI760E potentiostat at room temperature in DMF. *n*-Bu_4NPF_6 (0.1 M) was used as the supporting electrolyte, and a Glass Carbon electrode or platinum electrode was used as the working electrode. The auxiliary electrode was a Pt sheet. All potentials are referenced against the $Ag/AgNO_3$ redox couple. The scan rate was 100 mV s^{-1}.

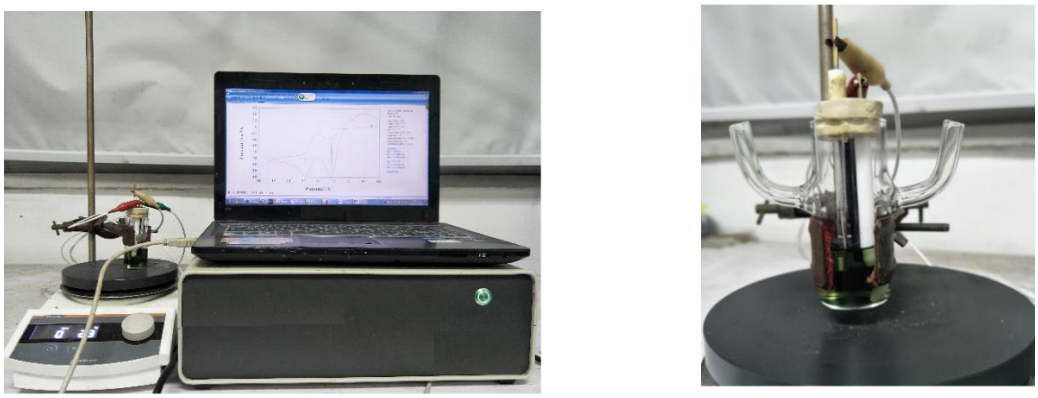


Figure S1. Photograph of setup used for cyclic voltammetry.

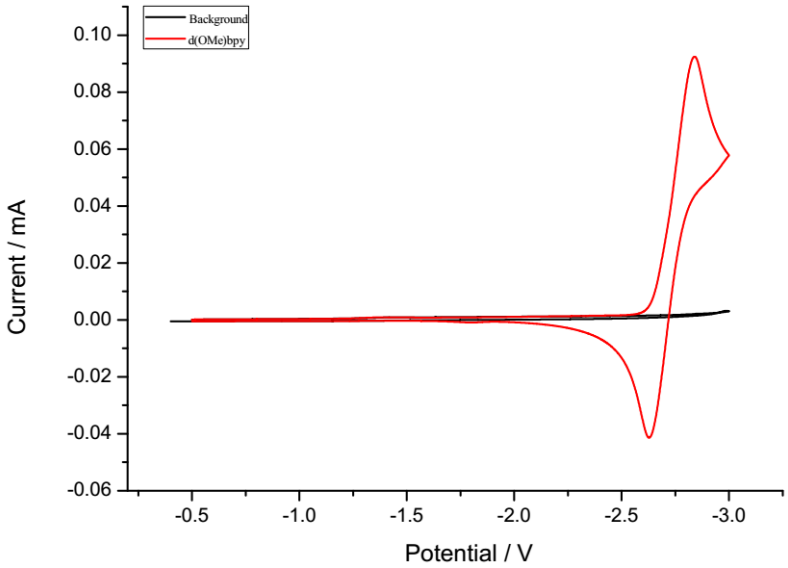


Figure S2. Cyclic voltammograms recorded on Glass Carbon electrode: **(Red line)** DMF containing 0.1 M of *n*-Bu_4NPF_6, 10 mM of d(OMe)bpy. **(Black line)** DMF containing 0.1 M *n*-Bu_4NPF_6.

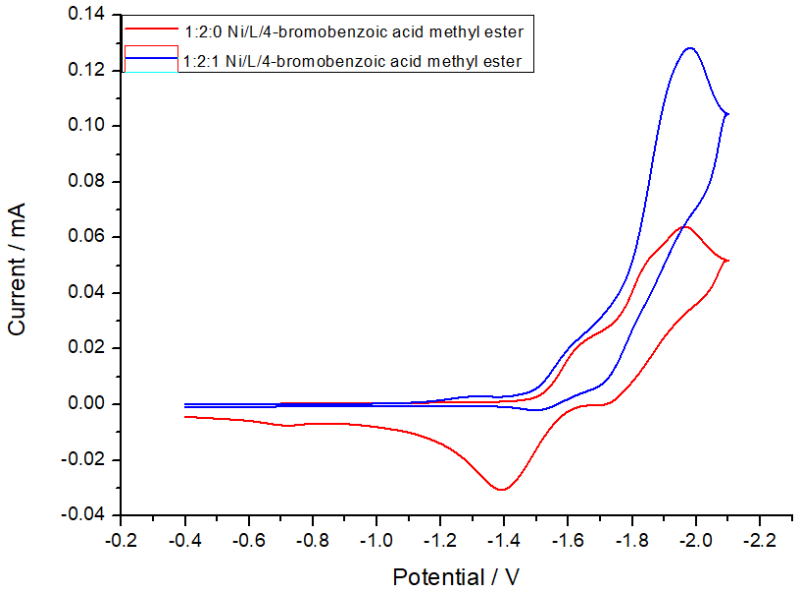


Figure S3. Cyclic voltammograms recorded on Glass Carbon electrode:

(Red line) DMF containing 0.1 M of *n*-Bu_4NPF_6, 10 mM of $NiBr_2$ glyme and 20 mM d(OMe)bpy.

(Blue line) Solution after addition of 10 mM **2a**.

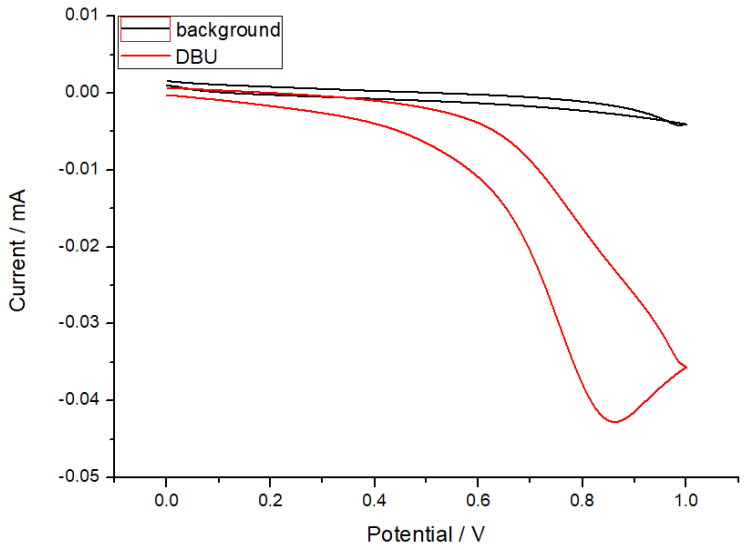


Figure S4. Cyclic voltammograms recorded on a platium electrode:

(Black line) DMF containing 0.1 M *n*-Bu_4NPF_6.

(Red line) solution after addition of 10 mM DBU.

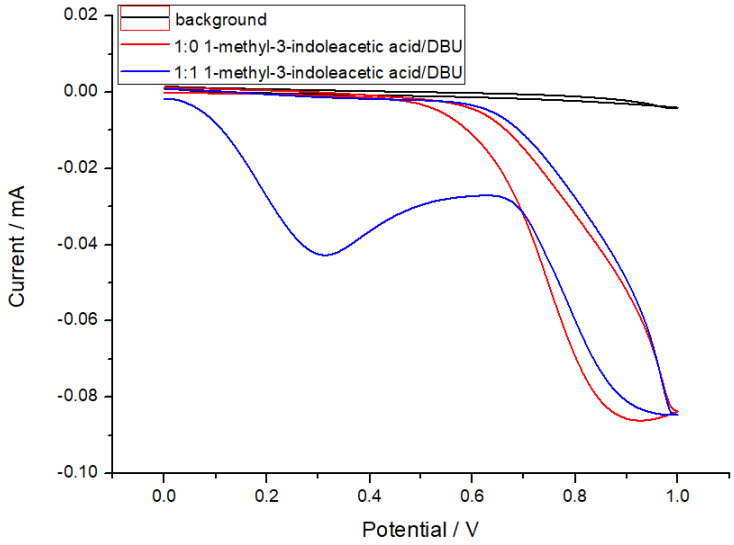


Figure S5. Cyclic voltammograms recorded on a platium electrode:

(Black line) DMF containing 0.1 M *n*-Bu_4NPF_6.

(Red line) solution after addition of 10 mM **1a**.

(Blue line) solution after addition of 10 mM DBU.

5. Potentials of Anode and Cathode During the Electrolysis

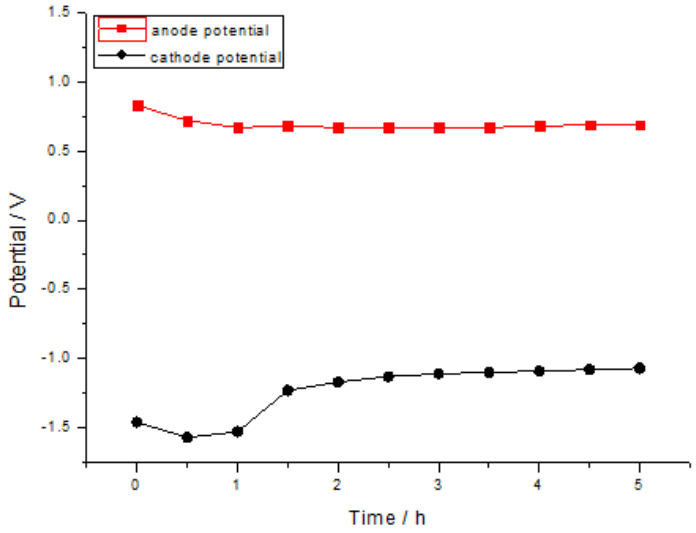
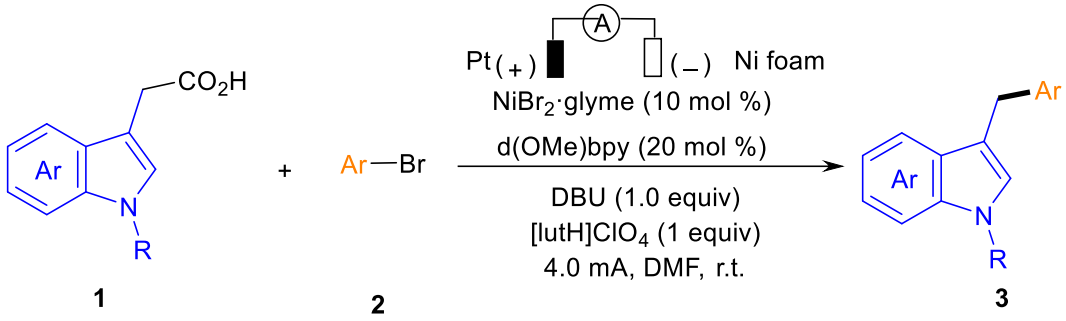


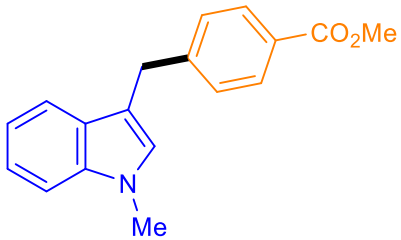
Figure S8. Electric potentials of anode and cathode from standard reaction conditions. All potentials are referenced against the $Ag/AgNO_3$ redox couple.

6. General Procedure and Characterization Data



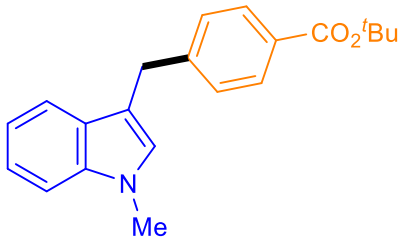
The dried nickel foam electrode (2.0 × 3.0 cm^2), platinum electrode (1.0 × 1.0 cm^2) and 10 mL hydrogenation tube charged with a proper stir bar are moved into the glove box. To the hydrogenation tube was added **1** (0.3 mmol, 1 equiv), **2** (0.60 mmol, 2 equiv), $NiBr_2$ glyme (10 mol %), d(OMe)bpy (20 mol %), $[lutH]ClO_4$ (0.3 mmol, 1 equiv), DBU (0.3 mmol, 1 equiv) in DMF (3 mL). The tube was sealed with a septum equipped with anode (Pt), cathode (Ni foam), and the reaction mixture was electrolyzed under a constant current of 4.0 mA for 10 h at room temperature. After the reaction was completed, the mixture was diluted with 20 mL of water and extracted with EtOAc (3×20 mL). The organic layer was washed with saturated NH_4Cl (aq.) (10 mL), dried over Na_2SO_4, filtered, and the solvent removed under reduced pressure. The crude product was purified by flash column chromatography (eluent: Petroleum ether), affording the desired product.

Methyl 4-((1-methyl-1*H*-indol-3-yl)methyl)benzoate (3a)[1]



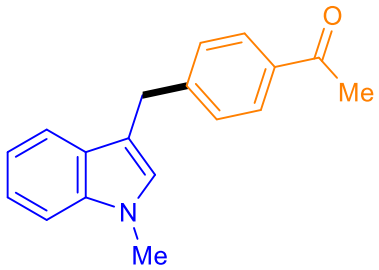
White solid (59.9 mg, 71% yield).**^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.0 Hz, 2H), 7.48 (d, *J* = 8.0 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 1H), 7.24 (t, *J* = 7.2 Hz, 1H), 7.09 (t, *J* = 7.2 Hz, 1H), 6.77 (s, 1H), 4.16 (s, 2H), 3.90 (s, 3H), 3.73 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 167.3, 147.1, 137.3, 129.9, 128.8, 128.0, 127.8, 127.4, 121.9, 119.2, 119.1, 113.3, 109.4, 52.1, 32.8, 31.8.

***Tert*-butyl 4-((1-methyl-1*H*-indol-3-yl)methyl)benzoate (3b)**



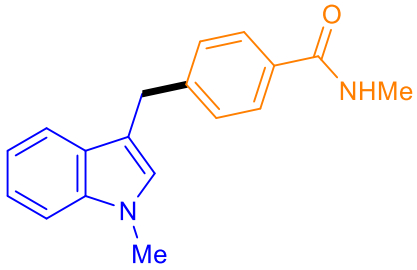
Colorless oil (67.5 mg, 70% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.0 Hz, 2H), 7.51 (d, *J* = 8.0 Hz, 1H), 7.37 (d, *J* = 8.0 Hz, 2H), 7.26 (t, *J* = 8.0 Hz, 1H), 7.11 (t, *J* = 7.8 Hz, 1H), 6.78 (s, 1H), 4.18 (s, 2H), 3.75 (s, 3H), 1.63 (s, 9H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 166.0, 146.5, 137.2, 129.8, 129.6, 128.6, 127.7, 127.3, 121.8, 119.2, 119.0, 113.5, 109.3, 80.8, 32.7, 31.7, 28.3. **HRMS** (EI) calculated for $C_{21}H_{23}NO_2$ $[M]^+$: 321.1723, found: 321.1730. **IR** (neat): ν 2975, 1706, 1609, 1472, 1414, 1367, 1290, 1252, 1162, 1114, 1016, 909, 848, 799, 761, 736, 707, 565, 524, 452, 426 cm^{-1}.

1-(4-((1-Methyl-1*H*-indol-3-yl)methyl)phenyl)ethan-1-one (3c)



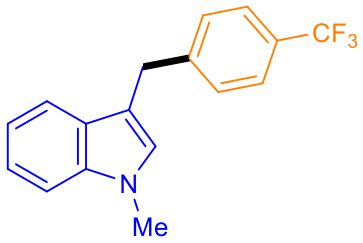
White solid (47.4 mg, 60% yield). Melting point 86.3–87.4 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.0 Hz, 2H), 7.48 (d, *J* = 8.4 Hz, 1H), 7.38 (d, *J* = 7.6 Hz, 2H), 7.31 (d, *J* = 8.4 Hz, 1H), 7.24 (t, *J* = 8.0 Hz, 1H), 7.09 (t, *J* = 6.8 Hz, 1H), 6.79 (s, 1H), 4.16 (s, 2H), 3.75 (s, 3H), 2.58 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 198.0, 147.4, 137.3, 135.2, 128.9, 128.6, 127.7, 127.3, 121.8, 119.1, 119.0, 113.2, 109.4, 32.7, 31.7, 26.7. **HRMS** (EI) calculated for $C_{18}H_{17}NO$ $[M]^+$: 263.1302, found: 263.1302. **IR** (neat): ν 3053, 2920, 1674, 1603, 1569, 1471, 1420, 1357, 1327, 1255, 1182, 1153, 1122, 1060, 1013, 954, 916, 852, 805, 784, 729, 687, 577, 471, 449, 425 cm^{-1}.

***N*-methyl-4-((1-methyl-1*H*-indol-3-yl)methyl)benzamide (3d)**



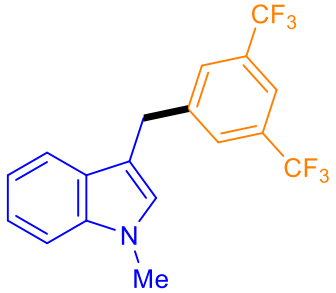
White solid (54.2 mg, 65% yield). Melting point 173.7–175.5 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 7.6 Hz, 2H), 7.45 (d, *J* = 8.0 Hz, 1H), 7.29 (d, *J* = 7.6 Hz, 3H), 7.21 (t, *J* = 7.6 Hz, 1H), 7.06 (t, *J* = 7.6 Hz, 1H), 6.74 (s, 1H), 6.24 (s, 1H), 4.11 (s, 2H), 3.71 (s, 3H), 2.95 (d, *J* = 4.8 Hz, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 168.4, 145.2, 137.3, 132.4, 128.9, 127.7, 127.3, 127.0, 121.8, 119.2, 119.0, 113.5, 109.3, 32.7, 31.5, 26.9. **HRMS** (ESI) calculated for $C_{18}H_{19}N_2O$ $[M+H]^+$: 279.1492, found: 279.1497. **IR** (neat): ν 3342, 2901, 1627, 1546, 1503, 1475, 1404, 1375, 1326, 1303, 1252, 1156, 1124, 1060, 1010, 921, 840, 791, 762, 736, 675, 645, 611, 565, 484, 423 cm^{-1}.

1-Methyl-3-(4-(trifluoromethyl)benzyl)-1*H*-indole (3e)[2]



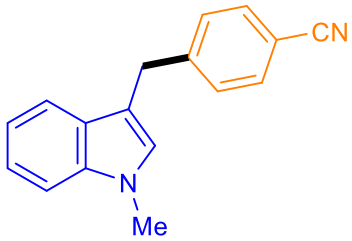
White solid (52.2 mg, 60% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8.0 Hz, 2H), 7.50 (m, 1H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.33 (m, 1H), 7.29–7.22 (m, 1H), 7.12 (m, 1H), 6.80 (s, 1H), 4.18 (s, 2H), 3.76 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 145.8, 137.4, 129.1, 128.3 (q, *J* = 32.0 Hz), 127.8, 127.4, 125.4 (q, *J* = 3.8 Hz), 124.6 (q, *J* = 272.0 Hz), 121.9, 119.2, 119.1, 113.2, 109.4, 32.8, 31.5. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.2.

3-(3,5-Bis(trifluoromethyl)benzyl)-1-methyl-1*H*-indol (3f)



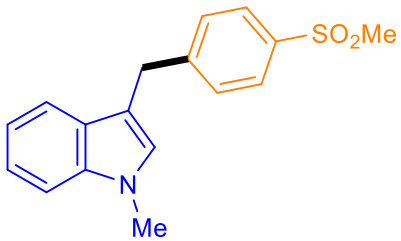
White solid (48.6 mg, 45% yield). Melting point 56–57 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.74–7.69 (m, 3H), 7.43 (m, 1H), 7.31–7.30 (m, 1H), 7.27–7.21 (m, 1H, contains residual solvent signal of $CDCl_3$), 7.09 (m, 1H), 6.79 (s, 1H), 4.20 (s, 2H), 3.75 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 144.1, 137.3, 131.5 (q, *J* = 33.0 Hz), 128.80, 128.77, 127.40, 127.36, 123.50 (q, *J* = 272.0 Hz), 122.0, 120.28–119.93 (m), 119.3, 118.7, 112.1, 109.5, 32.72, 31.4. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.9. **HRMS** (EI) calcd for $C_{18}H_{13}F_6N$ $[M]^+$: 357.0947, found: 357.0956. **IR** (neat): ν 3047, 2919, 1618, 1468, 1372, 1276, 1164, 1119, 734, 702, 679, 426 cm^{-1}.

4-((1-Methyl-1*H*-indol-3-yl)methyl)benzonitrile (**3g**)



White solid (45.0 mg, 62% yield). Melting point 75–77 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 8.0 Hz, 2H), 7.40 (m, 1H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.29 (m, 1H), 7.25–7.19 (m, 1H), 7.09–7.02 (m, 1H), 6.78 (s, 1H), 4.13 (s, 2H), 3.72 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 147.3, 137.3, 132.2, 129.4, 127.6, 127.4, 121.9, 119.2, 119.2, 119.0, 112.4, 109.8, 109.4, 32.7, 31.7. **HRMS** (ESI) calcd for $C_{17}H_{15}N_2$ $[M+H]^+$: 247.1230, found: 247.1230. **IR** (neat): ν 3049, 2912, 2222, 1604, 1501, 1370, 1326, 1238, 841, 814, 737, 546, 426 cm^{-1}.

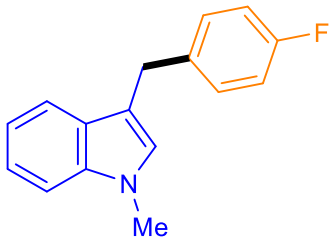
1-Methyl-3-(4-(methylsulfonyl)benzyl)-1*H*-indole (**3h**)



White solid (66.9 mg, 75% yield). Melting point 113–114 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.0 Hz, 2H), 7.47–7.40 (m, 3H), 7.29 (m, 1H), 7.22 (m, 1H), 7.06 (m, 1H), 6.80 (s, 1H), 4.16 (s, 2H), 3.73 (s, 3H), 2.99 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 148.3, 138.1, 137.3, 129.6, 127.6, 127.5, 127.4, 121.9, 119.1, 119.0, 112.5, 109.5, 44.6, 32.7, 31.6. **HRMS** (ESI) calculated for

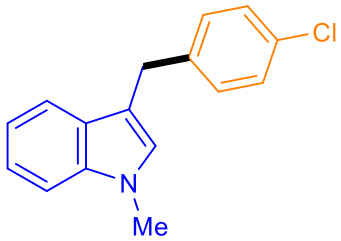
$C_{17}H_{18}NO_2S$ $[M+H]^+$: 300.1053, found: 300.1046. **IR** (neat): ν 2917, 1613, 1468, 1418, 1300, 1141, 1087, 956, 764, 750, 730, 520, 423 cm^{-1}.

3-(4-Fluorobenzyl)-1-methyl-1*H*-indole (**3i**)



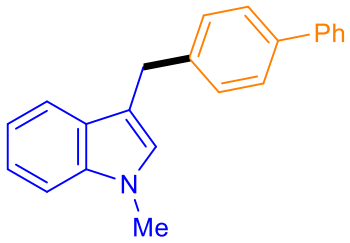
Pale-red oil (34.3 mg, 48% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.47 (d, *J* = 8.0 Hz, 1H), 7.28 (d, *J* = 8.0 Hz, 1H), 7.25–7.18 (m, 3H, contains residual solvent signal of $CDCl_3$), 7.06 (m, 1H), 6.97–6.90 (m, 2H), 6.73 (s, 1H), 4.05 (s, 2H), 3.71 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 161.3 (d, *J* = 242.0 Hz), 137.3, 137.1 (d, *J* = 3.0 Hz), 130.0 (d, *J* = 8.0 Hz), 127.7, 127.1, 121.7, 119.2, 118.9, 115.1 (d, *J* = 21.0 Hz), 114.2, 109.3, 32.6, 30.8. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -118.0. **HRMS** (EI) calculated for $C_{16}H_{14}FN$ $[M]^+$: 239.1105, found: 239.1101. **IR** (neat): ν 3049, 2910, 1601, 1552, 1504, 1372, 1216, 1153, 1011, 806, 735, 509, 425 cm^{-1}.

3-(4-Chlorobenzyl)-1-methyl-1*H*-indole (**3j**)



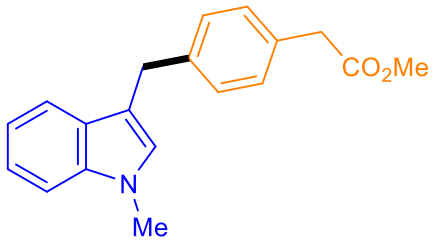
White solid (55.7 mg, 73% yield). Melting point 63–65 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 8.0 Hz, 1H), 7.27 (d, *J* = 8.0 Hz, 1H), 7.24–7.16 (m, 5H), 7.06 (m, 1H), 6.72 (s, 1H), 4.04 (s, 2H), 3.70 (s, 3H). **^{13}C{^{1}H} NMR** (101 MHz, $CDCl_3$) δ 140.0, 137.3, 131.6, 130.1, 128.5, 127.7, 127.2, 121.8, 119.2, 119.0, 113.7, 109.3, 32.7, 31.0. **HRMS** (EI) calculated for $C_{16}H_{14}ClN$ $[M]^+$: 255.0809, found: 255.0818. **IR** (neat): ν 3049, 2900, 1480, 1324, 1086, 1063, 1009, 799, 777, 733, 563, 475, 424 cm^{-1}.

3-([1,1'-Biphenyl]-4-ylmethyl)-1-methyl-1*H*-indole (3k)



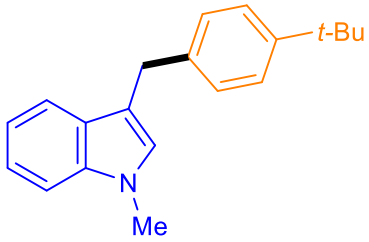
Colorless oil (67.2 mg, 76% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.40–7.29 (m, 7H), 7.29–7.22 (m, 4H, contains residual solvent signal of $CDCl_3$), 7.20–7.18 (m, 1H), 7.02 (m, 1H), 6.50 (s, 1H), 4.03 (s, 2H), 3.65 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 141.89, 141.85, 138.5, 137.1, 130.1, 129.4, 128.2, 127.43, 127.42, 126.9, 126.0, 121.5, 119.3, 118.7, 114.9, 109.1, 32.6, 29.0. **HRMS** (ESI) calculated for $C_{22}H_{20}N$ $[M+H]^+$: 298.1590, found: 298.1588. **IR** (neat): ν 3053, 2912, 1474, 1371, 1326, 1009, 907, 735, 701, 550, 426 cm^{-1}.

Methyl 2-(4-((1-methyl-1*H*-indol-3-yl)methyl)phenyl)acetate (3l)



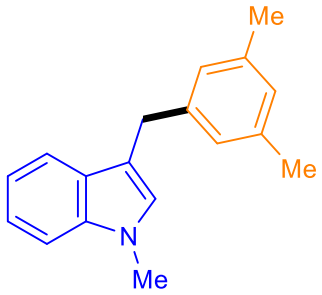
Colorless oil (62.4 mg, 71% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.0 Hz, 1H), 7.31–7.12 (m, 6H, contains residual solvent signal of $CDCl_3$), 7.06 (m, 1H), 6.73 (s, 1H), 4.07 (s, 2H), 3.70 (s, 3H), 3.66 (s, 3H), 3.57 (s, 2H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 172.3, 140.4, 137.2, 131.5, 129.3, 128.9, 127.9, 127.2, 121.6, 119.2, 118.8, 114.2, 109.2, 52.1, 40.0, 32.6, 31.2. **HRMS** (ESI) calculated for $C_{19}H_{20}NO_2$ $[M+H]^+$: 294.1489, found: 294.1488. **IR** (neat): ν 2948, 1732, 1551, 1512, 1470, 1326, 1151, 1010, 737, 565, 426 cm^{-1}.

3-(4-(*Tert*-butyl)benzyl)-1-methyl-1*H*-indole (3m)



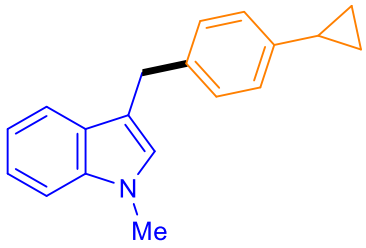
Colorless oil (41.4 mg, 50% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.0 Hz, 1H), 7.30–7.18 (m, 6H, contains residual solvent signal of $CDCl_3$), 7.07 (m, 1H), 6.74 (s, 1H), 4.06 (s, 2H), 3.70 (s, 3H), 1.29 (s, 9H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 148.6, 138.5, 137.2, 128.3, 128.0, 127.1, 125.3, 121.6, 119.3, 118.8, 114.5, 109.2, 34.4, 32.6, 31.5, 31.0. **HRMS** (EI) calculated for $C_{20}H_{23}N$ $[M]^+$: 277.1825, found: 277.1828. **IR** (neat): ν 2956, 1512, 1469, 1370, 1325, 1012, 735, 567, 547, 426 cm^{-1}.

3-(3,5-Dimethylbenzyl)-1-methyl-1H-indole (3n)



Colorless oil (38.9 mg, 52% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 7.6 Hz, 1H), 7.31 (d, *J* = 8.0 Hz, 1H), 7.27 – 7.22 (m, 1H), 7.12 (t, *J* = 7.6 Hz, 1H), 6.95 (s, 2H), 6.87 (s, 1H), 6.77 (s, 1H), 4.06 (s, 2H), 3.75 (s, 3H), 2.31 (s, 6H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 141.4, 137.9, 137.2, 128.0, 127.6, 127.2, 126.7, 121.6, 119.3, 118.8, 114.6, 109.2, 32.7, 31.4, 21.5. **HRMS** (EI) calculated for $C_{18}H_{19}N$ $[M]^+$: 249.1512, found: 249.1512. **IR** (neat): ν 3012, 2911, 1603, 1469, 1423, 1372, 1327, 1249, 1151, 1120, 1059, 1011, 848, 800, 735, 712, 626, 566, 541, 426 cm^{-1}.

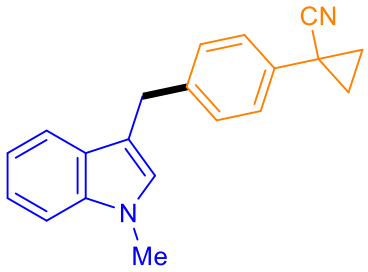
3-(4-Cyclopropylbenzyl)-1-methyl-1*H*-indole (3o)



White solid (47.8 mg, 61% yield). Melting point 73.9–75.1 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.0 Hz, 1H), 7.31 (d, *J* = 8.4 Hz, 1H), 7.26-7.20 (m, 3H), 7.10 (t, *J* = 7.2 Hz, 1H), 7.02 (d, *J* = 7.6 Hz, 2H), 6.75 (s, 1H), 4.08 (s, 2H), 3.73 (s, 3H), 1.93-1.86 (m, 1H), 0.97-0.93 (m, 2H), 0.71-0.67 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 141.5, 138.5, 137.2, 128.7, 127.9, 127.2, 125.7, 121.6, 119.3, 118.8, 114.6, 109.2, 32.7, 31.2, 15.2, 9.2. **HRMS** (EI) calculated for $C_{19}H_{19}N$ $[M]^+$: 261.1512,

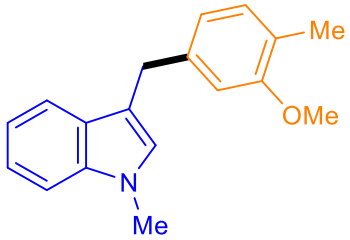
found: 261.1512. **IR** (neat): ν 2997, 2919, 1614, 1553, 1513, 1458, 1418, 1375, 1326, 1253, 1215, 1182, 1152, 1125, 1040, 1008, 919, 898, 804, 734, 567, 530, 429 cm^{-1}.

1-(4-((1-Methyl-1*H*-indol-3-yl)methyl)phenyl)cyclopropane-1-carbonitrile (3p)



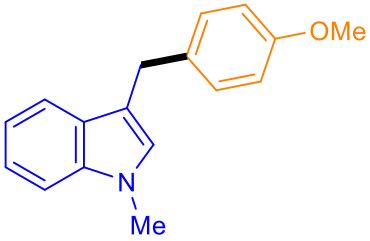
Light yellow oil (65.3 mg, 76% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 8.0 Hz, 1H), 7.33-7.21 (m, 6H), 7.10 (t, *J* = 7.6 Hz, 1H), 6.78 (s, 1H), 4.11 (s, 2H), 3.74 (s, 3H), 1.71-1.68 (m, 2H), 1.38-1.35 (m, 2H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 141.2, 137.2, 133.5, 129.2, 127.7, 127.2, 125.9, 122.9, 121.7, 119.2, 118.9, 113.8, 109.3, 32.7, 31.1, 18.0, 13.6. **HRMS** (DART) calculated for $C_{20}H_{19}N_2$ $[M+H]^+$: 287.1543, found: 287.1540. **IR** (neat): ν 2909, 2233, 1613, 1512, 1470, 1425, 1373, 1326, 1250, 1152, 1120, 1062, 1014, 944, 910, 780, 736, 665, 565, 524, 505, 427 cm^{-1}.

3-(3-Methoxy-4-methylbenzyl)-1-methyl-1*H*-indole (3q)



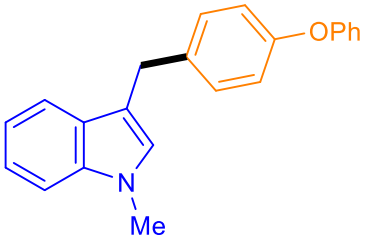
Light yellow oil (33.4 mg, 42% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.61 – 7.55 (m, 1H), 7.33 – 7.28 (m, 1H), 7.26 – 7.22 (m, 1H), 7.14 – 7.03 (m, 2H), 6.81 (d, *J* = 6.4 Hz, 2H), 6.76 (s, 1H), 4.09 (s, 2H), 3.79 (s, 3H), 3.74 (s, 3H), 2.21 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 157.8, 140.3, 137.3, 130.5, 128.0, 127.2, 124.1, 121.7, 120.6, 119.3, 118.9, 114.7, 110.7, 109.2, 55.4, 32.7, 31.7, 16.0. **HRMS** (EI) calculated for $C_{18}H_{19}NO$ $[M]^+$: 265.1461, found: 265.1465. **IR** (neat): ν 2914, 1723, 1612, 1583, 1506, 1464, 1411, 1373, 1327, 1252, 1150, 1129, 1039, 1011, 944, 855, 791, 736, 683, 598, 558, 448, 427cm^{-1}.

3-(4-Methoxybenzyl)-1-methyl-1*H*-indole (3r)[3]



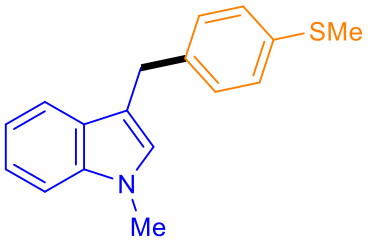
Colorless oil (48.6 mg, 65% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.0 Hz, 1H), 7.26 (m, 1H), 7.22–7.17 (m, 3H), 7.05 (m, 1H), 6.81 (d, *J* = 8.8 Hz, 2H), 6.70 (s, 1H), 4.03 (s, 2H), 3.75 (s, 3H), 3.69 (s, 3H). **^{13}C{^{1}H} NMR** (101 MHz, $CDCl_3$) δ 157.9, 137.3, 133.6, 129.6, 127.9, 127.1, 121.6, 119.3, 118.8, 114.8, 113.8, 109.2, 55.3, 32.6, 30.7.

1-Methyl-3-(4-phenoxybenzyl)-1*H*-indole (3s)



White solid (62.5 mg, 67% yield). Melting point 92–94 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 8.0 Hz, 1H), 7.32–7.26 (m, 3H), 7.25–7.19 (m, 3H), 7.10–7.03 (m, 2H), 6.98 (d, *J* = 7.6 Hz, 2H), 6.92 (d, *J* = 8.4 Hz, 2H), 6.76 (s, 1H), 4.07 (s, 2H), 3.71 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 157.7, 155.2, 137.3, 136.5, 129.9, 129.7, 127.8, 127.1, 123.0, 121.7, 119.3, 119.1, 118.9, 118.6, 114.4, 109.2, 32.7, 30.9. **HRMS** (EI) calculated for $C_{22}H_{19}NO$ $[M]^+$: 313.1461, found: 313.1467. **IR** (neat): ν 2917, 1583, 1477, 1325, 1221, 1012, 866, 757, 734, 691, 655, 561, 491, 424 cm^{-1}.

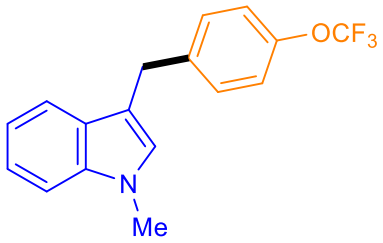
1-Methyl-3-(4-(methylthio)benzyl)-1*H*-indole (3t)



Colorless oil (36.1 mg, 45% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.0 Hz, 1H), 7.31 (d, *J* = 8.0 Hz, 1H), 7.27 – 7.18 (m, 5H), 7.10 (t, *J* = 7.6 Hz, 1H), 6.77 (s, 1H), 4.09 (s, 2H), 3.74 (s, 3H), 2.48 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 138.7, 137.3, 135.4, 129.3, 127.8, 127.2, 127.2, 121.7, 119.3, 118.9, 114.2, 109.3, 32.7, 31.1, 16.4. **HRMS** (EI) calculated for $C_{17}H_{17}NS$ $[M]^+$:

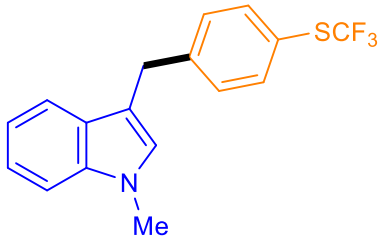
267.1076, found: 267.1081. **IR** (neat): ν 2915, 1613, 1470, 1423, 1372, 1325, 1250, 1200, 1152, 1093, 1058, 1012, 965, 844, 794, 736, 665, 564, 523, 488, 427 cm^{-1}.

1-Methyl-3-(4-(trifluoromethoxy)benzyl)-1*H*-indole (**3u**)



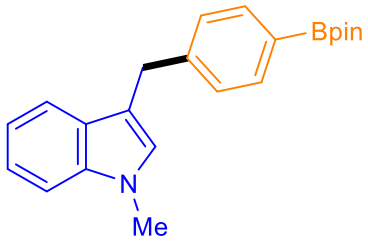
White solid (40.0 mg, 44% yield). Melting point 71–73 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.47 (d, *J* = 8.0 Hz, 1H), 7.31–7.25 (m, 3H), 7.24–7.21 (m, 1H), 7.13–7.05 (m, 3H), 6.76 (s, 1H), 4.09 (s, 2H), 3.73 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 147.5, 140.2, 137.2, 129.9, 127.7, 127.2, 121.8, 120.9, 120.6 (q, *J* = 255.0 Hz), 119.1, 119.0, 113.6, 109.3, 32.7, 30.9. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -58.0. **HRMS** (EI) calculated for $C_{17}H_{14}F_3NO$ $[M]^+$: 305.1022, found: 305.1025. **IR** (neat): ν 2919, 1552, 1504, 1471, 1427, 1221, 1150, 1100, 1014, 915, 810, 782, 731, 681, 424 cm^{-1}.

1-Methyl-3-(4-((trifluoromethyl)thio)benzyl)-1*H*-indole (3v)



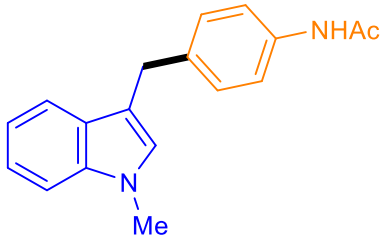
Colorless oil (56 mg, 58% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.4 Hz, 2H), 7.49 (d, *J* = 8.0 Hz, 1H), 7.38 – 7.31 (m, 3H), 7.25 (t, *J* = 7.6 Hz, 1H), 7.10 (t, *J* = 7.6 Hz, 1H), 6.81 (s, 1H), 4.15 (s, 2H), 3.76 (s, 3H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$) δ 145.0, 137.3, 136.6, 129.9, 129.8 (q, *J* = 306.25 Hz), 127.8, 127.4, 121.9, 121.47, 121.45, 119.2, 119.1, 113.2, 109.4, 32.8, 31.4. ^{19}F NMR (376 MHz, CDCl3) δ -43.04. **HRMS** (EI) calculated for $C_{17}H_{14}F_3NS$ $[M]^+$: 321.0794, found: 321.0804. **IR** (neat): ν 2913, 1593, 1471, 1374, 1328, 1254, 1108, 1014, 921, 797, 737, 673, 565, 524, 502, 426 cm^{-1}.

1-Methyl-3-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzyl)-1*H*-indole (3w)



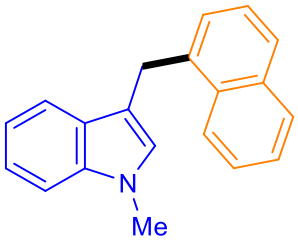
Colorless oil (62.5 mg, 60% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.80 – 7.72 (m, 2H), 7.51 (d, *J* = 8.0 Hz, 1H), 7.34 – 7.27 (m, 3H), 7.25 – 7.20 (m, 1H), 7.07 (t, *J* = 7.6 Hz, 1H), 6.73 (s, 1H), 4.12 (s, 2H), 3.72 (s, 3H), 1.35 (s, 12H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 144.9, 137.3, 135.0, 128.3, 127.9, 127.3, 121.7, 119.3, 118.9, 114.1, 109.2, 83.8, 32.7, 31.9, 25.0. **HRMS** (ESI) calculated for $C_{22}H_{27}BNO_2$ $[M+H]^+$: 348.2129, found: 348.2129. **IR** (neat): ν 2977, 2921, 1609, 1515, 1469, 1394, 1356, 1318, 1267, 1212, 1141, 1085, 1012, 961, 857, 782, 736, 666, 561, 521, 443, 427 cm^{-1}.

***N*-(4-((1-methyl-1*H*-indol-3-yl)methyl)phenyl)acetamide (3x)**



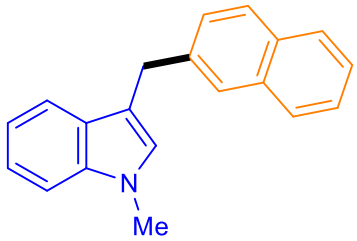
White solid (41.8 mg, 50% yield). Melting point 154.1–155.2 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.51 (d, *J* = 8.0 Hz, 1H), 7.48 (s, 1H), 7.40 (d, *J* = 8.5 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 1H), 7.24 – 7.19 (m, 3H), 7.08 (t, *J* = 7.5 Hz, 1H), 6.74 (s, 1H), 4.06 (s, 2H), 3.71 (s, 3H), 2.13 (s, 3H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$) δ 168.5, 137.6, 137.3, 135.9, 129.2, 127.8, 127.2, 121.7, 120.2, 119.3, 118.9, 114.3, 109.3, 32.7, 31.1, 24.6. **HRMS** (ESI) calculated for $C_{18}H_{18}N_2ONa$ $[M+Na]^+$: 301.1311, found: 301.1303. **IR** (neat): ν 2922, 1655, 1598, 1532, 1510, 1471, 1410, 1370, 1311, 1264, 1125, 1065, 1007, 963, 924, 863, 824, 781, 734, 674, 601, 564, 523, 493, 426 cm^{-1}.

1-Methyl-3-(naphthalen-1-ylmethyl)-1*H*-indole (**3y**)



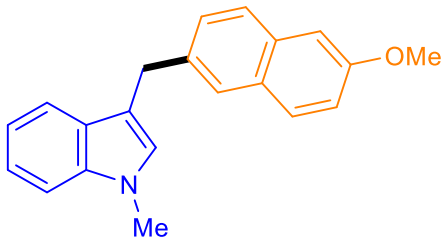
White solid (40.0 mg, 50% yield). Melting point 72–73 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 8.0 Hz, 1H), 7.88–7.83 (m, 1H), 7.76–7.71 (m, 1H), 7.63 (d, *J* = 8.0 Hz, 1H), 7.47–7.34 (m, 4H), 7.30–7.19 (m, 2H), 7.14–7.07 (m, 1H), 6.50 (s, 1H), 4.52 (s, 2H), 3.61 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 137.2, 137.1, 133.9, 132.3, 128.6, 127.9, 127.6, 126.9, 126.7, 125.8, 125.7, 125.5, 124.5, 121.7, 119.2, 118.9, 113.9, 109.2, 32.6, 28.9. **HRMS** (EI) calculated for $C_{20}H_{17}N$ $[M]^+$: 271.1356, found: 271.1355. **IR** (neat): ν 3049, 2908, 1688, 1469, 1370, 1327, 1244, 1011, 785, 771, 734, 606, 520, 426, 410 cm^{-1}.

1-Methyl-3-(naphthalen-2-ylmethyl)-1*H*-indole (**3z**)



White solid (60.2 mg, 74% yield). Melting point 71–73 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.92–7.82 (m, 4H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.56–7.49 (m, 3H), 7.42–7.30 (m, 2H), 7.22–7.15 (m, 1H), 6.84 (s, 1H), 4.36 (s, 2H), 3.78 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 139.1, 137.3, 133.8, 132.2, 127.98, 127.96, 127.8, 127.72, 127.66, 127.4, 126.7, 125.9, 125.3, 121.7, 119.3, 118.9, 114.3, 109.3, 32.7, 31.9. **HRMS** (EI) calculated for $C_{20}H_{17}N$ $[M]^+$: 271.1356, found: 271.1355. **IR** (neat): ν 3051, 2912, 1466, 1327, 1253, 824, 810, 736, 565, 471, 426 cm^{-1}.

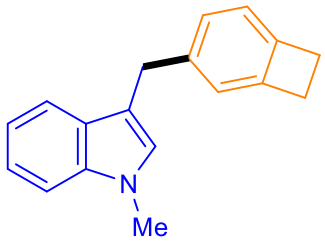
3-((6-Methoxynaphthalen-2-yl)methyl)-1-methyl-1*H*-indole (3aa)



White solid (47 mg, 52% yield). Melting point 89.3–90.5 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.8 Hz, 3H), 7.57 (d, *J* = 8.4 Hz, 1H), 7.42 (d, *J* = 8.4 Hz, 1H), 7.30 (s, 1H), 7.23 (d, *J* = 8.4 Hz, 1H), 7.16 – 7.04 (m, 3H), 6.77 (s, 1H), 4.25 (s, 2H), 3.92 (s, 3H), 3.72 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 157.3, 137.3, 136.7, 133.2, 129.21, 129.15, 128.3, 128.0, 127.4, 126.9, 126.6, 121.7, 119.4, 118.9, 118.7, 114.5, 109.3, 105.8, 55.4, 32.7, 31.7. **HRMS** (EI) calculated for $C_{21}H_{19}NO$ $[M]^+$:301.1461, found: 301.1465. **IR** (neat): ν 2930, 1686, 1605, 1503, 1477, 1374, 1325,

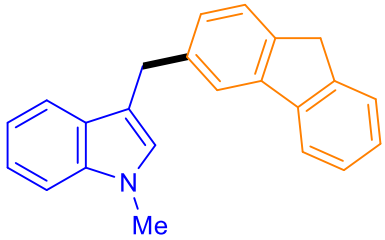
1288, 1264, 1230, 1205, 1151, 1117, 1060, 1026, 943, 911, 886, 854, 811, 795, 738, 663, 615, 590, 485, 423 cm^{-1}.

3-(Bicyclo[4.2.0]octa-1,3,5-trien-3-ylmethyl)-1-methyl-1*H*-indole (**3ab**)



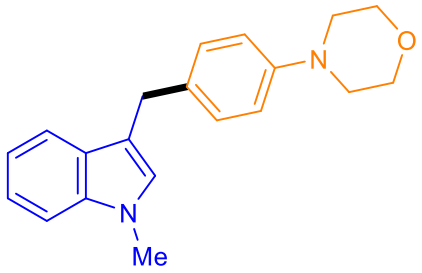
Light red oil (56.7 mg, 77% yield). ^{1}**H NMR** (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.0 Hz, 1H), 7.27–7.23 (m, 1H), 7.22–7.17 (m, 1H), 7.12 (d, *J* = 7.6 Hz, 1H), 7.06 (m, 1H), 6.98–6.90 (m, 2H), 6.72 (s, 1H), 4.05 (s, 2H), 3.68 (s, 3H), 3.10 (s, 4H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 145.8, 143.2, 140.1, 137.2, 127.9, 127.2, 127.1, 123.0, 122.4, 121.6, 119.3, 118.8, 115.0, 109.2, 32.6, 32.1, 29.5, 29.3. **HRMS** (DART) calculated for $C_{18}H_{18}N$ $[M+H]^+$: 248.1434, found: 248.1431. **IR** (neat): ν 2921, 1470, 1422, 1372, 1324, 1249, 1201, 1120, 1057, 1010, 800, 735, 426 cm^{-1}.

3-((9H-Fluoren-3-yl)methyl)-1-methyl-1*H*-indole (3ac)



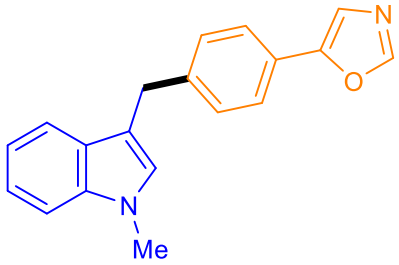
White solid (63.1 mg, 68% yield). Melting point 101.1–102.2 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 7.6 Hz, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.63 (d, *J* = 8.0 Hz, 1H), 7.56 (d, *J* = 7.6 Hz, 1H), 7.51 (s, 1H), 7.43 – 7.23 (m, 5H), 7.18 – 7.12 (m, 1H), 6.82 (s, 1H), 4.23 (s, 2H), 3.88 (s, 2H), 3.75 (d, *J* = 1.2 Hz, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 143.6, 143.3, 141.9, 140.3, 139.7, 137.3, 128.0, 127.4, 127.3, 126.8, 126.4, 125.5, 125.1, 121.7, 119.8, 119.7, 119.4, 118.9, 114.6, 109.3, 36.9, 32.7, 31.8. **HRMS** (DART) calculated for $C_{23}H_{20}N$ $[M+H]^+$: 310.1590, found: 310.1587. **IR** (neat): ν 3049, 2889, 1613, 1469, 1424, 1372, 1327, 1250, 1195, 1152, 1129, 1059, 1009, 951, 906, 837, 763, 730, 646, 612, 575, 520, 423 cm^{-1}.

4-(4-((1-Methyl-1*H*-indol-3-yl)methyl)phenyl)morpholine (3ad)



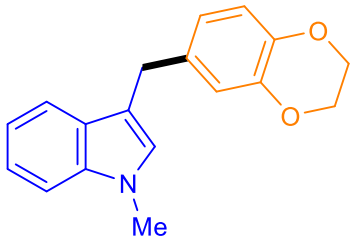
Yellow solid (50.6 mg, 55% yield). Melting point 172.9–174.1 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8.0 Hz, 1H), 7.30 (d, *J* = 8.2 Hz, 1H), 7.23 (t, *J* = 8.1 Hz, 3H), 7.09 (t, *J* = 7.4 Hz, 1H), 6.86 (d, *J* = 8.1 Hz, 2H), 6.75 (s, 1H), 4.06 (s, 2H), 3.87 (t, *J* = 4.7 Hz, 4H), 3.73 (s, 3H), 3.13 (t, *J* = 4.8 Hz, 4H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 149.51, 137.25, 133.22, 129.46, 127.91, 127.11, 121.60, 119.33, 118.78, 115.99, 114.84, 109.20, 67.07, 49.83, 32.67, 30.69. **HRMS** (ESI) calculated for $C_{20}H_{23}N_2O$ $[M+H]^+$: 307.1805, found: 307.1809. **IR** (neat): ν 2961, 2823, 1611, 1514, 1477, 1447, 1369, 1326, 1304, 1266, 1227, 1146, 1119, 1052, 1009, 926, 840, 813, 792, 739, 623, 579, 543, 521, 424 cm^{-1}.

5-(4-((1-Methyl-1*H*-indol-3-yl)methyl)phenyl)oxazole (3ae)



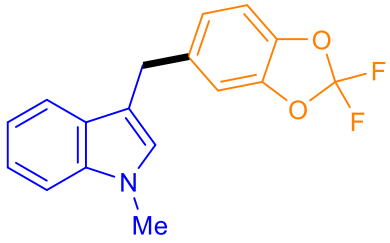
White solid (74.4 mg, 86% yield). Melting point 146.6–148.3 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.90 (s, 1H), 7.59 (d, *J* = 7.6 Hz, 2H), 7.53 (d, *J* = 8.0 Hz, 1H), 7.43 – 7.29 (m, 4H), 7.26 (t, *J* = 7.6 Hz, 1H), 7.11 (t, *J* = 7.6 Hz, 1H), 6.80 (s, 1H), 4.15 (s, 2H), 3.75 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 151.8, 150.3, 142.3, 137.3, 129.3, 127.8, 127.2, 125.5, 124.5, 121.8, 121.0, 119.2, 119.0, 113.7, 109.3, 32.7, 31.5. **HRMS** (ESI) calculated for $C_{19}H_{17}N_2O$ $[M+H]^+$: 289.1335, found: 289.1344. **IR** (neat): ν 3097, 2910, 1614, 1509, 1480, 1423, 1376, 1325, 1252, 1152, 1101, 1063, 1041, 1012, 940, 918, 871, 819, 781, 731, 681, 648, 567, 524, 496, 448, 423 cm^{-1}.

3-((2,3-Dihydrobenzo[b][1,4]dioxin-6-yl)methyl)-1-methyl-1*H*-indole (3af)



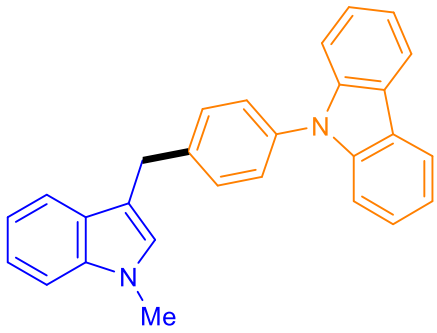
Light yellow oil (48.6 mg, 58% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 8.0 Hz, 1H), 7.32 (d, *J* = 8.0 Hz, 1H), 7.25 (d, *J* = 8.4 Hz, 1H), 7.12 (t, *J* = 7.2 Hz, 1H), 6.84 (s, 1H), 6.82 (s, 3H), 4.25 (s, 4H), 4.04 (s, 2H), 3.76 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 143.4, 141.7, 137.2, 135.0, 127.9, 127.1, 121.64, 121.62, 119.3, 118.8, 117.4, 117.1, 114.5, 109.2, 64.5, 64.4, 32.7, 30.8. **HRMS** (EI) calculated for $C_{18}H_{17}NO_2$ $[M]^+$: 279.1254, found: 279.1254. **IR** (neat): ν 2927, 2874, 1684, 1588, 1503, 1469, 1428, 1373, 1281, 1255, 1200, 1122, 1066, 1011, 915, 885, 803, 735, 682, 644, 593, 552, 462, 427 cm^{-1}.

3-((2,2-Difluorobenzo[d][1,3]dioxol-5-yl)methyl)-1-methyl-1*H*-indole (3ag)



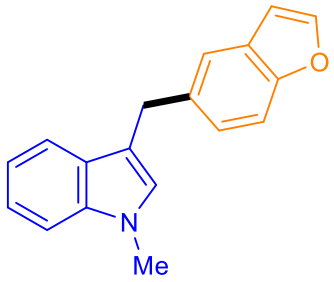
Colorless oil (59.1 mg, 66% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 8.0 Hz, 1H), 7.29–7.27 (m, 1H), 7.23–7.19 (m, 1H), 7.07 (t, *J* = 6.8 Hz, 1H), 6.98–6.89 (m, 3H), 6.77 (s, 1H), 4.06 (s, 2H), 3.72 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 143.9, 142.0, 137.8, 137.3, 131.7 (t, *J* = 252 Hz), 127.6, 127.2, 123.4, 121.9, 119.06, 119.05, 113.5, 109.9, 109.4, 109.0, 32.7, 31.4. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -50.1. **HRMS** (EI) calculated for $C_{17}H_{13}F_2NO_2$ $[M]^+$: 301.0909, found: 301.0911. **IR** (neat): ν 2913, 1494, 1445, 1229, 1136, 1034, 949, 736, 702, 425 cm^{-1}.

9-(4-((1-Methyl-1*H*-indol-3-yl)methyl)phenyl)-9H-carbazole (3ah)



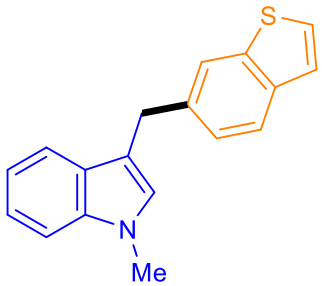
White solid (98.5 mg, 85% yield). Melting point 145–146 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.0 Hz, 2H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.51–7.42 (m, 4H), 7.40–7.37 (m, 4H), 7.34–7.30 (m, 1H), 7.29–7.22 (m, 3H), 7.12 (m, 1H), 6.88 (s, 1H), 4.21 (s, 2H), 3.77 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 141.03, 140.98, 137.3, 135.4, 130.0, 127.9, 127.3, 127.0, 125.9, 123.3, 121.8, 120.3, 119.8, 119.2, 119.0, 113.8, 109.9, 109.3, 32.7, 31.3. **HRMS** (ESI) calculated for $C_{28}H_{23}N_2$ $[M+H]^+$: 387.1856, found: 387.1853. **IR** (neat): ν 3047, 2915, 1593, 1512, 1450, 1331, 1313, 1231, 752, 723, 655, 430 cm^{-1}.

3-(Benzofuran-5-ylmethyl)-1-methyl-1*H*-indole (**3ai**)



Colorless oil (61.5 mg, 79% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 2.4 Hz, 1H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.46 (s, 1H), 7.39 (m, 1H), 7.30–7.15 (m, 3H, contains residual solvent signal of $CDCl_3$), 7.09–7.02 (m, 1H), 6.72 (s, 1H), 6.65 (m, 1H), 4.17 (s, 2H), 3.67 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 153.7, 145.1, 137.3, 136.0, 127.9, 127.6, 127.2, 125.3, 121.7, 120.8, 119.3, 118.9, 114.9, 111.1, 109.2, 106.6, 32.6, 31.5. **HRMS** (EI) calculated for $C_{18}H_{15}ON$ $[M]^+$: 261.1148, found: 261.1149. **IR** (neat): ν 3049, 2910, 1465, 1372, 1325, 1258, 1192, 1107, 1029, 881, 764, 732, 423 cm^{-1}.

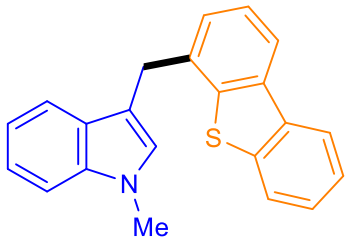
3-(Benzo[*b*]thiophen-6-ylmethyl)-1-methyl-1*H*-indole (**3aj**)



Colorless oil (45.4 mg, 55% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.73 (s, 1H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.51 (d, *J* = 8.0 Hz, 1H), 7.33–7.15 (m, 5H), 7.05 (t, *J* = 7.2 Hz, 1H), 6.72 (s, 1H), 4.20 (s, 2H), 3.66 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 140.2, 137.94, 137.90, 137.3, 127.9, 127.4, 125.7, 125.5, 123.7, 123.4, 122.1, 121.7, 119.3, 118.9, 114.3, 109.3, 32.7, 31.6. **HRMS** (EI) calculated for

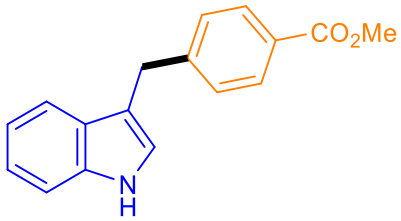
$C_{18}H_{15}NS$ [M]$^+$: 277.0920, found: 277.0931. **IR** (neat): ν 3048, 2905, 1468, 1371, 1323, 1249, 1010, 902, 784, 735, 691, 584, 423 cm^{-1}.

3-(Dibenzo[b,d]thiophen-4-ylmethyl)-1-methyl-1*H*-indole (**3ak**)



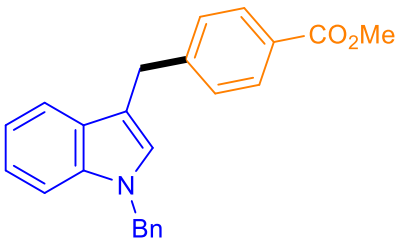
White solid (65.2 mg, 67% yield). Melting point 88–90 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.22–8.17 (m, 1H), 8.09 (d, *J* = 7.6 Hz, 1H), 7.93–7.88 (m, 1H), 7.63 (d, *J* = 8.0 Hz, 1H), 7.54–7.47 (m, 2H), 7.47–7.33 (m, 3H), 7.31–7.26 (m, 1H), 7.14 (t, *J* = 8.0 Hz, 1H), 6.91 (s, 1H), 4.43 (s, 2H), 3.76 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 139.4, 139.2, 137.2, 136.1, 135.8, 135.7, 128.0, 127.8, 126.8, 126.6, 124.9, 124.4, 122.9, 121.8, 121.7, 119.5, 119.3, 119.0, 111.8, 109.3, 32.7, 30.9. **HRMS** (EI) calculated for $C_{22}H_{17}NS$ [M]$^+$: 327.1076, found: 327.1083. **IR** (neat): ν 3051, 2921, 1471, 1440, 1323, 1250, 1042, 1011, 748, 728, 565, 425 cm^{-1}.

Methyl 4-((1*H*-indol-3-yl)methyl)benzoate (**3al**)[1]



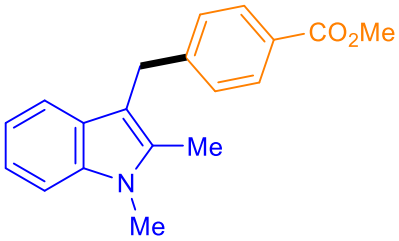
White solid (38.6 mg, 49% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.05 (br, 1H), 7.94 (d, *J* = 8.4 Hz, 2H), 7.45 (d, *J* = 8.0 Hz, 1H), 7.37–7.31 (m, 3H), 7.18 (t, *J* = 7.6 Hz, 1H), 7.06 (t, *J* = 7.6 Hz, 1H), 6.91 (s, 1H), 4.15 (s, 2H), 3.88 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 167.3, 146.9, 136.5, 129.8, 128.7, 127.9, 127.3, 122.5, 122.2, 119.5, 119.0, 114.7, 111.2, 52.0, 31.7.

Methyl 4-((1-benzyl-1*H*-indol-3-yl)methyl)benzoate (**3am**)



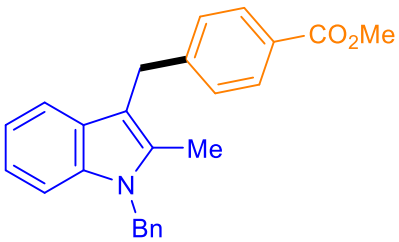
White solid (74.5 mg, 71% yield). Melting point 108–110 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.0 Hz, 2H), 7.46 (d, *J* = 8.0 Hz, 1H), 7.34 (d, *J* = 8.0 Hz, 2H), 7.29–7.22 (m, 4H, contains residual solvent signal of $CDCl_3$), 7.16 (t, *J* = 7.6 Hz, 1H), 7.10–7.02 (m, 3H), 6.86 (s, 1H), 5.25 (s, 2H), 4.15 (s, 2H), 3.88 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 167.2, 146.9, 137.6, 136.9, 129.8, 128.8, 128.7, 128.0, 127.9, 127.6, 126.8, 126.7, 122.0, 119.3, 113.9, 109.8, 52.0, 50.0, 31.7. **HRMS** (ESI) calculated for $C_{24}H_{22}NO_2$ $[M+H]^+$: 356.1645, found: 356.1641. **IR** (neat): ν 3026, 2804, 1709, 1608, 1466, 1279, 1175, 1104, 713, 697, 518, 453, 430 cm^{-1}.

Methyl 4-((1,2-dimethyl-1*H*-indol-3-yl)methyl)benzoate (**3an**)



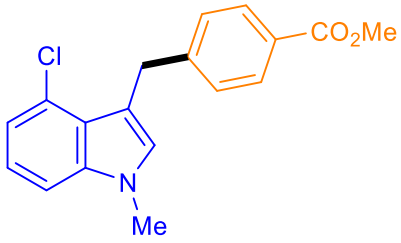
White solid (55.4 mg, 63% yield). Melting point 93–95 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.4 Hz, 2H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.27–7.20 (m, 3H), 7.14 (t, *J* = 8.0 Hz, 1H), 7.01 (t, *J* = 8.0 Hz, 1H), 4.12 (s, 2H), 3.85 (s, 3H), 3.65 (s, 3H), 2.33 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 167.2, 147.6, 136.7, 133.8, 129.7, 128.3, 127.8, 127.7, 120.8, 119.0, 118.1, 108.9, 108.7, 52.0, 30.6, 29.6, 10.4. **HRMS** (ESI) calculated for $C_{19}H_{20}NO_2$ $[M+H]^+$: 294.1489, found: 294.1490. **IR** (neat): ν 2911, 1709, 1605, 1469, 1427, 1368, 1275, 1175, 1103, 1015, 759, 733, 714 cm^{-1}.

Methyl 4-((1-benzyl-2-methyl-1*H*-indol-3-yl)methyl)benzoate (**3ao**)[4]



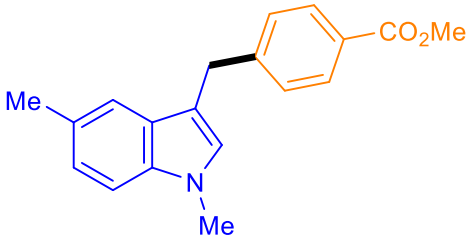
White solid (61.1 mg, 56% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.0 Hz, 2H), 7.40 (d, *J* = 7.6 Hz, 1H), 7.32–7.19 (m, 7H), 7.15–7.08 (m, 1H), 7.04 (m, 1H), 6.96 (d, *J* = 6.8 Hz, 1H), 5.32 (s, 2H), 4.16 (s, 2H), 3.87 (s, 3H), 2.29 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 167.2, 147.4, 138.0, 136.6, 133.7, 129.7, 128.8, 128.3, 128.0, 127.8, 127.3, 126.0, 121.1, 119.3, 118.3, 109.7, 109.1, 52.0, 46.6, 30.6, 10.4.

Methyl 4-((4-chloro-1-methyl-1*H*-indol-3-yl)methyl)benzoate (**3ap**)



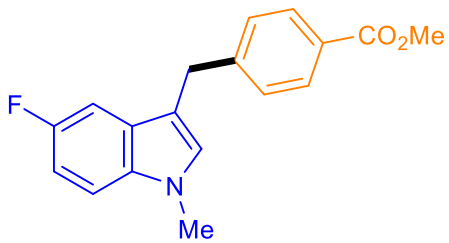
White solid (69.7 mg, 74% yield). Melting point 76–77 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.4 Hz, 2H), 7.29 (d, *J* = 8.4 Hz, 2H), 7.16–7.14 (m, 1H), 7.08–7.01 (m, 2H), 6.62 (s, 1H), 4.40 (s, 2H), 3.88 (s, 3H), 3.66 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 167.3, 147.6, 138.6, 129.7, 129.0, 128.8, 127.8, 126.5, 124.4, 122.3, 120.1, 113.6, 108.1, 52.0, 32.9, 32.5. **HRMS** (ESI) calculated for $C_{18}H_{17}NO_2Cl$ $[M+H]^+$: 314.0942, found: 314.0939. **IR** (neat): ν 2943, 1719, 1608, 1419, 1280, 1174, 1101, 1020, 863, 769, 734, 700 cm^{-1}.

Methyl 4-((1,5-dimethyl-1*H*-indol-3-yl)methyl)benzoate (**3aq**)



Colorless oil (68.3 mg, 78% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.23 (s, 1H), 7.16 (d, *J* = 8.4 Hz, 1H), 7.03 (d, *J* = 8.4 Hz, 1H), 6.69 (s, 1H), 4.09 (s, 2H), 3.87 (s, 3H), 3.67 (s, 3H), 2.41 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 167.3, 147.2, 135.7, 129.8, 128.7, 128.2, 128.0, 127.9, 127.4, 123.4, 118.7, 112.6, 109.0, 52.0, 32.7, 31.6, 21.5. **HRMS** (ESI) calculated for $C_{19}H_{20}NO_2$ $[M+H]^+$: 294.1489, found: 294.1489. **IR** (neat): ν 2913, 1714, 1608, 1491, 1432, 1377, 1274, 1175, 1103, 1018, 784, 714, 605, 590, 426 cm^{-1}.

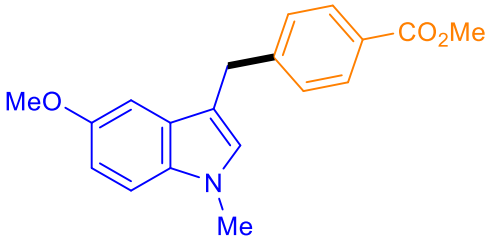
Methyl 4-((5-fluoro-1-methyl-1*H*-indol-3-yl)methyl)benzoate (**3ar**)



White solid (21.6 mg, 24% yield). Melting point 98–99 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.4 Hz, 2H), 7.32 (d, *J* = 8.4 Hz, 2H), 7.19 (m, 1H), 7.07 (dd, *J* = 9.6, 2.4 Hz, 1H), 6.95 (td, *J* = 9.2, 2.4 Hz, 1H), 6.81 (s, 1H), 4.08 (s, 2H), 3.89 (s, 3H), 3.72 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz,

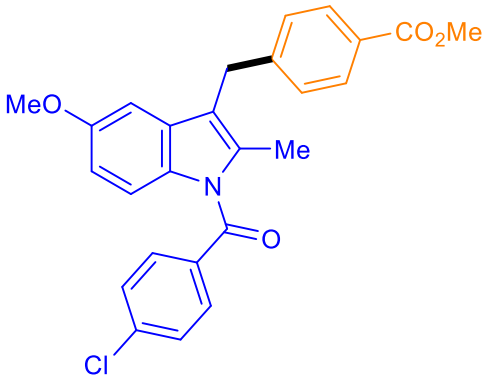
$CDCl_3$) δ 167.1, 157.6 (d, *J* = 233.0 Hz), 146.6, 133.9, 129.8, 128.9, 128.6, 128.0, 127.9 (d, *J* = 9.0 Hz), 113.2 (d, *J* = 5.0 Hz), 110.1 (d, *J* = 35.0 Hz), 110.0, 103.9 (d, *J* = 23.0 Hz), 52.0, 32.9, 31.6. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -125.5. **HRMS** (ESI) calculated for $C_{18}H_{17}NO_2F$ $[M+H]^+$: 298.1238, found: 298.1240. **IR** (neat): ν 2921, 1713, 1610, 1573, 1486, 1425, 1278, 1246, 1108, 900, 744, 429 cm^{-1}.

Methyl 4-((5-methoxy-1-methyl-1*H*-indol-3-yl)methyl)benzoate (**3as**)



White solid (65.0 mg, 71% yield). Melting point 96–98 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.4 Hz, 2H), 7.34 (d, *J* = 8.4 Hz, 2H), 7.22–7.15 (m, 1H), 6.91–6.85 (m, 2H), 6.72 (s, 1H), 4.10 (s, 2H), 3.89 (s, 3H), 3.79 (s, 3H), 3.70 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 167.2, 153.8, 147.0, 132.6, 129.7, 128.7, 128.0, 127.9, 112.6, 111.8, 110.04, 110.00, 101.0, 56.0, 52.0, 32.8, 31.7. **HRMS** (ESI) calculated for $C_{19}H_{20}NO_3$ $[M+H]^+$: 310.1438, found: 310.1432. **IR** (neat): ν 2915, 1708, 1610, 1460, 1423, 1282, 1256, 1225, 1107, 1054, 1027, 891, 827, 744 cm^{-1}.

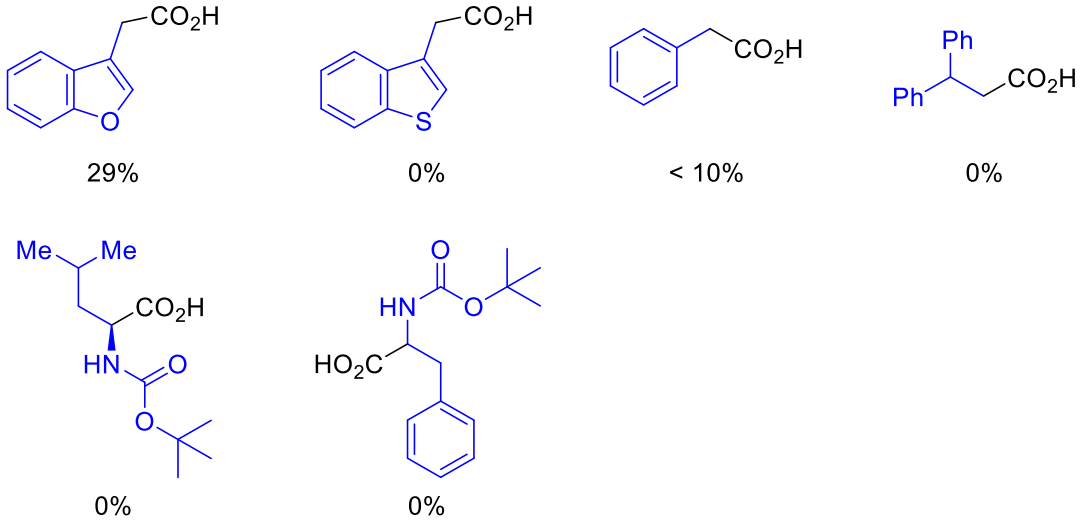
Methyl4-((1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1*H*-indol-3-yl)methyl)benzoate (**3at**)



White solid (67.2 mg, 50% yield). Melting point 143–144 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.4 Hz, 2H), 7.67 (d, *J* = 8.4 Hz, 2H), 7.48 (d, *J* = 8.0 Hz, 2H), 7.28 (d, *J* = 8.0 Hz, 2H), 6.88 (d, *J* = 8.8 Hz, 1H), 6.74 (s, 1H), 6.65 (m, 1H), 4.08 (s, 2H), 3.89 (s, 3H), 3.73 (s, 3H), 2.38 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 168.4, 167.0, 155.9, 145.3, 139.2, 135.3, 134.1, 131.2, 131.1, 131.0, 129.9, 129.2, 128.26, 128.23, 117.4, 115.0, 111.3, 101.7, 55.7, 52.1, 30.1, 13.4. **HRMS** (ESI)

calculated for $C_{26}H_{23}NO_4Cl$ $[M+H]^+$: 448.1310, found: 448.1302. **IR** (neat): ν 3392, 2954, 2848, 1722, 1669, 1474, 1397, 1314, 1270, 1225, 1174, 1103, 1082, 1064, 804, 703, 651, 475 cm^{-1}.

7. Unsuccessful substrates



Scheme S1. Unsuccessful aliphatic carboxylic acids.

8. Crystallographic Data of Compound 3o

Table 1. Crystal data and structure refinement for **3o**.

Identification code	d8v211031	
Empirical formula	C19 H19 N	
Formula weight	261.35	
Temperature	213(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P b c a	
Unit cell dimensions	a = 8.3081(5) Å	= 90°.
	b = 7.9162(5) Å	= 90°.
	c = 44.227(2) Å	= 90°.
Volume	2908.7(3) $Å^3$	
Z	8	
Density (calculated)	1.194 Mg/m^3	
Absorption coefficient	0.069 mm^{-1}	
F(000)	1120	
Crystal size	0.200 x 0.150 x 0.120 mm^3	
Theta range for data collection	2.619 to 25.999 °.	
Index ranges	-10<=h<=9, -9<=k<=7, -54<=l<=54	
Reflections collected	13191	
Independent reflections	2834 [R(int) = 0.0368]	
Completeness to theta = 25.242 °	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6362	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2834 / 0 / 183	
Goodness-of-fit on F^2	1.042	
Final R indices [I>2sigma(I)]	R1 = 0.0439, wR2 = 0.1058	
R indices (all data)	R1 = 0.0566, wR2 = 0.1159	
Extinction coefficient	0.018(3)	
Largest diff. peak and hole	0.191 and -0.156 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)
for d8v211031. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

_	x	y	z	U(eq)
_				
N(1)	4347(2)	-35(2)	4190(1)	43(1)
C(1)	4925(2)	1248(2)	4370(1)	36(1)
C(2)	4756(2)	1510(2)	4678(1)	50(1)
C(3)	5480(2)	2928(3)	4798(1)	58(1)
C(4)	6345(2)	4054(2)	4618(1)	56(1)
C(5)	6497(2)	3793(2)	4311(1)	43(1)
C(6)	5778(2)	2370(2)	4182(1)	34(1)
C(7)	5696(2)	1716(2)	3880(1)	34(1)
C(8)	4828(2)	261(2)	3898(1)	40(1)
C(9)	3503(3)	-1525(2)	4295(1)	72(1)
C(10)	6462(2)	2418(2)	3601(1)	40(1)
C(11)	5644(2)	3919(2)	3454(1)	30(1)
C(12)	4514(2)	4923(2)	3599(1)	32(1)
C(13)	3825(2)	6296(2)	3455(1)	31(1)
C(14)	4249(2)	6740(2)	3161(1)	30(1)
C(15)	5374(2)	5730(2)	3015(1)	35(1)
C(16)	6042(2)	4344(2)	3158(1)	34(1)
C(17)	3476(2)	8236(2)	3019(1)	36(1)
C(18)	4441(2)	9562(2)	2858(1)	54(1)
C(19)	3353(2)	8455(2)	2684(1)	56(1)
_				

Table 3. Bond lengths [Å] and angles [°] for d8v211031.

N(1)-C(8)	1.3688(19)
N(1)-C(1)	1.3779(19)
N(1)-C(9)	1.449(2)
C(1)-C(2)	1.385(2)
C(1)-C(6)	1.4069(19)
C(2)-C(3)	1.379(3)
C(2)-H(2)	0.9400
C(3)-C(4)	1.395(3)
C(3)-H(3)	0.9400
C(4)-C(5)	1.380(2)
C(4)-H(4)	0.9400
C(5)-C(6)	1.395(2)
C(5)-H(5)	0.9400
C(6)-C(7)	1.4342(19)
C(7)-C(8)	1.361(2)
C(7)-C(10)	1.4970(19)
C(8)-H(8)	0.9400
C(9)-H(9A)	0.9700
C(9)-H(9B)	0.9700
C(9)-H(9C)	0.9700
C(10)-C(11)	1.5151(19)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(11)-C(12)	1.3874(18)
C(11)-C(16)	1.3905(19)
C(12)-C(13)	1.3840(19)
C(12)-H(12)	0.9400
C(13)-C(14)	1.3907(18)
C(13)-H(13)	0.9400
C(14)-C(15)	1.3895(19)
C(14)-C(17)	1.4870(19)
C(15)-C(16)	1.383(2)
C(15)-H(15)	0.9400
C(16)-H(16)	0.9400
C(17)-C(19)	1.495(2)
C(17)-C(18)	1.500(2)

C(17)-H(17)	0.9900
C(18)-C(19)	1.477(3)
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800

C(8)-N(1)-C(1)	108.45(12)
C(8)-N(1)-C(9)	125.67(15)
C(1)-N(1)-C(9)	125.66(14)
N(1)-C(1)-C(2)	130.08(14)
N(1)-C(1)-C(6)	107.42(13)
C(2)-C(1)-C(6)	122.49(15)
C(3)-C(2)-C(1)	117.03(15)
C(3)-C(2)-H(2)	121.5
C(1)-C(2)-H(2)	121.5
C(2)-C(3)-C(4)	121.75(15)
C(2)-C(3)-H(3)	119.1
C(4)-C(3)-H(3)	119.1
C(5)-C(4)-C(3)	120.88(16)
C(5)-C(4)-H(4)	119.6
C(3)-C(4)-H(4)	119.6
C(4)-C(5)-C(6)	118.82(15)
C(4)-C(5)-H(5)	120.6
C(6)-C(5)-H(5)	120.6
C(5)-C(6)-C(1)	119.03(13)
C(5)-C(6)-C(7)	133.65(13)
C(1)-C(6)-C(7)	107.32(13)
C(8)-C(7)-C(6)	106.00(12)
C(8)-C(7)-C(10)	126.02(14)
C(6)-C(7)-C(10)	127.92(13)
C(7)-C(8)-N(1)	110.81(13)
C(7)-C(8)-H(8)	124.6
N(1)-C(8)-H(8)	124.6
N(1)-C(9)-H(9A)	109.5
N(1)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
N(1)-C(9)-H(9C)	109.5

H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(7)-C(10)-C(11)	117.04(12)
C(7)-C(10)-H(10A)	108.0
C(11)-C(10)-H(10A)	108.0
C(7)-C(10)-H(10B)	108.0
C(11)-C(10)-H(10B)	108.0
H(10A)-C(10)-H(10B)	107.3
C(12)-C(11)-C(16)	117.24(12)
C(12)-C(11)-C(10)	123.67(12)
C(16)-C(11)-C(10)	119.09(12)
C(13)-C(12)-C(11)	121.08(12)
C(13)-C(12)-H(12)	119.5
C(11)-C(12)-H(12)	119.5
C(12)-C(13)-C(14)	121.60(12)
C(12)-C(13)-H(13)	119.2
C(14)-C(13)-H(13)	119.2
C(15)-C(14)-C(13)	117.38(12)
C(15)-C(14)-C(17)	123.48(12)
C(13)-C(14)-C(17)	119.13(12)
C(16)-C(15)-C(14)	120.86(12)
C(16)-C(15)-H(15)	119.6
C(14)-C(15)-H(15)	119.6
C(15)-C(16)-C(11)	121.82(13)
C(15)-C(16)-H(16)	119.1
C(11)-C(16)-H(16)	119.1
C(14)-C(17)-C(19)	122.76(13)
C(14)-C(17)-C(18)	121.83(13)
C(19)-C(17)-C(18)	59.08(11)
C(14)-C(17)-H(17)	114.1
C(19)-C(17)-H(17)	114.1
C(18)-C(17)-H(17)	114.1
C(19)-C(18)-C(17)	60.30(11)
C(19)-C(18)-H(18A)	117.7
C(17)-C(18)-H(18A)	117.7
C(19)-C(18)-H(18B)	117.7
C(17)-C(18)-H(18B)	117.7
H(18A)-C(18)-H(18B)	114.9

C(18)-C(19)-C(17)	60.62(10)
C(18)-C(19)-H(19A)	117.7
C(17)-C(19)-H(19A)	117.7
C(18)-C(19)-H(19B)	117.7
C(17)-C(19)-H(19B)	117.7
H(19A)-C(19)-H(19B)	114.8

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for d8v211031. The anisotropic displacement factor exponent takes the form: $-2\ ^2[\ h^2\ a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	40(1)	35(1)	52(1)	12(1)	-5(1)	-7(1)
C(1)	31(1)	38(1)	40(1)	10(1)	-2(1)	5(1)
C(2)	46(1)	60(1)	43(1)	17(1)	5(1)	12(1)
C(3)	65(1)	74(1)	34(1)	-4(1)	0(1)	19(1)
C(4)	59(1)	55(1)	54(1)	-15(1)	-6(1)	1(1)
C(5)	41(1)	41(1)	48(1)	-3(1)	0(1)	-3(1)
C(6)	29(1)	32(1)	39(1)	4(1)	-1(1)	3(1)
C(7)	33(1)	31(1)	37(1)	5(1)	-2(1)	4(1)
C(8)	42(1)	36(1)	43(1)	2(1)	-11(1)	0(1)
C(9)	75(1)	57(1)	84(1)	25(1)	-8(1)	-29(1)
C(10)	41(1)	40(1)	39(1)	5(1)	6(1)	10(1)
C(11)	29(1)	30(1)	31(1)	0(1)	0(1)	-1(1)
C(12)	35(1)	34(1)	27(1)	1(1)	4(1)	0(1)
C(13)	33(1)	31(1)	30(1)	-3(1)	5(1)	1(1)
C(14)	30(1)	29(1)	31(1)	0(1)	1(1)	-2(1)
C(15)	37(1)	38(1)	29(1)	2(1)	6(1)	0(1)
C(16)	33(1)	36(1)	34(1)	-2(1)	7(1)	4(1)
C(17)	38(1)	36(1)	35(1)	6(1)	4(1)	4(1)
C(18)	48(1)	47(1)	69(1)	25(1)	8(1)	5(1)
C(19)	67(1)	61(1)	40(1)	10(1)	-5(1)	18(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for d8v211031.

	x	y	z	U(eq)
H(2)	4172	755	4800	59
H(3)	5389	3141	5006	69
H(4)	6832	5004	4707	67
H(5)	7074	4559	4190	52
H(8)	4591	-445	3733	48
H(9A)	3015	-2099	4124	108
H(9B)	2672	-1195	4437	108
H(9C)	4258	-2279	4394	108
H(10A)	6525	1509	3451	48
H(10B)	7567	2746	3651	48
H(12)	4212	4667	3799	39
H(13)	3050	6943	3558	37
H(15)	5685	5992	2816	42
H(16)	6787	3671	3053	41
H(17)	2543	8684	3133	44
H(18A)	4122	10744	2886	65
H(18B)	5602	9377	2838	65
H(19A)	3842	7587	2556	68
H(19B)	2362	8953	2604	68

Table 6. Torsion angles [℃] for d8v211031.

C(8)-N(1)-C(1)-C(2)	179.85(15)
C(9)-N(1)-C(1)-C(2)	-5.4(3)
C(8)-N(1)-C(1)-C(6)	0.40(15)
C(9)-N(1)-C(1)-C(6)	175.14(15)
N(1)-C(1)-C(2)-C(3)	179.94(15)
C(6)-C(1)-C(2)-C(3)	-0.7(2)
C(1)-C(2)-C(3)-C(4)	0.1(2)
C(2)-C(3)-C(4)-C(5)	0.5(3)
C(3)-C(4)-C(5)-C(6)	-0.5(2)
C(4)-C(5)-C(6)-C(1)	-0.1(2)
C(4)-C(5)-C(6)-C(7)	-179.75(15)
N(1)-C(1)-C(6)-C(5)	-179.79(13)
C(2)-C(1)-C(6)-C(5)	0.7(2)
N(1)-C(1)-C(6)-C(7)	-0.06(15)
C(2)-C(1)-C(6)-C(7)	-179.56(13)
C(5)-C(6)-C(7)-C(8)	179.37(15)
C(1)-C(6)-C(7)-C(8)	-0.30(15)
C(5)-C(6)-C(7)-C(10)	2.0(3)
C(1)-C(6)-C(7)-C(10)	-177.70(13)
C(6)-C(7)-C(8)-N(1)	0.56(16)
C(10)-C(7)-C(8)-N(1)	178.02(13)
C(1)-N(1)-C(8)-C(7)	-0.62(17)
C(9)-N(1)-C(8)-C(7)	-175.35(15)
C(8)-C(7)-C(10)-C(11)	104.81(17)
C(6)-C(7)-C(10)-C(11)	-78.29(19)
C(7)-C(10)-C(11)-C(12)	17.0(2)
C(7)-C(10)-C(11)-C(16)	-163.58(13)
C(16)-C(11)-C(12)-C(13)	-0.4(2)
C(10)-C(11)-C(12)-C(13)	179.01(13)
C(11)-C(12)-C(13)-C(14)	-1.0(2)
C(12)-C(13)-C(14)-C(15)	1.3(2)
C(12)-C(13)-C(14)-C(17)	-179.50(12)
C(13)-C(14)-C(15)-C(16)	-0.2(2)
C(17)-C(14)-C(15)-C(16)	-179.45(13)
C(14)-C(15)-C(16)-C(11)	-1.1(2)
C(12)-C(11)-C(16)-C(15)	1.4(2)

C(10)-C(11)-C(16)-C(15)	-178.02(13)
C(15)-C(14)-C(17)-C(19)	22.7(2)
C(13)-C(14)-C(17)-C(19)	-156.48(15)
C(15)-C(14)-C(17)-C(18)	-48.6(2)
C(13)-C(14)-C(17)-C(18)	132.16(15)
C(14)-C(17)-C(18)-C(19)	111.75(16)
C(14)-C(17)-C(19)-C(18)	-110.23(16)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for d8v211031 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

9. Crystallographic Data of Compound 3ae

Table 1. Crystal data and structure refinement for **3ae**.

Identification code	mo_d8v211027_0m	
Empirical formula	C19 H16 N2 O	
Formula weight	288.34	
Temperature	213(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 25.192(2) Å	= 90°.
	b = 5.6061(5) Å	= 110.115(3)°.
	c = 33.579(3) Å	= 90°.
Volume	4453.1(7) $Å^3$	
Z	12	
Density (calculated)	1.290 Mg/m^3	
Absorption coefficient	0.081 mm^{-1}	
F(000)	1824	
Crystal size	0.200 x 0.150 x 0.120 mm^3	
Theta range for data collection	1.830 to 26.000 °.	
Index ranges	-31<=h<=30, -6<=k<=6, -41<=l<=41	
Reflections collected	75235	
Independent reflections	17400 [R(int) = 0.0491]	
Completeness to theta = 25.242 °	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6865	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	17400 / 1 / 1195	
Goodness-of-fit on F^2	1.043	
Final R indices [I>2sigma(I)]	R1 = 0.0446, wR2 = 0.0950	
R indices (all data)	R1 = 0.0673, wR2 = 0.1086	
Absolute structure parameter	-0.6(8)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.155 and -0.180 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)
for mo_d8v211027_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

_	x	y	z	U(eq)
O(1)	6957(1)	640(6)	2472(1)	46(1)
O(1A)	9621(1)	10931(6)	9120(1)	49(1)
O(1B)	482(1)	768(6)	5851(1)	50(1)
O(1C)	6318(1)	10874(6)	5871(1)	44(1)
O(1D)	6156(1)	5687(6)	10726(1)	47(1)
O(1E)	7233(1)	5821(6)	7593(1)	48(1)
N(1)	6929(1)	3679(9)	2046(1)	52(1)
N(2)	8705(1)	6030(7)	5306(1)	43(1)
N(1A)	9608(1)	8003(9)	9558(1)	60(1)
N(2A)	8050(1)	5287(8)	6302(1)	48(1)
N(1B)	436(1)	3883(9)	5436(1)	55(1)
N(2B)	2128(1)	6076(8)	8693(1)	48(1)
N(1C)	6386(1)	7739(9)	6290(1)	53(1)
N(2C)	4531(1)	5749(7)	3034(1)	40(1)
N(1D)	6132(1)	8640(9)	11160(1)	54(1)
N(2D)	4720(1)	11506(7)	7908(1)	39(1)
N(1E)	7236(1)	2821(10)	7167(1)	56(1)
N(2E)	8699(1)	207(8)	10418(1)	49(1)
C(1)	6805(2)	1501(11)	2073(1)	51(1)
C(2)	7186(1)	4366(9)	2465(1)	45(1)
C(3)	7209(1)	2544(8)	2725(1)	32(1)
C(4)	7426(1)	2198(7)	3179(1)	32(1)
C(5)	7780(1)	3893(8)	3444(1)	36(1)
C(6)	7993(1)	3586(8)	3876(1)	37(1)
C(7)	7862(1)	1572(8)	4064(1)	37(1)
C(8)	7504(1)	-114(8)	3801(1)	41(1)
C(9)	7290(1)	180(8)	3368(1)	38(1)
C(10)	8114(2)	1117(9)	4535(1)	48(1)
C(11)	8239(1)	3256(9)	4820(1)	43(1)
C(12)	8756(1)	4060(9)	5068(1)	46(1)

C(13)	8135(1)	6437(8)	5210(1)	37(1)
C(14)	7869(1)	8242(9)	5365(1)	45(1)
C(15)	7287(2)	8337(10)	5200(1)	51(1)
C(16)	6977(1)	6714(10)	4894(1)	52(1)
C(17)	7244(1)	4922(10)	4749(1)	45(1)
C(18)	7833(1)	4786(8)	4904(1)	37(1)
C(19)	9162(1)	7449(11)	5586(1)	61(1)
C(1A)	9746(2)	10145(10)	9524(1)	54(1)
C(2A)	9368(2)	7234(10)	9137(1)	54(1)
C(3A)	9374(1)	8992(8)	8867(1)	38(1)
C(4A)	9189(1)	9306(8)	8413(1)	35(1)
C(5A)	8857(1)	7534(8)	8151(1)	38(1)
C(6A)	8668(1)	7801(8)	7715(1)	41(1)
C(7A)	8802(1)	9837(8)	7529(1)	40(1)
C(8A)	9138(1)	11540(9)	7792(1)	45(1)
C(9A)	9327(1)	11296(8)	8226(1)	42(1)
C(10A)	8568(2)	10290(10)	7057(1)	52(1)
C(11A)	8472(1)	8149(9)	6777(1)	41(1)
C(12A)	7969(2)	7190(9)	6526(1)	48(1)
C(13A)	8619(1)	4888(8)	6406(1)	37(1)
C(14A)	8914(2)	3183(9)	6271(1)	47(1)
C(15A)	9489(2)	3204(9)	6444(1)	51(1)
C(16A)	9780(1)	4892(10)	6747(1)	50(1)
C(17A)	9492(1)	6632(10)	6878(1)	43(1)
C(18A)	8898(1)	6668(8)	6706(1)	36(1)
C(19A)	7609(1)	3793(10)	6016(1)	64(1)
C(1B)	304(2)	1706(11)	5455(1)	56(1)
C(2B)	726(2)	4508(9)	5855(1)	48(1)
C(3B)	756(1)	2627(8)	6109(1)	37(1)
C(4B)	988(1)	2213(8)	6562(1)	34(1)
C(5B)	1345(1)	3896(8)	6829(1)	38(1)
C(6B)	1549(1)	3563(8)	7260(1)	39(1)
C(7B)	1418(1)	1526(8)	7446(1)	41(1)
C(8B)	1064(2)	-142(9)	7178(1)	45(1)
C(9B)	854(1)	168(8)	6745(1)	42(1)
C(10B)	1656(2)	1108(9)	7918(1)	52(1)
C(11B)	1736(2)	3238(9)	8201(1)	44(1)
C(12B)	2224(2)	4121(9)	8470(1)	51(1)

C(13B)	1554(1)	6404(8)	8557(1)	39(1)
C(14B)	1250(2)	8181(9)	8681(1)	47(1)
C(15B)	675(2)	8198(10)	8482(1)	52(1)
C(16B)	407(2)	6536(11)	8169(1)	52(1)
C(17B)	710(1)	4777(10)	8051(1)	47(1)
C(18B)	1296(1)	4715(8)	8245(1)	38(1)
C(19B)	2551(2)	7555(11)	8995(1)	70(1)
C(1C)	6500(2)	9962(10)	6267(1)	47(1)
C(2C)	6092(2)	7111(9)	5871(1)	47(1)
C(3C)	6049(1)	8990(8)	5613(1)	36(1)
C(4C)	5812(1)	9426(7)	5160(1)	33(1)
C(5C)	5448(1)	7742(8)	4898(1)	35(1)
C(6C)	5224(1)	8085(8)	4466(1)	38(1)
C(7C)	5356(1)	10120(8)	4280(1)	36(1)
C(8C)	5720(1)	11779(8)	4544(1)	41(1)
C(9C)	5943(1)	11461(8)	4975(1)	39(1)
C(10C)	5108(2)	10634(9)	3809(1)	43(1)
C(11C)	4990(1)	8493(8)	3523(1)	37(1)
C(12C)	4474(1)	7654(9)	3265(1)	43(1)
C(13C)	5097(1)	5238(8)	3141(1)	34(1)
C(14C)	5371(1)	3514(9)	2994(1)	41(1)
C(15C)	5952(1)	3396(10)	3165(1)	46(1)
C(16C)	6259(2)	5021(10)	3477(1)	48(1)
C(17C)	5992(1)	6790(9)	3621(1)	41(1)
C(18C)	5401(1)	6940(8)	3449(1)	33(1)
C(19C)	4080(1)	4322(9)	2742(1)	50(1)
C(1D)	6277(2)	6466(11)	11129(1)	52(1)
C(2D)	5895(2)	9395(9)	10744(1)	49(1)
C(3D)	5905(1)	7610(8)	10478(1)	36(1)
C(4D)	5722(1)	7317(7)	10018(1)	33(1)
C(5D)	5400(1)	9084(8)	9754(1)	38(1)
C(6D)	5222(1)	8833(8)	9320(1)	40(1)
C(7D)	5356(1)	6816(8)	9134(1)	41(1)
C(8D)	5686(2)	5085(8)	9401(1)	45(1)
C(9D)	5865(2)	5301(8)	9836(1)	43(1)
C(10D)	5127(2)	6426(9)	8660(1)	51(1)
C(11D)	5084(2)	8604(9)	8387(1)	43(1)
C(12D)	4607(2)	9572(10)	8122(1)	46(1)

C(13D)	5301(1)	11743(8)	8046(1)	36(1)
C(14D)	5623(1)	13469(9)	7934(1)	43(1)
C(15D)	6199(2)	13390(10)	8139(1)	52(1)
C(16D)	6444(2)	11655(11)	8442(1)	59(1)
C(17D)	6123(2)	9938(10)	8546(1)	49(1)
C(18D)	5541(1)	9982(8)	8349(1)	38(1)
C(19D)	4314(1)	13023(10)	7613(1)	52(1)
C(1E)	7092(2)	4966(10)	7193(1)	48(1)
C(2E)	7499(1)	2147(9)	7589(1)	47(1)
C(3E)	7502(1)	3930(8)	7850(1)	35(1)
C(4E)	7701(1)	4285(8)	8305(1)	34(1)
C(5E)	8033(1)	2539(8)	8573(1)	35(1)
C(6E)	8219(1)	2806(8)	9007(1)	40(1)
C(7E)	8086(1)	4841(8)	9192(1)	42(1)
C(8E)	7751(1)	6561(9)	8925(1)	45(1)
C(9E)	7559(1)	6299(9)	8490(1)	42(1)
C(10E)	8310(2)	5277(10)	9664(1)	60(1)
C(11E)	8347(2)	3102(9)	9933(1)	45(1)
C(12E)	8826(2)	2079(9)	10214(1)	48(1)
C(13E)	8125(1)	-99(8)	10274(1)	39(1)
C(14E)	7797(2)	-1762(9)	10379(1)	51(1)
C(15E)	7227(2)	-1682(10)	10169(1)	56(1)
C(16E)	6979(2)	47(11)	9859(1)	56(1)
C(17E)	7303(1)	1761(10)	9757(1)	47(1)
C(18E)	7890(1)	1720(8)	9967(1)	39(1)
C(19E)	9102(2)	-1343(11)	10726(1)	65(1)

_

Table 3. Bond lengths [Å] and angles [ᵠ] for mo_d8v211027_0m.

O(1)-C(1)	1.350(5)
O(1)-C(3)	1.375(5)
O(1A)-C(1A)	1.356(5)
O(1A)-C(3A)	1.388(5)
O(1B)-C(1B)	1.355(5)
O(1B)-C(3B)	1.378(5)
O(1C)-C(1C)	1.350(5)
O(1C)-C(3C)	1.386(5)
O(1D)-C(1D)	1.354(5)
O(1D)-C(3D)	1.376(5)
O(1E)-C(1E)	1.354(5)
O(1E)-C(3E)	1.387(5)
N(1)-C(1)	1.271(7)
N(1)-C(2)	1.385(5)
N(2)-C(13)	1.378(4)
N(2)-C(12)	1.395(6)
N(2)-C(19)	1.448(5)
N(1A)-C(1A)	1.266(7)
N(1A)-C(2A)	1.400(5)
N(2A)-C(12A)	1.360(6)
N(2A)-C(13A)	1.373(4)
N(2A)-C(19A)	1.458(5)
N(1B)-C(1B)	1.273(7)
N(1B)-C(2B)	1.388(5)
N(2B)-C(13B)	1.372(4)
N(2B)-C(12B)	1.393(6)
N(2B)-C(19B)	1.452(6)
N(1C)-C(1C)	1.287(7)
N(1C)-C(2C)	1.391(5)
N(2C)-C(12C)	1.357(6)
N(2C)-C(13C)	1.374(4)
N(2C)-C(19C)	1.456(5)
N(1D)-C(1D)	1.286(7)
N(1D)-C(2D)	1.381(5)
N(2D)-C(13D)	1.380(4)
N(2D)-C(12D)	1.383(6)

N(2D)-C(19D)	1.434(5)
N(1E)-C(1E)	1.268(7)
N(1E)-C(2E)	1.393(5)
N(2E)-C(12E)	1.352(6)
N(2E)-C(13E)	1.368(4)
N(2E)-C(19E)	1.462(6)
C(1)-H(1)	0.9400
C(2)-C(3)	1.332(6)
C(2)-H(2)	0.9400
C(3)-C(4)	1.447(5)
C(4)-C(5)	1.394(5)
C(4)-C(9)	1.396(6)
C(5)-C(6)	1.375(5)
C(5)-H(5)	0.9400
C(6)-C(7)	1.388(6)
C(6)-H(6)	0.9400
C(7)-C(8)	1.392(6)
C(7)-C(10)	1.509(5)
C(8)-C(9)	1.375(5)
C(8)-H(8)	0.9400
C(9)-H(9)	0.9400
C(10)-C(11)	1.499(6)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(11)-C(12)	1.359(5)
C(11)-C(18)	1.434(5)
C(12)-H(12)	0.9400
C(13)-C(18)	1.398(6)
C(13)-C(14)	1.410(6)
C(14)-C(15)	1.378(5)
C(14)-H(14)	0.9400
C(15)-C(16)	1.394(6)
C(15)-H(15)	0.9400
C(16)-C(17)	1.386(7)
C(16)-H(16)	0.9400
C(17)-C(18)	1.397(4)
C(17)-H(17)	0.9400
C(19)-H(19A)	0.9700

C(19)-H(19B)	0.9700
C(19)-H(19C)	0.9700
C(1A)-H(1A)	0.9400
C(2A)-C(3A)	1.343(6)
C(2A)-H(2A)	0.9400
C(3A)-C(4A)	1.444(5)
C(4A)-C(9A)	1.383(6)
C(4A)-C(5A)	1.397(6)
C(5A)-C(6A)	1.383(5)
C(5A)-H(5A)	0.9400
C(6A)-C(7A)	1.398(6)
C(6A)-H(6A)	0.9400
C(7A)-C(8A)	1.377(6)
C(7A)-C(10A)	1.510(5)
C(8A)-C(9A)	1.374(5)
C(8A)-H(8A)	0.9400
C(9A)-H(9A)	0.9400
C(10A)-C(11A)	1.493(7)
C(10A)-H(10C)	0.9800
C(10A)-H(10D)	0.9800
C(11A)-C(12A)	1.365(6)
C(11A)-C(18A)	1.441(5)
C(12A)-H(12A)	0.9400
C(13A)-C(14A)	1.377(6)
C(13A)-C(18A)	1.422(6)
C(14A)-C(15A)	1.364(5)
C(14A)-H(14A)	0.9400
C(15A)-C(16A)	1.397(6)
C(15A)-H(15A)	0.9400
C(16A)-C(17A)	1.375(6)
C(16A)-H(16A)	0.9400
C(17A)-C(18A)	1.405(4)
C(17A)-H(17A)	0.9400
C(19A)-H(19D)	0.9700
C(19A)-H(19E)	0.9700
C(19A)-H(19F)	0.9700
C(1B)-H(1B)	0.9400
C(2B)-C(3B)	1.343(6)

C(2B)-H(2B)	0.9400
C(3B)-C(4B)	1.449(5)
C(4B)-C(9B)	1.395(6)
C(4B)-C(5B)	1.396(5)
C(5B)-C(6B)	1.372(5)
C(5B)-H(5B)	0.9400
C(6B)-C(7B)	1.394(6)
C(6B)-H(6B)	0.9400
C(7B)-C(8B)	1.388(6)
C(7B)-C(10B)	1.509(5)
C(8B)-C(9B)	1.375(5)
C(8B)-H(8B)	0.9400
C(9B)-H(9B)	0.9400
C(10B)-C(11B)	1.496(6)
C(10B)-H(10E)	0.9800
C(10B)-H(10F)	0.9800
C(11B)-C(12B)	1.344(5)
C(11B)-C(18B)	1.433(5)
C(12B)-H(12B)	0.9400
C(13B)-C(18B)	1.396(6)
C(13B)-C(14B)	1.403(6)
C(14B)-C(15B)	1.370(5)
C(14B)-H(14B)	0.9400
C(15B)-C(16B)	1.392(7)
C(15B)-H(15B)	0.9400
C(16B)-C(17B)	1.385(7)
C(16B)-H(16B)	0.9400
C(17B)-C(18B)	1.394(5)
C(17B)-H(17B)	0.9400
C(19B)-H(19G)	0.9700
C(19B)-H(19H)	0.9700
C(19B)-H(19I)	0.9700
C(1C)-H(1C)	0.9400
C(2C)-C(3C)	1.343(6)
C(2C)-H(2C)	0.9400
C(3C)-C(4C)	1.452(5)
C(4C)-C(9C)	1.392(6)
C(4C)-C(5C)	1.397(5)

C(5C)-C(6C)	1.380(5)
C(5C)-H(5C)	0.9400
C(6C)-C(7C)	1.393(6)
C(6C)-H(6C)	0.9400
C(7C)-C(8C)	1.389(6)
C(7C)-C(10C)	1.517(5)
C(8C)-C(9C)	1.373(5)
C(8C)-H(8C)	0.9400
C(9C)-H(9C)	0.9400
C(10C)-C(11C)	1.501(6)
C(10C)-H(10G)	0.9800
C(10C)-H(10H)	0.9800
C(11C)-C(12C)	1.374(5)
C(11C)-C(18C)	1.437(5)
C(12C)-H(12C)	0.9400
C(13C)-C(14C)	1.375(5)
C(13C)-C(18C)	1.422(5)
C(14C)-C(15C)	1.379(5)
C(14C)-H(14C)	0.9400
C(15C)-C(16C)	1.402(6)
C(15C)-H(15C)	0.9400
C(16C)-C(17C)	1.375(6)
C(16C)-H(16C)	0.9400
C(17C)-C(18C)	1.404(4)
C(17C)-H(17C)	0.9400
C(19C)-H(19J)	0.9700
C(19C)-H(19K)	0.9700
C(19C)-H(19L)	0.9700
C(1D)-H(1D)	0.9400
C(2D)-C(3D)	1.348(6)
C(2D)-H(2D)	0.9400
C(3D)-C(4D)	1.462(5)
C(4D)-C(9D)	1.389(6)
C(4D)-C(5D)	1.389(5)
C(5D)-C(6D)	1.377(5)
C(5D)-H(5D)	0.9400
C(6D)-C(7D)	1.389(6)
C(6D)-H(6D)	0.9400

C(7D)-C(8D)	1.387(6)
C(7D)-C(10D)	1.511(5)
C(8D)-C(9D)	1.379(5)
C(8D)-H(8D)	0.9400
C(9D)-H(9D)	0.9400
C(10D)-C(11D)	1.508(6)
C(10D)-H(10I)	0.9800
C(10D)-H(10J)	0.9800
C(11D)-C(12D)	1.341(6)
C(11D)-C(18D)	1.426(5)
C(12D)-H(12D)	0.9400
C(13D)-C(14D)	1.396(6)
C(13D)-C(18D)	1.397(6)
C(14D)-C(15D)	1.376(5)
C(14D)-H(14D)	0.9400
C(15D)-C(16D)	1.389(7)
C(15D)-H(15D)	0.9400
C(16D)-C(17D)	1.377(7)
C(16D)-H(16D)	0.9400
C(17D)-C(18D)	1.386(5)
C(17D)-H(17D)	0.9400
C(19D)-H(19M)	0.9700
C(19D)-H(19N)	0.9700
C(19D)-H(19O)	0.9700
C(1E)-H(1E)	0.9400
C(2E)-C(3E)	1.329(6)
C(2E)-H(2E)	0.9400
C(3E)-C(4E)	1.448(5)
C(4E)-C(9E)	1.393(6)
C(4E)-C(5E)	1.397(5)
C(5E)-C(6E)	1.380(5)
C(5E)-H(5E)	0.9400
C(6E)-C(7E)	1.392(6)
C(6E)-H(6E)	0.9400
C(7E)-C(8E)	1.387(6)
C(7E)-C(10E)	1.511(5)
C(8E)-C(9E)	1.380(5)
C(8E)-H(8E)	0.9400

C(9E)-H(9E)	0.9400
C(10E)-C(11E)	1.500(7)
C(10E)-H(10K)	0.9800
C(10E)-H(10L)	0.9800
C(11E)-C(12E)	1.377(6)
C(11E)-C(18E)	1.425(5)
C(12E)-H(12E)	0.9400
C(13E)-C(14E)	1.370(6)
C(13E)-C(18E)	1.427(6)
C(14E)-C(15E)	1.365(5)
C(14E)-H(14E)	0.9400
C(15E)-C(16E)	1.402(7)
C(15E)-H(15E)	0.9400
C(16E)-C(17E)	1.377(7)
C(16E)-H(16E)	0.9400
C(17E)-C(18E)	1.402(4)
C(17E)-H(17E)	0.9400
C(19E)-H(19P)	0.9700
C(19E)-H(19Q)	0.9700
C(19E)-H(19R)	0.9700

C(1)-O(1)-C(3)	104.3(4)
C(1A)-O(1A)-C(3A)	105.0(4)
C(1B)-O(1B)-C(3B)	104.4(4)
C(1C)-O(1C)-C(3C)	104.7(4)
C(1D)-O(1D)-C(3D)	104.5(4)
C(1E)-O(1E)-C(3E)	104.6(4)
C(1)-N(1)-C(2)	103.6(4)
C(13)-N(2)-C(12)	106.9(3)
C(13)-N(2)-C(19)	126.3(4)
C(12)-N(2)-C(19)	126.7(3)
C(1A)-N(1A)-C(2A)	103.8(4)
C(12A)-N(2A)-C(13A)	109.3(4)
C(12A)-N(2A)-C(19A)	126.2(3)
C(13A)-N(2A)-C(19A)	124.4(4)
C(1B)-N(1B)-C(2B)	104.3(4)
C(13B)-N(2B)-C(12B)	106.5(3)
C(13B)-N(2B)-C(19B)	126.3(4)

C(12B)-N(2B)-C(19B)	127.2(3)
C(1C)-N(1C)-C(2C)	103.7(4)
C(12C)-N(2C)-C(13C)	108.5(3)
C(12C)-N(2C)-C(19C)	127.2(3)
C(13C)-N(2C)-C(19C)	124.1(4)
C(1D)-N(1D)-C(2D)	104.2(4)
C(13D)-N(2D)-C(12D)	106.6(3)
C(13D)-N(2D)-C(19D)	126.7(4)
C(12D)-N(2D)-C(19D)	126.7(3)
C(1E)-N(1E)-C(2E)	103.5(4)
C(12E)-N(2E)-C(13E)	108.9(4)
C(12E)-N(2E)-C(19E)	126.3(3)
C(13E)-N(2E)-C(19E)	124.7(4)
N(1)-C(1)-O(1)	115.0(4)
N(1)-C(1)-H(1)	122.5
O(1)-C(1)-H(1)	122.5
C(3)-C(2)-N(1)	110.6(4)
C(3)-C(2)-H(2)	124.7
N(1)-C(2)-H(2)	124.7
C(2)-C(3)-O(1)	106.6(3)
C(2)-C(3)-C(4)	135.3(4)
O(1)-C(3)-C(4)	118.2(4)
C(5)-C(4)-C(9)	117.8(3)
C(5)-C(4)-C(3)	120.4(4)
C(9)-C(4)-C(3)	121.7(4)
C(6)-C(5)-C(4)	121.2(4)
C(6)-C(5)-H(5)	119.4
C(4)-C(5)-H(5)	119.4
C(5)-C(6)-C(7)	121.0(4)
C(5)-C(6)-H(6)	119.5
C(7)-C(6)-H(6)	119.5
C(6)-C(7)-C(8)	117.9(3)
C(6)-C(7)-C(10)	122.2(4)
C(8)-C(7)-C(10)	119.9(4)
C(9)-C(8)-C(7)	121.5(4)
C(9)-C(8)-H(8)	119.2
C(7)-C(8)-H(8)	119.2
C(8)-C(9)-C(4)	120.6(4)

C(8)-C(9)-H(9)	119.7
C(4)-C(9)-H(9)	119.7
C(11)-C(10)-C(7)	117.0(4)
C(11)-C(10)-H(10A)	108.0
C(7)-C(10)-H(10A)	108.0
C(11)-C(10)-H(10B)	108.0
C(7)-C(10)-H(10B)	108.0
H(10A)-C(10)-H(10B)	107.3
C(12)-C(11)-C(18)	106.2(4)
C(12)-C(11)-C(10)	127.0(4)
C(18)-C(11)-C(10)	126.6(3)
C(11)-C(12)-N(2)	110.8(3)
C(11)-C(12)-H(12)	124.6
N(2)-C(12)-H(12)	124.6
N(2)-C(13)-C(18)	108.8(4)
N(2)-C(13)-C(14)	128.5(4)
C(18)-C(13)-C(14)	122.6(3)
C(15)-C(14)-C(13)	117.1(4)
C(15)-C(14)-H(14)	121.4
C(13)-C(14)-H(14)	121.4
C(14)-C(15)-C(16)	121.2(4)
C(14)-C(15)-H(15)	119.4
C(16)-C(15)-H(15)	119.4
C(17)-C(16)-C(15)	121.1(3)
C(17)-C(16)-H(16)	119.4
C(15)-C(16)-H(16)	119.4
C(16)-C(17)-C(18)	119.4(4)
C(16)-C(17)-H(17)	120.3
C(18)-C(17)-H(17)	120.3
C(17)-C(18)-C(13)	118.5(4)
C(17)-C(18)-C(11)	134.3(4)
C(13)-C(18)-C(11)	107.2(3)
N(2)-C(19)-H(19A)	109.5
N(2)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
N(2)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5

N(1A)-C(1A)-O(1A)	115.0(5)
N(1A)-C(1A)-H(1A)	122.5
O(1A)-C(1A)-H(1A)	122.5
C(3A)-C(2A)-N(1A)	110.7(5)
C(3A)-C(2A)-H(2A)	124.6
N(1A)-C(2A)-H(2A)	124.6
C(2A)-C(3A)-O(1A)	105.6(3)
C(2A)-C(3A)-C(4A)	136.7(4)
O(1A)-C(3A)-C(4A)	117.7(4)
C(9A)-C(4A)-C(5A)	118.5(3)
C(9A)-C(4A)-C(3A)	122.5(4)
C(5A)-C(4A)-C(3A)	119.0(4)
C(6A)-C(5A)-C(4A)	120.2(4)
C(6A)-C(5A)-H(5A)	119.9
C(4A)-C(5A)-H(5A)	119.9
C(5A)-C(6A)-C(7A)	120.8(4)
C(5A)-C(6A)-H(6A)	119.6
C(7A)-C(6A)-H(6A)	119.6
C(8A)-C(7A)-C(6A)	118.0(4)
C(8A)-C(7A)-C(10A)	119.3(4)
C(6A)-C(7A)-C(10A)	122.6(4)
C(9A)-C(8A)-C(7A)	121.6(4)
C(9A)-C(8A)-H(8A)	119.2
C(7A)-C(8A)-H(8A)	119.2
C(8A)-C(9A)-C(4A)	120.8(4)
C(8A)-C(9A)-H(9A)	119.6
C(4A)-C(9A)-H(9A)	119.6
C(11A)-C(10A)-C(7A)	116.5(4)
C(11A)-C(10A)-H(10C)	108.2
C(7A)-C(10A)-H(10C)	108.2
C(11A)-C(10A)-H(10D)	108.2
C(7A)-C(10A)-H(10D)	108.2
H(10C)-C(10A)-H(10D)	107.3
C(12A)-C(11A)-C(18A)	104.9(4)
C(12A)-C(11A)-C(10A)	128.3(4)
C(18A)-C(11A)-C(10A)	126.8(3)
N(2A)-C(12A)-C(11A)	111.5(3)
N(2A)-C(12A)-H(12A)	124.2

C(11A)-C(12A)-H(12A)	124.2
N(2A)-C(13A)-C(14A)	131.6(4)
N(2A)-C(13A)-C(18A)	106.5(4)
C(14A)-C(13A)-C(18A)	121.9(3)
C(15A)-C(14A)-C(13A)	117.9(4)
C(15A)-C(14A)-H(14A)	121.0
C(13A)-C(14A)-H(14A)	121.0
C(14A)-C(15A)-C(16A)	122.0(4)
C(14A)-C(15A)-H(15A)	119.0
C(16A)-C(15A)-H(15A)	119.0
C(17A)-C(16A)-C(15A)	120.7(3)
C(17A)-C(16A)-H(16A)	119.6
C(15A)-C(16A)-H(16A)	119.6
C(16A)-C(17A)-C(18A)	118.9(4)
C(16A)-C(17A)-H(17A)	120.6
C(18A)-C(17A)-H(17A)	120.6
C(17A)-C(18A)-C(13A)	118.6(4)
C(17A)-C(18A)-C(11A)	133.6(4)
C(13A)-C(18A)-C(11A)	107.8(3)
N(2A)-C(19A)-H(19D)	109.5
N(2A)-C(19A)-H(19E)	109.5
H(19D)-C(19A)-H(19E)	109.5
N(2A)-C(19A)-H(19F)	109.5
H(19D)-C(19A)-H(19F)	109.5
H(19E)-C(19A)-H(19F)	109.5
N(1B)-C(1B)-O(1B)	114.6(4)
N(1B)-C(1B)-H(1B)	122.7
O(1B)-C(1B)-H(1B)	122.7
C(3B)-C(2B)-N(1B)	110.0(4)
C(3B)-C(2B)-H(2B)	125.0
N(1B)-C(2B)-H(2B)	125.0
C(2B)-C(3B)-O(1B)	106.7(3)
C(2B)-C(3B)-C(4B)	135.1(4)
O(1B)-C(3B)-C(4B)	118.2(4)
C(9B)-C(4B)-C(5B)	118.2(3)
C(9B)-C(4B)-C(3B)	121.5(4)
C(5B)-C(4B)-C(3B)	120.3(4)
C(6B)-C(5B)-C(4B)	120.7(4)

C(6B)-C(5B)-H(5B)	119.6
C(4B)-C(5B)-H(5B)	119.6
C(5B)-C(6B)-C(7B)	121.4(4)
C(5B)-C(6B)-H(6B)	119.3
C(7B)-C(6B)-H(6B)	119.3
C(8B)-C(7B)-C(6B)	117.4(4)
C(8B)-C(7B)-C(10B)	120.8(4)
C(6B)-C(7B)-C(10B)	121.7(4)
C(9B)-C(8B)-C(7B)	121.9(4)
C(9B)-C(8B)-H(8B)	119.1
C(7B)-C(8B)-H(8B)	119.1
C(8B)-C(9B)-C(4B)	120.3(4)
C(8B)-C(9B)-H(9B)	119.8
C(4B)-C(9B)-H(9B)	119.8
C(11B)-C(10B)-C(7B)	117.5(4)
C(11B)-C(10B)-H(10E)	107.9
C(7B)-C(10B)-H(10E)	107.9
C(11B)-C(10B)-H(10F)	107.9
C(7B)-C(10B)-H(10F)	107.9
H(10E)-C(10B)-H(10F)	107.2
C(12B)-C(11B)-C(18B)	106.1(4)
C(12B)-C(11B)-C(10B)	127.9(4)
C(18B)-C(11B)-C(10B)	125.9(4)
C(11B)-C(12B)-N(2B)	111.4(3)
C(11B)-C(12B)-H(12B)	124.3
N(2B)-C(12B)-H(12B)	124.3
N(2B)-C(13B)-C(18B)	108.9(4)
N(2B)-C(13B)-C(14B)	128.2(4)
C(18B)-C(13B)-C(14B)	122.8(3)
C(15B)-C(14B)-C(13B)	117.0(4)
C(15B)-C(14B)-H(14B)	121.5
C(13B)-C(14B)-H(14B)	121.5
C(14B)-C(15B)-C(16B)	121.3(4)
C(14B)-C(15B)-H(15B)	119.4
C(16B)-C(15B)-H(15B)	119.4
C(17B)-C(16B)-C(15B)	121.4(3)
C(17B)-C(16B)-H(16B)	119.3
C(15B)-C(16B)-H(16B)	119.3

C(16B)-C(17B)-C(18B)	118.8(4)
C(16B)-C(17B)-H(17B)	120.6
C(18B)-C(17B)-H(17B)	120.6
C(17B)-C(18B)-C(13B)	118.6(4)
C(17B)-C(18B)-C(11B)	134.4(4)
C(13B)-C(18B)-C(11B)	107.0(3)
N(2B)-C(19B)-H(19G)	109.5
N(2B)-C(19B)-H(19H)	109.5
H(19G)-C(19B)-H(19H)	109.5
N(2B)-C(19B)-H(19I)	109.5
H(19G)-C(19B)-H(19I)	109.5
H(19H)-C(19B)-H(19I)	109.5
N(1C)-C(1C)-O(1C)	114.8(4)
N(1C)-C(1C)-H(1C)	122.6
O(1C)-C(1C)-H(1C)	122.6
C(3C)-C(2C)-N(1C)	110.5(4)
C(3C)-C(2C)-H(2C)	124.7
N(1C)-C(2C)-H(2C)	124.7
C(2C)-C(3C)-O(1C)	106.3(3)
C(2C)-C(3C)-C(4C)	136.1(4)
O(1C)-C(3C)-C(4C)	117.6(4)
C(9C)-C(4C)-C(5C)	118.6(3)
C(9C)-C(4C)-C(3C)	122.1(4)
C(5C)-C(4C)-C(3C)	119.3(4)
C(6C)-C(5C)-C(4C)	120.7(4)
C(6C)-C(5C)-H(5C)	119.7
C(4C)-C(5C)-H(5C)	119.7
C(5C)-C(6C)-C(7C)	120.7(4)
C(5C)-C(6C)-H(6C)	119.6
C(7C)-C(6C)-H(6C)	119.6
C(8C)-C(7C)-C(6C)	118.1(3)
C(8C)-C(7C)-C(10C)	118.8(4)
C(6C)-C(7C)-C(10C)	123.1(4)
C(9C)-C(8C)-C(7C)	121.7(4)
C(9C)-C(8C)-H(8C)	119.1
C(7C)-C(8C)-H(8C)	119.1
C(8C)-C(9C)-C(4C)	120.2(4)
C(8C)-C(9C)-H(9C)	119.9

C(4C)-C(9C)-H(9C)	119.9
C(11C)-C(10C)-C(7C)	115.8(4)
C(11C)-C(10C)-H(10G)	108.3
C(7C)-C(10C)-H(10G)	108.3
C(11C)-C(10C)-H(10H)	108.3
C(7C)-C(10C)-H(10H)	108.3
H(10G)-C(10C)-H(10H)	107.4
C(12C)-C(11C)-C(18C)	105.4(4)
C(12C)-C(11C)-C(10C)	127.8(3)
C(18C)-C(11C)-C(10C)	126.7(3)
N(2C)-C(12C)-C(11C)	111.5(3)
N(2C)-C(12C)-H(12C)	124.3
C(11C)-C(12C)-H(12C)	124.3
N(2C)-C(13C)-C(14C)	130.9(4)
N(2C)-C(13C)-C(18C)	107.6(3)
C(14C)-C(13C)-C(18C)	121.5(3)
C(13C)-C(14C)-C(15C)	118.4(4)
C(13C)-C(14C)-H(14C)	120.8
C(15C)-C(14C)-H(14C)	120.8
C(14C)-C(15C)-C(16C)	120.9(4)
C(14C)-C(15C)-H(15C)	119.6
C(16C)-C(15C)-H(15C)	119.5
C(17C)-C(16C)-C(15C)	121.4(3)
C(17C)-C(16C)-H(16C)	119.3
C(15C)-C(16C)-H(16C)	119.3
C(16C)-C(17C)-C(18C)	118.4(4)
C(16C)-C(17C)-H(17C)	120.8
C(18C)-C(17C)-H(17C)	120.8
C(17C)-C(18C)-C(13C)	119.2(4)
C(17C)-C(18C)-C(11C)	133.7(4)
C(13C)-C(18C)-C(11C)	107.0(3)
N(2C)-C(19C)-H(19J)	109.5
N(2C)-C(19C)-H(19K)	109.5
H(19J)-C(19C)-H(19K)	109.5
N(2C)-C(19C)-H(19L)	109.5
H(19J)-C(19C)-H(19L)	109.5
H(19K)-C(19C)-H(19L)	109.5
N(1D)-C(1D)-O(1D)	114.4(5)

N(1D)-C(1D)-H(1D)	122.8
O(1D)-C(1D)-H(1D)	122.8
C(3D)-C(2D)-N(1D)	110.0(4)
C(3D)-C(2D)-H(2D)	125.0
N(1D)-C(2D)-H(2D)	125.0
C(2D)-C(3D)-O(1D)	106.8(3)
C(2D)-C(3D)-C(4D)	135.5(4)
O(1D)-C(3D)-C(4D)	117.6(3)
C(9D)-C(4D)-C(5D)	118.8(3)
C(9D)-C(4D)-C(3D)	121.4(4)
C(5D)-C(4D)-C(3D)	119.8(3)
C(6D)-C(5D)-C(4D)	120.6(4)
C(6D)-C(5D)-H(5D)	119.7
C(4D)-C(5D)-H(5D)	119.7
C(5D)-C(6D)-C(7D)	121.2(4)
C(5D)-C(6D)-H(6D)	119.4
C(7D)-C(6D)-H(6D)	119.4
C(8D)-C(7D)-C(6D)	117.6(4)
C(8D)-C(7D)-C(10D)	120.4(4)
C(6D)-C(7D)-C(10D)	121.9(4)
C(9D)-C(8D)-C(7D)	121.9(4)
C(9D)-C(8D)-H(8D)	119.1
C(7D)-C(8D)-H(8D)	119.1
C(8D)-C(9D)-C(4D)	119.9(4)
C(8D)-C(9D)-H(9D)	120.1
C(4D)-C(9D)-H(9D)	120.1
C(11D)-C(10D)-C(7D)	116.4(4)
C(11D)-C(10D)-H(10I)	108.2
C(7D)-C(10D)-H(10I)	108.2
C(11D)-C(10D)-H(10J)	108.2
C(7D)-C(10D)-H(10J)	108.2
H(10I)-C(10D)-H(10J)	107.3
C(12D)-C(11D)-C(18D)	106.8(4)
C(12D)-C(11D)-C(10D)	126.2(4)
C(18D)-C(11D)-C(10D)	126.9(4)
C(11D)-C(12D)-N(2D)	111.2(3)
C(11D)-C(12D)-H(12D)	124.4
N(2D)-C(12D)-H(12D)	124.4

N(2D)-C(13D)-C(14D)	128.5(4)
N(2D)-C(13D)-C(18D)	108.7(4)
C(14D)-C(13D)-C(18D)	122.7(3)
C(15D)-C(14D)-C(13D)	116.9(4)
C(15D)-C(14D)-H(14D)	121.5
C(13D)-C(14D)-H(14D)	121.5
C(14D)-C(15D)-C(16D)	121.1(4)
C(14D)-C(15D)-H(15D)	119.5
C(16D)-C(15D)-H(15D)	119.5
C(17D)-C(16D)-C(15D)	121.5(4)
C(17D)-C(16D)-H(16D)	119.2
C(15D)-C(16D)-H(16D)	119.2
C(16D)-C(17D)-C(18D)	119.0(4)
C(16D)-C(17D)-H(17D)	120.5
C(18D)-C(17D)-H(17D)	120.5
C(17D)-C(18D)-C(13D)	118.8(4)
C(17D)-C(18D)-C(11D)	134.5(4)
C(13D)-C(18D)-C(11D)	106.7(3)
N(2D)-C(19D)-H(19M)	109.5
N(2D)-C(19D)-H(19N)	109.5
H(19M)-C(19D)-H(19N)	109.5
N(2D)-C(19D)-H(19O)	109.5
H(19M)-C(19D)-H(19O)	109.5
H(19N)-C(19D)-H(19O)	109.5
N(1E)-C(1E)-O(1E)	114.9(4)
N(1E)-C(1E)-H(1E)	122.5
O(1E)-C(1E)-H(1E)	122.5
C(3E)-C(2E)-N(1E)	111.1(4)
C(3E)-C(2E)-H(2E)	124.4
N(1E)-C(2E)-H(2E)	124.4
C(2E)-C(3E)-O(1E)	105.9(3)
C(2E)-C(3E)-C(4E)	136.2(4)
O(1E)-C(3E)-C(4E)	117.9(4)
C(9E)-C(4E)-C(5E)	118.0(3)
C(9E)-C(4E)-C(3E)	122.2(4)
C(5E)-C(4E)-C(3E)	119.7(4)
C(6E)-C(5E)-C(4E)	121.0(4)
C(6E)-C(5E)-H(5E)	119.5

C(4E)-C(5E)-H(5E)	119.5
C(5E)-C(6E)-C(7E)	120.9(4)
C(5E)-C(6E)-H(6E)	119.5
C(7E)-C(6E)-H(6E)	119.6
C(8E)-C(7E)-C(6E)	118.0(4)
C(8E)-C(7E)-C(10E)	119.4(4)
C(6E)-C(7E)-C(10E)	122.6(4)
C(9E)-C(8E)-C(7E)	121.6(4)
C(9E)-C(8E)-H(8E)	119.2
C(7E)-C(8E)-H(8E)	119.2
C(8E)-C(9E)-C(4E)	120.5(4)
C(8E)-C(9E)-H(9E)	119.7
C(4E)-C(9E)-H(9E)	119.7
C(11E)-C(10E)-C(7E)	115.1(4)
C(11E)-C(10E)-H(10K)	108.5
C(7E)-C(10E)-H(10K)	108.5
C(11E)-C(10E)-H(10L)	108.5
C(7E)-C(10E)-H(10L)	108.5
H(10K)-C(10E)-H(10L)	107.5
C(12E)-C(11E)-C(18E)	105.2(4)
C(12E)-C(11E)-C(10E)	127.4(4)
C(18E)-C(11E)-C(10E)	127.3(4)
N(2E)-C(12E)-C(11E)	111.4(3)
N(2E)-C(12E)-H(12E)	124.3
C(11E)-C(12E)-H(12E)	124.3
N(2E)-C(13E)-C(14E)	130.7(4)
N(2E)-C(13E)-C(18E)	107.0(4)
C(14E)-C(13E)-C(18E)	122.2(3)
C(15E)-C(14E)-C(13E)	117.8(4)
C(15E)-C(14E)-H(14E)	121.1
C(13E)-C(14E)-H(14E)	121.1
C(14E)-C(15E)-C(16E)	121.8(4)
C(14E)-C(15E)-H(15E)	119.1
C(16E)-C(15E)-H(15E)	119.1
C(17E)-C(16E)-C(15E)	121.0(4)
C(17E)-C(16E)-H(16E)	119.5
C(15E)-C(16E)-H(16E)	119.5
C(16E)-C(17E)-C(18E)	118.5(4)

C(16E)-C(17E)-H(17E)	120.8
C(18E)-C(17E)-H(17E)	120.8
C(17E)-C(18E)-C(11E)	133.8(4)
C(17E)-C(18E)-C(13E)	118.7(4)
C(11E)-C(18E)-C(13E)	107.4(3)
N(2E)-C(19E)-H(19P)	109.5
N(2E)-C(19E)-H(19Q)	109.5
H(19P)-C(19E)-H(19Q)	109.5
N(2E)-C(19E)-H(19R)	109.5
H(19P)-C(19E)-H(19R)	109.5
H(19Q)-C(19E)-H(19R)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mo_d8v211027_0m. The anisotropic displacement factor exponent takes the form: $-2\ ^2[\ h^2\ a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	50(1)	40(2)	43(2)	-9(1)	8(1)	-6(1)
O(1A)	56(1)	48(2)	43(2)	-5(1)	17(1)	-4(1)
O(1B)	60(2)	40(2)	50(2)	-9(2)	18(1)	-4(1)
O(1C)	50(1)	44(2)	36(2)	-3(1)	11(1)	-2(1)
O(1D)	59(2)	39(2)	40(2)	4(1)	12(1)	2(1)
O(1E)	54(1)	43(2)	44(2)	8(2)	13(1)	8(1)
N(1)	50(2)	60(3)	42(2)	6(2)	10(1)	0(2)
N(2)	35(1)	47(2)	44(2)	5(2)	8(1)	-3(1)
N(1A)	66(2)	67(3)	45(2)	4(2)	19(2)	1(2)
N(2A)	35(2)	59(2)	46(2)	8(2)	9(1)	-5(2)
N(1B)	63(2)	57(3)	43(2)	2(2)	16(2)	2(2)
N(2B)	36(2)	53(2)	47(2)	11(2)	7(1)	-2(2)
N(1C)	57(2)	62(3)	36(2)	3(2)	10(1)	5(2)
N(2C)	35(1)	51(2)	35(2)	-1(2)	12(1)	-4(1)
N(1D)	62(2)	60(3)	36(2)	-6(2)	10(2)	1(2)
N(2D)	40(2)	42(2)	35(2)	-2(2)	13(1)	-1(1)
N(1E)	52(2)	69(3)	40(2)	-1(2)	10(2)	2(2)
N(2E)	41(2)	57(2)	46(2)	-5(2)	9(1)	6(2)
C(1)	42(2)	73(4)	35(2)	-9(2)	8(2)	-4(2)
C(2)	47(2)	40(3)	42(2)	2(2)	9(2)	-2(2)
C(3)	28(1)	30(2)	37(2)	-6(2)	9(1)	-3(1)
C(4)	29(1)	29(2)	39(2)	0(2)	13(1)	3(1)
C(5)	35(2)	32(2)	39(2)	4(2)	12(1)	-2(2)
C(6)	36(2)	34(2)	39(2)	-1(2)	9(1)	-2(2)
C(7)	38(2)	35(2)	39(2)	2(2)	16(1)	6(2)
C(8)	48(2)	29(2)	47(2)	7(2)	19(2)	0(2)
C(9)	38(2)	32(2)	43(2)	-4(2)	11(1)	-6(2)
C(10)	66(2)	40(3)	41(2)	10(2)	23(2)	13(2)
C(11)	47(2)	45(3)	35(2)	10(2)	14(2)	2(2)
C(12)	40(2)	53(3)	44(2)	14(2)	13(2)	6(2)
C(13)	36(2)	41(2)	34(2)	5(2)	11(1)	-4(2)
C(14)	50(2)	46(3)	40(2)	-3(2)	14(2)	-4(2)

C(15)	48(2)	50(3)	57(2)	-7(2)	20(2)	0(2)
C(16)	35(2)	61(3)	56(2)	0(2)	10(2)	2(2)
C(17)	42(2)	46(3)	43(2)	-5(2)	8(2)	-5(2)
C(18)	40(2)	40(2)	30(2)	7(2)	9(1)	0(2)
C(19)	44(2)	69(3)	58(3)	12(2)	3(2)	-12(2)
C(1A)	57(2)	61(3)	42(2)	-4(2)	14(2)	7(2)
C(2A)	64(2)	53(3)	46(2)	0(2)	21(2)	-10(2)
C(3A)	37(2)	36(2)	44(2)	-4(2)	19(1)	-1(2)
C(4A)	35(2)	34(2)	42(2)	0(2)	19(1)	4(2)
C(5A)	39(2)	32(2)	46(2)	3(2)	20(2)	2(2)
C(6A)	45(2)	34(2)	46(2)	0(2)	19(2)	5(2)
C(7A)	49(2)	32(2)	44(2)	6(2)	25(2)	12(2)
C(8A)	59(2)	32(2)	53(2)	5(2)	31(2)	0(2)
C(9A)	49(2)	32(2)	49(2)	-2(2)	22(2)	-2(2)
C(10A)	68(2)	46(3)	47(2)	7(2)	26(2)	13(2)
C(11A)	48(2)	43(3)	35(2)	10(2)	18(2)	11(2)
C(12A)	44(2)	52(3)	54(2)	13(2)	25(2)	14(2)
C(13A)	37(2)	38(2)	35(2)	6(2)	12(1)	1(2)
C(14A)	53(2)	42(3)	47(2)	-9(2)	20(2)	-10(2)
C(15A)	54(2)	47(3)	58(3)	-1(2)	28(2)	6(2)
C(16A)	37(2)	56(3)	56(3)	-3(2)	17(2)	1(2)
C(17A)	41(2)	43(3)	43(2)	-3(2)	11(2)	-5(2)
C(18A)	41(2)	36(2)	32(2)	4(2)	14(1)	0(2)
C(19A)	44(2)	68(3)	67(3)	12(3)	2(2)	-20(2)
C(1B)	53(2)	70(4)	44(2)	-9(2)	16(2)	1(2)
C(2B)	59(2)	44(3)	41(2)	2(2)	17(2)	-2(2)
C(3B)	36(2)	35(2)	42(2)	-3(2)	18(1)	0(2)
C(4B)	34(2)	29(2)	42(2)	2(2)	19(1)	8(1)
C(5B)	38(2)	35(2)	44(2)	6(2)	18(1)	2(2)
C(6B)	42(2)	33(2)	43(2)	4(2)	16(1)	8(2)
C(7B)	52(2)	37(2)	41(2)	8(2)	24(2)	15(2)
C(8B)	60(2)	30(2)	53(2)	10(2)	29(2)	6(2)
C(9B)	50(2)	31(2)	51(2)	-2(2)	25(2)	1(2)
C(10B)	74(2)	45(3)	44(2)	14(2)	29(2)	20(2)
C(11B)	50(2)	45(3)	42(2)	10(2)	21(2)	8(2)
C(12B)	42(2)	60(3)	53(2)	23(2)	20(2)	13(2)
C(13B)	38(2)	42(2)	36(2)	9(2)	12(1)	-2(2)
C(14B)	57(2)	42(3)	44(2)	-1(2)	19(2)	-2(2)

C(15B)	52(2)	48(3)	60(3)	-7(2)	22(2)	2(2)
C(16B)	36(2)	64(3)	54(3)	2(3)	12(2)	5(2)
C(17B)	42(2)	52(3)	44(2)	-4(2)	11(2)	-7(2)
C(18B)	42(2)	40(2)	32(2)	7(2)	13(1)	2(2)
C(19B)	53(2)	76(3)	63(3)	18(3)	-4(2)	-19(2)
C(1C)	50(2)	52(3)	35(2)	-3(2)	10(2)	7(2)
C(2C)	56(2)	43(3)	38(2)	1(2)	12(2)	-2(2)
C(3C)	36(2)	35(2)	37(2)	-4(2)	14(1)	3(2)
C(4C)	35(2)	31(2)	36(2)	-1(2)	14(1)	4(1)
C(5C)	40(2)	27(2)	40(2)	4(2)	18(1)	0(1)
C(6C)	46(2)	36(2)	35(2)	0(2)	16(1)	0(2)
C(7C)	47(2)	31(2)	36(2)	2(2)	20(1)	7(2)
C(8C)	53(2)	30(2)	48(2)	2(2)	27(2)	-1(2)
C(9C)	44(2)	30(2)	44(2)	-2(2)	16(2)	-3(2)
C(10C)	58(2)	37(2)	37(2)	2(2)	19(2)	7(2)
C(11C)	45(2)	40(2)	27(2)	6(2)	13(1)	8(2)
C(12C)	43(2)	52(3)	39(2)	7(2)	21(2)	8(2)
C(13C)	36(2)	39(2)	26(2)	6(2)	11(1)	-4(2)
C(14C)	50(2)	37(2)	38(2)	-8(2)	18(2)	-8(2)
C(15C)	45(2)	47(3)	51(2)	-3(2)	22(2)	6(2)
C(16C)	38(2)	53(3)	54(2)	-1(2)	15(2)	5(2)
C(17C)	39(2)	46(3)	35(2)	-2(2)	8(2)	-2(2)
C(18C)	36(2)	36(2)	28(2)	4(2)	12(1)	0(2)
C(19C)	41(2)	60(3)	48(2)	-1(2)	12(2)	-15(2)
C(1D)	52(2)	65(3)	35(2)	1(2)	10(2)	-5(2)
C(2D)	62(2)	43(3)	41(2)	-4(2)	14(2)	2(2)
C(3D)	35(2)	33(2)	43(2)	1(2)	15(1)	-2(2)
C(4D)	37(2)	26(2)	38(2)	2(2)	16(1)	-5(1)
C(5D)	42(2)	36(2)	40(2)	-2(2)	21(1)	-1(2)
C(6D)	45(2)	37(2)	40(2)	2(2)	17(1)	-2(2)
C(7D)	52(2)	37(2)	40(2)	-2(2)	24(2)	-13(2)
C(8D)	66(2)	28(2)	52(2)	-7(2)	32(2)	-5(2)
C(9D)	54(2)	30(2)	49(2)	0(2)	22(2)	0(2)
C(10D)	86(3)	35(2)	36(2)	-6(2)	27(2)	-21(2)
C(11D)	57(2)	42(3)	33(2)	-4(2)	21(2)	-6(2)
C(12D)	44(2)	58(3)	40(2)	-13(2)	21(2)	-13(2)
C(13D)	37(2)	39(2)	34(2)	-5(2)	16(1)	3(2)
C(14D)	45(2)	43(3)	44(2)	3(2)	21(2)	-1(2)

C(15D)	45(2)	51(3)	66(3)	7(2)	26(2)	-4(2)
C(16D)	37(2)	69(4)	67(3)	-1(3)	14(2)	-3(2)
C(17D)	47(2)	54(3)	42(2)	6(2)	10(2)	4(2)
C(18D)	45(2)	38(2)	32(2)	-4(2)	16(2)	-2(2)
C(19D)	44(2)	58(3)	50(2)	-6(2)	10(2)	9(2)
C(1E)	49(2)	53(3)	37(2)	8(2)	9(2)	1(2)
C(2E)	48(2)	49(3)	41(2)	0(2)	9(2)	7(2)
C(3E)	29(2)	35(2)	38(2)	4(2)	8(1)	0(2)
C(4E)	28(1)	35(2)	39(2)	-2(2)	13(1)	-4(2)
C(5E)	35(2)	30(2)	41(2)	-5(2)	14(1)	1(2)
C(6E)	41(2)	37(2)	39(2)	2(2)	11(1)	1(2)
C(7E)	50(2)	36(2)	42(2)	-3(2)	20(2)	-9(2)
C(8E)	55(2)	34(2)	52(2)	-6(2)	27(2)	-1(2)
C(9E)	44(2)	34(2)	47(2)	4(2)	17(2)	5(2)
C(10E)	81(3)	57(3)	44(2)	-11(2)	25(2)	-19(2)
C(11E)	53(2)	50(3)	32(2)	-13(2)	14(2)	-14(2)
C(12E)	46(2)	53(3)	47(2)	-14(2)	18(2)	-12(2)
C(13E)	38(2)	43(2)	35(2)	-5(2)	11(1)	2(2)
C(14E)	59(2)	47(3)	50(2)	9(2)	24(2)	10(2)
C(15E)	48(2)	58(3)	67(3)	-4(2)	24(2)	-8(2)
C(16E)	40(2)	60(3)	64(3)	0(3)	12(2)	-1(2)
C(17E)	46(2)	45(3)	45(2)	0(2)	8(2)	2(2)
C(18E)	41(2)	40(2)	34(2)	-7(2)	12(1)	-2(2)
C(19E)	54(2)	65(3)	64(3)	-3(3)	6(2)	23(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for mo_d8v211027_0m.

	x	y	z	U(eq)
H(1)	6621	561	1833	62
H(2)	7326	5904	2553	53
H(5)	7876	5272	3324	43
H(6)	8232	4756	4047	44
H(8)	7407	-1485	3922	49
H(9)	7050	-989	3198	46
H(10A)	7855	82	4616	57
H(10B)	8467	229	4589	57
H(12)	9101	3380	5077	55
H(14)	8079	9334	5571	54
H(15)	7095	9518	5297	61
H(16)	6581	6837	4783	63
H(17)	7029	3810	4548	54
H(19A)	9117	9096	5491	91
H(19B)	9520	6841	5581	91
H(19C)	9154	7360	5872	91
H(1A)	9921	11118	9761	65
H(2A)	9222	5697	9055	65
H(5A)	8762	6157	8271	45
H(6A)	8446	6596	7541	49
H(8A)	9241	12902	7673	54
H(9A)	9553	12497	8397	50
H(10C)	8208	11135	6993	62
H(10D)	8828	11360	6984	62
H(12A)	7613	7771	6511	58
H(14A)	8724	2042	6067	56
H(15A)	9697	2048	6357	61
H(16A)	10176	4839	6862	59
H(17A)	9688	7777	7079	52
H(19D)	7242	4498	5974	96

H(19E)	7625	2214	6138	96
H(19F)	7666	3673	5745	96
H(1B)	98	819	5214	67
H(2B)	878	6024	5947	58
H(5B)	1446	5272	6713	46
H(6B)	1783	4734	7435	47
H(8B)	965	-1522	7295	54
H(9B)	619	-1004	6571	51
H(10E)	1406	-11	7992	63
H(10F)	2024	321	7983	63
H(12B)	2583	3497	8505	61
H(14B)	1432	9309	8890	57
H(15B)	457	9355	8558	63
H(16B)	13	6609	8035	63
H(17B)	523	3645	7844	57
H(19G)	2520	9179	8890	105
H(19H)	2925	6941	9032	105
H(19I)	2491	7533	9265	105
H(1C)	6695	10878	6507	56
H(2C)	5945	5585	5781	56
H(5C)	5353	6362	5018	42
H(6C)	4981	6932	4294	46
H(8C)	5816	13156	4423	49
H(9C)	6186	12620	5146	47
H(10G)	4754	11516	3753	52
H(10H)	5370	11678	3732	52
H(12C)	4125	8315	3251	52
H(14C)	5166	2441	2781	49
H(15C)	6146	2209	3072	56
H(16C)	6655	4900	3589	58
H(17C)	6202	7873	3830	50
H(19J)	4152	4114	2478	76
H(19K)	3721	5127	2687	76
H(19L)	4068	2774	2868	76
H(1D)	6451	5499	11367	63
H(2D)	5749	10929	10660	59
H(5D)	5303	10462	9873	45
H(6D)	5005	10049	9146	48

H(8D)	5791	3726	9282	55
H(9D)	6083	4087	10010	52
H(10I)	5369	5257	8588	61
H(10J)	4750	5719	8585	61
H(12D)	4242	9009	8086	55
H(14D)	5454	14631	7727	51
H(15D)	6430	14529	8073	62
H(16D)	6838	11654	8579	70
H(17D)	6296	8755	8747	59
H(19M)	4373	14658	7713	78
H(19N)	3935	12521	7589	78
H(19O)	4358	12915	7338	78
H(1E)	6902	5893	6953	58
H(2E)	7654	630	7677	57
H(5E)	8132	1160	8455	42
H(6E)	8438	1598	9182	48
H(8E)	7652	7937	9044	54
H(9E)	7330	7489	8317	50
H(10K)	8688	5980	9740	72
H(10L)	8066	6450	9733	72
H(12E)	9196	2614	10258	58
H(14E)	7958	-2920	10588	61
H(15E)	6994	-2817	10234	68
H(16E)	6586	35	9718	68
H(17E)	7134	2931	9552	57
H(19P)	9481	-705	10793	97
H(19Q)	9086	-2931	10608	97
H(19R)	9008	-1422	10983	97

–

Table 6. Torsion angles [℃] for mo_d8v211027_0m.

C(2)-N(1)-C(1)-O(1)	-0.2(5)
C(3)-O(1)-C(1)-N(1)	-0.2(4)
C(1)-N(1)-C(2)-C(3)	0.6(4)
N(1)-C(2)-C(3)-O(1)	-0.7(4)
N(1)-C(2)-C(3)-C(4)	179.6(3)
C(1)-O(1)-C(3)-C(2)	0.5(4)
C(1)-O(1)-C(3)-C(4)	-179.7(3)
C(2)-C(3)-C(4)-C(5)	-13.0(6)
O(1)-C(3)-C(4)-C(5)	167.3(3)
C(2)-C(3)-C(4)-C(9)	167.1(4)
O(1)-C(3)-C(4)-C(9)	-12.6(5)
C(9)-C(4)-C(5)-C(6)	0.4(5)
C(3)-C(4)-C(5)-C(6)	-179.5(3)
C(4)-C(5)-C(6)-C(7)	0.0(5)
C(5)-C(6)-C(7)-C(8)	-0.5(5)
C(5)-C(6)-C(7)-C(10)	176.5(3)
C(6)-C(7)-C(8)-C(9)	0.5(5)
C(10)-C(7)-C(8)-C(9)	-176.5(3)
C(7)-C(8)-C(9)-C(4)	-0.1(5)
C(5)-C(4)-C(9)-C(8)	-0.4(5)
C(3)-C(4)-C(9)-C(8)	179.5(3)
C(6)-C(7)-C(10)-C(11)	32.9(5)
C(8)-C(7)-C(10)-C(11)	-150.2(3)
C(7)-C(10)-C(11)-C(12)	-113.3(4)
C(7)-C(10)-C(11)-C(18)	70.5(5)
C(18)-C(11)-C(12)-N(2)	-0.2(5)
C(10)-C(11)-C(12)-N(2)	-177.0(4)
C(13)-N(2)-C(12)-C(11)	1.4(4)
C(19)-N(2)-C(12)-C(11)	-176.1(4)
C(12)-N(2)-C(13)-C(18)	-2.0(4)
C(19)-N(2)-C(13)-C(18)	175.5(4)
C(12)-N(2)-C(13)-C(14)	-179.2(4)
C(19)-N(2)-C(13)-C(14)	-1.7(7)
N(2)-C(13)-C(14)-C(15)	176.6(4)
C(18)-C(13)-C(14)-C(15)	-0.2(6)
C(13)-C(14)-C(15)-C(16)	0.0(6)

C(14)-C(15)-C(16)-C(17)	1.1(7)
C(15)-C(16)-C(17)-C(18)	-1.9(7)
C(16)-C(17)-C(18)-C(13)	1.6(6)
C(16)-C(17)-C(18)-C(11)	-178.2(5)
N(2)-C(13)-C(18)-C(17)	-178.0(4)
C(14)-C(13)-C(18)-C(17)	-0.6(6)
N(2)-C(13)-C(18)-C(11)	1.9(4)
C(14)-C(13)-C(18)-C(11)	179.3(4)
C(12)-C(11)-C(18)-C(17)	178.8(5)
C(10)-C(11)-C(18)-C(17)	-4.4(8)
C(12)-C(11)-C(18)-C(13)	-1.1(5)
C(10)-C(11)-C(18)-C(13)	175.8(4)
C(2A)-N(1A)-C(1A)-O(1A)	0.3(5)
C(3A)-O(1A)-C(1A)-N(1A)	-0.5(5)
C(1A)-N(1A)-C(2A)-C(3A)	0.0(5)
N(1A)-C(2A)-C(3A)-O(1A)	-0.3(4)
N(1A)-C(2A)-C(3A)-C(4A)	-178.9(4)
C(1A)-O(1A)-C(3A)-C(2A)	0.4(4)
C(1A)-O(1A)-C(3A)-C(4A)	179.4(3)
C(2A)-C(3A)-C(4A)-C(9A)	-171.0(4)
O(1A)-C(3A)-C(4A)-C(9A)	10.6(5)
C(2A)-C(3A)-C(4A)-C(5A)	9.0(6)
O(1A)-C(3A)-C(4A)-C(5A)	-169.5(3)
C(9A)-C(4A)-C(5A)-C(6A)	-0.8(5)
C(3A)-C(4A)-C(5A)-C(6A)	179.2(3)
C(4A)-C(5A)-C(6A)-C(7A)	-0.2(5)
C(5A)-C(6A)-C(7A)-C(8A)	1.5(5)
C(5A)-C(6A)-C(7A)-C(10A)	-175.2(3)
C(6A)-C(7A)-C(8A)-C(9A)	-1.7(5)
C(10A)-C(7A)-C(8A)-C(9A)	175.1(3)
C(7A)-C(8A)-C(9A)-C(4A)	0.6(6)
C(5A)-C(4A)-C(9A)-C(8A)	0.7(5)
C(3A)-C(4A)-C(9A)-C(8A)	-179.4(3)
C(8A)-C(7A)-C(10A)-C(11A)	149.8(4)
C(6A)-C(7A)-C(10A)-C(11A)	-33.6(5)
C(7A)-C(10A)-C(11A)-C(12A)	110.6(5)
C(7A)-C(10A)-C(11A)-C(18A)	-70.8(5)
C(13A)-N(2A)-C(12A)-C(11A)	1.2(5)

C(19A)-N(2A)-C(12A)-C(11A)	177.8(4)
C(18A)-C(11A)-C(12A)-N(2A)	-1.3(5)
C(10A)-C(11A)-C(12A)-N(2A)	177.6(4)
C(12A)-N(2A)-C(13A)-C(14A)	179.1(4)
C(19A)-N(2A)-C(13A)-C(14A)	2.5(7)
C(12A)-N(2A)-C(13A)-C(18A)	-0.6(4)
C(19A)-N(2A)-C(13A)-C(18A)	-177.3(4)
N(2A)-C(13A)-C(14A)-C(15A)	-178.0(4)
C(18A)-C(13A)-C(14A)-C(15A)	1.7(6)
C(13A)-C(14A)-C(15A)-C(16A)	-0.4(7)
C(14A)-C(15A)-C(16A)-C(17A)	-0.9(7)
C(15A)-C(16A)-C(17A)-C(18A)	0.8(7)
C(16A)-C(17A)-C(18A)-C(13A)	0.5(6)
C(16A)-C(17A)-C(18A)-C(11A)	178.1(4)
N(2A)-C(13A)-C(18A)-C(17A)	178.0(4)
C(14A)-C(13A)-C(18A)-C(17A)	-1.8(6)
N(2A)-C(13A)-C(18A)-C(11A)	-0.2(4)
C(14A)-C(13A)-C(18A)-C(11A)	-180.0(4)
C(12A)-C(11A)-C(18A)-C(17A)	-176.9(4)
C(10A)-C(11A)-C(18A)-C(17A)	4.2(7)
C(12A)-C(11A)-C(18A)-C(13A)	0.9(4)
C(10A)-C(11A)-C(18A)-C(13A)	-178.0(4)
C(2B)-N(1B)-C(1B)-O(1B)	-0.7(5)
C(3B)-O(1B)-C(1B)-N(1B)	0.7(5)
C(1B)-N(1B)-C(2B)-C(3B)	0.5(4)
N(1B)-C(2B)-C(3B)-O(1B)	0.0(4)
N(1B)-C(2B)-C(3B)-C(4B)	-178.5(3)
C(1B)-O(1B)-C(3B)-C(2B)	-0.4(4)
C(1B)-O(1B)-C(3B)-C(4B)	178.4(3)
C(2B)-C(3B)-C(4B)-C(9B)	166.7(4)
O(1B)-C(3B)-C(4B)-C(9B)	-11.7(5)
C(2B)-C(3B)-C(4B)-C(5B)	-12.0(6)
O(1B)-C(3B)-C(4B)-C(5B)	169.6(3)
C(9B)-C(4B)-C(5B)-C(6B)	-1.2(5)
C(3B)-C(4B)-C(5B)-C(6B)	177.5(3)
C(4B)-C(5B)-C(6B)-C(7B)	1.2(5)
C(5B)-C(6B)-C(7B)-C(8B)	-1.0(5)
C(5B)-C(6B)-C(7B)-C(10B)	177.9(3)

C(6B)-C(7B)-C(8B)-C(9B)	0.8(5)
C(10B)-C(7B)-C(8B)-C(9B)	-178.1(3)
C(7B)-C(8B)-C(9B)-C(4B)	-0.8(5)
C(5B)-C(4B)-C(9B)-C(8B)	1.0(5)
C(3B)-C(4B)-C(9B)-C(8B)	-177.7(3)
C(8B)-C(7B)-C(10B)-C(11B)	-145.7(4)
C(6B)-C(7B)-C(10B)-C(11B)	35.4(5)
C(7B)-C(10B)-C(11B)-C(12B)	-116.1(5)
C(7B)-C(10B)-C(11B)-C(18B)	65.8(5)
C(18B)-C(11B)-C(12B)-N(2B)	0.6(5)
C(10B)-C(11B)-C(12B)-N(2B)	-177.8(4)
C(13B)-N(2B)-C(12B)-C(11B)	0.7(5)
C(19B)-N(2B)-C(12B)-C(11B)	-176.9(4)
C(12B)-N(2B)-C(13B)-C(18B)	-1.7(4)
C(19B)-N(2B)-C(13B)-C(18B)	175.9(4)
C(12B)-N(2B)-C(13B)-C(14B)	-178.5(4)
C(19B)-N(2B)-C(13B)-C(14B)	-0.9(7)
N(2B)-C(13B)-C(14B)-C(15B)	176.7(4)
C(18B)-C(13B)-C(14B)-C(15B)	0.4(6)
C(13B)-C(14B)-C(15B)-C(16B)	-0.5(7)
C(14B)-C(15B)-C(16B)-C(17B)	1.0(7)
C(15B)-C(16B)-C(17B)-C(18B)	-1.3(7)
C(16B)-C(17B)-C(18B)-C(13B)	1.2(6)
C(16B)-C(17B)-C(18B)-C(11B)	-178.6(5)
N(2B)-C(13B)-C(18B)-C(17B)	-177.7(4)
C(14B)-C(13B)-C(18B)-C(17B)	-0.7(6)
N(2B)-C(13B)-C(18B)-C(11B)	2.1(5)
C(14B)-C(13B)-C(18B)-C(11B)	179.1(4)
C(12B)-C(11B)-C(18B)-C(17B)	178.1(5)
C(10B)-C(11B)-C(18B)-C(17B)	-3.5(8)
C(12B)-C(11B)-C(18B)-C(13B)	-1.7(5)
C(10B)-C(11B)-C(18B)-C(13B)	176.8(4)
C(2C)-N(1C)-C(1C)-O(1C)	-0.9(5)
C(3C)-O(1C)-C(1C)-N(1C)	0.8(4)
C(1C)-N(1C)-C(2C)-C(3C)	0.6(4)
N(1C)-C(2C)-C(3C)-O(1C)	-0.1(4)
N(1C)-C(2C)-C(3C)-C(4C)	178.2(3)
C(1C)-O(1C)-C(3C)-C(2C)	-0.4(4)

C(1C)-O(1C)-C(3C)-C(4C)	-179.0(3)
C(2C)-C(3C)-C(4C)-C(9C)	-165.1(4)
O(1C)-C(3C)-C(4C)-C(9C)	13.0(5)
C(2C)-C(3C)-C(4C)-C(5C)	13.9(6)
O(1C)-C(3C)-C(4C)-C(5C)	-167.9(3)
C(9C)-C(4C)-C(5C)-C(6C)	0.3(5)
C(3C)-C(4C)-C(5C)-C(6C)	-178.8(3)
C(4C)-C(5C)-C(6C)-C(7C)	-0.2(5)
C(5C)-C(6C)-C(7C)-C(8C)	0.4(5)
C(5C)-C(6C)-C(7C)-C(10C)	-177.9(3)
C(6C)-C(7C)-C(8C)-C(9C)	-0.5(5)
C(10C)-C(7C)-C(8C)-C(9C)	177.8(3)
C(7C)-C(8C)-C(9C)-C(4C)	0.6(6)
C(5C)-C(4C)-C(9C)-C(8C)	-0.5(5)
C(3C)-C(4C)-C(9C)-C(8C)	178.6(3)
C(8C)-C(7C)-C(10C)-C(11C)	148.8(3)
C(6C)-C(7C)-C(10C)-C(11C)	-32.9(5)
C(7C)-C(10C)-C(11C)-C(12C)	113.7(4)
C(7C)-C(10C)-C(11C)-C(18C)	-69.1(5)
C(13C)-N(2C)-C(12C)-C(11C)	1.3(4)
C(19C)-N(2C)-C(12C)-C(11C)	176.8(4)
C(18C)-C(11C)-C(12C)-N(2C)	-1.1(4)
C(10C)-C(11C)-C(12C)-N(2C)	176.5(4)
C(12C)-N(2C)-C(13C)-C(14C)	-179.1(4)
C(19C)-N(2C)-C(13C)-C(14C)	5.3(6)
C(12C)-N(2C)-C(13C)-C(18C)	-1.0(4)
C(19C)-N(2C)-C(13C)-C(18C)	-176.6(3)
N(2C)-C(13C)-C(14C)-C(15C)	-179.3(4)
C(18C)-C(13C)-C(14C)-C(15C)	2.8(6)
C(13C)-C(14C)-C(15C)-C(16C)	-1.2(6)
C(14C)-C(15C)-C(16C)-C(17C)	-0.2(7)
C(15C)-C(16C)-C(17C)-C(18C)	0.1(6)
C(16C)-C(17C)-C(18C)-C(13C)	1.5(6)
C(16C)-C(17C)-C(18C)-C(11C)	179.4(4)
N(2C)-C(13C)-C(18C)-C(17C)	178.7(3)
C(14C)-C(13C)-C(18C)-C(17C)	-3.0(6)
N(2C)-C(13C)-C(18C)-C(11C)	0.3(4)
C(14C)-C(13C)-C(18C)-C(11C)	178.6(3)

C(12C)-C(11C)-C(18C)-C(17C)	-177.6(4)
C(10C)-C(11C)-C(18C)-C(17C)	4.7(7)
C(12C)-C(11C)-C(18C)-C(13C)	0.5(4)
C(10C)-C(11C)-C(18C)-C(13C)	-177.2(3)
C(2D)-N(1D)-C(1D)-O(1D)	-0.1(5)
C(3D)-O(1D)-C(1D)-N(1D)	-0.2(4)
C(1D)-N(1D)-C(2D)-C(3D)	0.4(5)
N(1D)-C(2D)-C(3D)-O(1D)	-0.6(4)
N(1D)-C(2D)-C(3D)-C(4D)	179.8(4)
C(1D)-O(1D)-C(3D)-C(2D)	0.5(4)
C(1D)-O(1D)-C(3D)-C(4D)	-179.8(3)
C(2D)-C(3D)-C(4D)-C(9D)	170.8(4)
O(1D)-C(3D)-C(4D)-C(9D)	-8.8(5)
C(2D)-C(3D)-C(4D)-C(5D)	-9.0(6)
O(1D)-C(3D)-C(4D)-C(5D)	171.4(3)
C(9D)-C(4D)-C(5D)-C(6D)	0.5(5)
C(3D)-C(4D)-C(5D)-C(6D)	-179.7(3)
C(4D)-C(5D)-C(6D)-C(7D)	0.2(5)
C(5D)-C(6D)-C(7D)-C(8D)	-1.3(5)
C(5D)-C(6D)-C(7D)-C(10D)	175.3(3)
C(6D)-C(7D)-C(8D)-C(9D)	1.8(6)
C(10D)-C(7D)-C(8D)-C(9D)	-174.8(3)
C(7D)-C(8D)-C(9D)-C(4D)	-1.1(6)
C(5D)-C(4D)-C(9D)-C(8D)	0.0(5)
C(3D)-C(4D)-C(9D)-C(8D)	-179.8(3)
C(8D)-C(7D)-C(10D)-C(11D)	-145.4(4)
C(6D)-C(7D)-C(10D)-C(11D)	38.1(5)
C(7D)-C(10D)-C(11D)-C(12D)	-115.2(5)
C(7D)-C(10D)-C(11D)-C(18D)	67.0(5)
C(18D)-C(11D)-C(12D)-N(2D)	0.4(5)
C(10D)-C(11D)-C(12D)-N(2D)	-177.7(4)
C(13D)-N(2D)-C(12D)-C(11D)	0.3(5)
C(19D)-N(2D)-C(12D)-C(11D)	-177.5(4)
C(12D)-N(2D)-C(13D)-C(14D)	-178.1(4)
C(19D)-N(2D)-C(13D)-C(14D)	-0.3(6)
C(12D)-N(2D)-C(13D)-C(18D)	-0.9(4)
C(19D)-N(2D)-C(13D)-C(18D)	176.9(4)
N(2D)-C(13D)-C(14D)-C(15D)	176.1(4)

C(18D)-C(13D)-C(14D)-C(15D)	-0.7(6)
C(13D)-C(14D)-C(15D)-C(16D)	0.4(7)
C(14D)-C(15D)-C(16D)-C(17D)	0.6(7)
C(15D)-C(16D)-C(17D)-C(18D)	-1.4(7)
C(16D)-C(17D)-C(18D)-C(13D)	1.2(6)
C(16D)-C(17D)-C(18D)-C(11D)	-177.0(5)
N(2D)-C(13D)-C(18D)-C(17D)	-177.5(4)
C(14D)-C(13D)-C(18D)-C(17D)	-0.1(6)
N(2D)-C(13D)-C(18D)-C(11D)	1.2(4)
C(14D)-C(13D)-C(18D)-C(11D)	178.5(4)
C(12D)-C(11D)-C(18D)-C(17D)	177.3(5)
C(10D)-C(11D)-C(18D)-C(17D)	-4.5(8)
C(12D)-C(11D)-C(18D)-C(13D)	-1.0(5)
C(10D)-C(11D)-C(18D)-C(13D)	177.2(4)
C(2E)-N(1E)-C(1E)-O(1E)	0.1(5)
C(3E)-O(1E)-C(1E)-N(1E)	0.0(4)
C(1E)-N(1E)-C(2E)-C(3E)	-0.2(5)
N(1E)-C(2E)-C(3E)-O(1E)	0.2(4)
N(1E)-C(2E)-C(3E)-C(4E)	179.2(3)
C(1E)-O(1E)-C(3E)-C(2E)	-0.1(4)
C(1E)-O(1E)-C(3E)-C(4E)	-179.3(3)
C(2E)-C(3E)-C(4E)-C(9E)	-169.3(4)
O(1E)-C(3E)-C(4E)-C(9E)	9.7(5)
C(2E)-C(3E)-C(4E)-C(5E)	8.8(6)
O(1E)-C(3E)-C(4E)-C(5E)	-172.2(3)
C(9E)-C(4E)-C(5E)-C(6E)	-0.4(5)
C(3E)-C(4E)-C(5E)-C(6E)	-178.6(3)
C(4E)-C(5E)-C(6E)-C(7E)	-0.9(5)
C(5E)-C(6E)-C(7E)-C(8E)	1.5(5)
C(5E)-C(6E)-C(7E)-C(10E)	-176.1(3)
C(6E)-C(7E)-C(8E)-C(9E)	-0.9(5)
C(10E)-C(7E)-C(8E)-C(9E)	176.8(4)
C(7E)-C(8E)-C(9E)-C(4E)	-0.4(6)
C(5E)-C(4E)-C(9E)-C(8E)	1.1(5)
C(3E)-C(4E)-C(9E)-C(8E)	179.2(3)
C(8E)-C(7E)-C(10E)-C(11E)	144.5(4)
C(6E)-C(7E)-C(10E)-C(11E)	-37.9(5)
C(7E)-C(10E)-C(11E)-C(12E)	116.2(5)

C(7E)-C(10E)-C(11E)-C(18E)	-67.0(6)
C(13E)-N(2E)-C(12E)-C(11E)	0.8(5)
C(19E)-N(2E)-C(12E)-C(11E)	177.7(4)
C(18E)-C(11E)-C(12E)-N(2E)	-0.6(5)
C(10E)-C(11E)-C(12E)-N(2E)	176.7(4)
C(12E)-N(2E)-C(13E)-C(14E)	178.8(4)
C(19E)-N(2E)-C(13E)-C(14E)	1.8(7)
C(12E)-N(2E)-C(13E)-C(18E)	-0.7(4)
C(19E)-N(2E)-C(13E)-C(18E)	-177.7(4)
N(2E)-C(13E)-C(14E)-C(15E)	-177.6(4)
C(18E)-C(13E)-C(14E)-C(15E)	1.8(6)
C(13E)-C(14E)-C(15E)-C(16E)	-0.6(7)
C(14E)-C(15E)-C(16E)-C(17E)	-0.9(7)
C(15E)-C(16E)-C(17E)-C(18E)	1.0(7)
C(16E)-C(17E)-C(18E)-C(11E)	176.9(5)
C(16E)-C(17E)-C(18E)-C(13E)	0.2(6)
C(12E)-C(11E)-C(18E)-C(17E)	-176.8(5)
C(10E)-C(11E)-C(18E)-C(17E)	5.9(8)
C(12E)-C(11E)-C(18E)-C(13E)	0.1(4)
C(10E)-C(11E)-C(18E)-C(13E)	-177.2(4)
N(2E)-C(13E)-C(18E)-C(17E)	177.9(4)
C(14E)-C(13E)-C(18E)-C(17E)	-1.7(6)
N(2E)-C(13E)-C(18E)-C(11E)	0.4(4)
C(14E)-C(13E)-C(18E)-C(11E)	-179.2(4)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for mo_d8v211027_0m [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(1E)-H(1E)...N(1C)	0.94	2.39	3.327(6)	172.0
C(1D)-H(1D)...N(1)#1	0.94	2.41	3.337(6)	169.8
C(1C)-H(1C)...N(1E)#2	0.94	2.42	3.359(6)	173.6
C(1B)-H(1B)...N(1B)#3	0.94	2.39	3.331(5)	174.9
C(1A)-H(1A)...N(1A)#4	0.94	2.43	3.357(5)	170.2
C(1)-H(1)...N(1D)#5	0.94	2.42	3.358(6)	172.1
C(1E)-H(1E)...N(1C)	0.94	2.39	3.327(6)	172.0
C(1D)-H(1D)...N(1)#1	0.94	2.41	3.337(6)	169.8
C(1C)-H(1C)...N(1E)#2	0.94	2.42	3.359(6)	173.6
C(1B)-H(1B)...N(1B)#3	0.94	2.39	3.331(5)	174.9
C(1A)-H(1A)...N(1A)#4	0.94	2.43	3.357(5)	170.2
C(1)-H(1)...N(1D)#5	0.94	2.42	3.358(6)	172.1
C(1)-H(1)...N(1D)#5	0.94	2.42	3.358(6)	172.1
C(1A)-H(1A)...N(1A)#4	0.94	2.43	3.357(5)	170.2
C(1B)-H(1B)...N(1B)#3	0.94	2.39	3.331(5)	174.9
C(1C)-H(1C)...N(1E)#2	0.94	2.42	3.359(6)	173.6
C(1D)-H(1D)...N(1)#1	0.94	2.41	3.337(6)	169.8
C(1E)-H(1E)...N(1C)	0.94	2.39	3.327(6)	172.0
C(1)-H(1)...N(1D)#5	0.94	2.42	3.358(6)	172.1
C(1A)-H(1A)...N(1A)#4	0.94	2.43	3.357(5)	170.2
C(1B)-H(1B)...N(1B)#3	0.94	2.39	3.331(5)	174.9
C(1C)-H(1C)...N(1E)#2	0.94	2.42	3.359(6)	173.6
C(1D)-H(1D)...N(1)#1	0.94	2.41	3.337(6)	169.8
C(1E)-H(1E)...N(1C)	0.94	2.39	3.327(6)	172.0

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z+1 #2 x,y+1,z #3 -x,y-1/2,-z+1 #4 -x+2,y+1/2,-z+2

#5 x,y-1,z-1

10. References

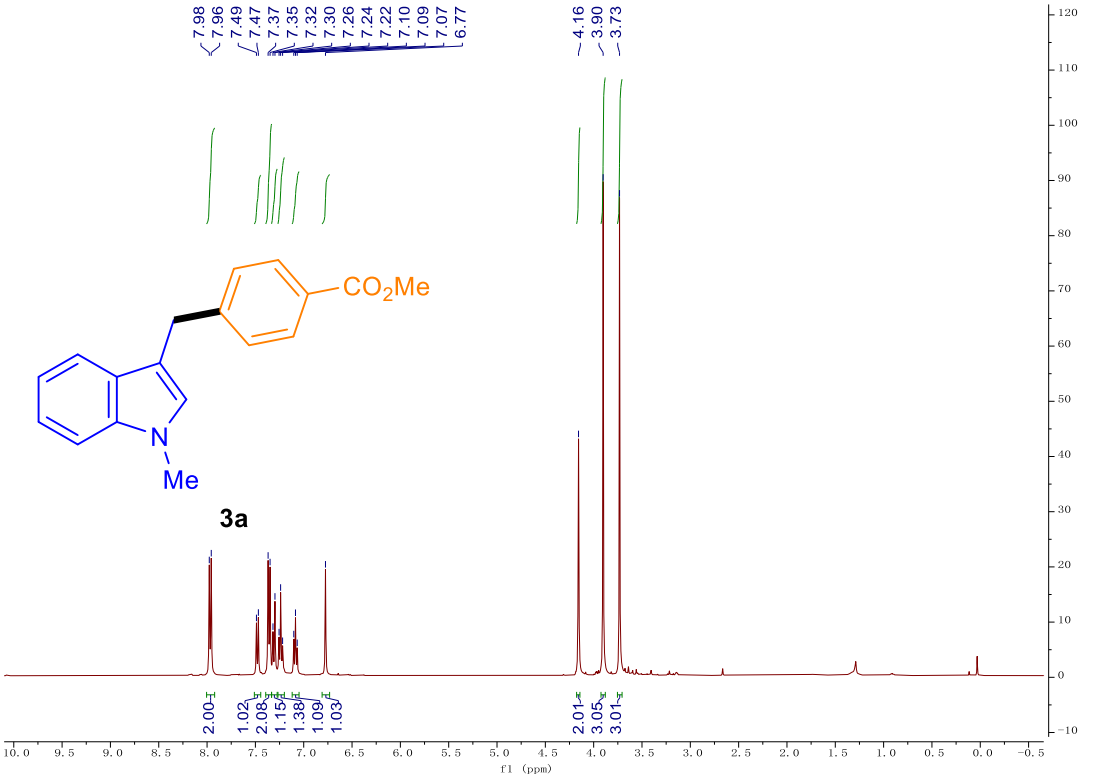
[1] N. T. Chandrika, M. Y. Fosso, Y. Alimova, A. May, O. A. Gonzalez, S. Garneau-Tsodikova, *Med. Chem. Comm*. **2019**, *10*, 926−933.

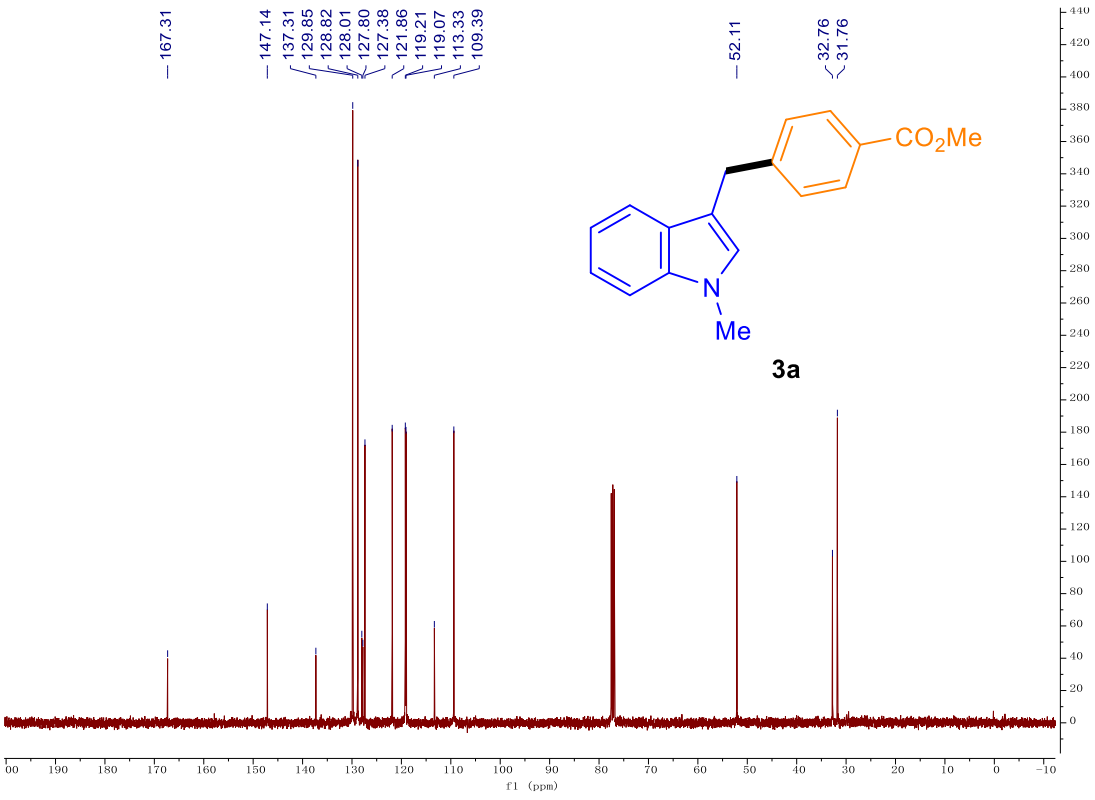
[2] S. Nomiyama, T. Hondo, T. Tsuchimoto, *Adv. Syn. Cat.* **2016**, *358*, 1136−1149.

[3] H. Hikawa, F. Kotaki, S. Kikkawa, I. Azumaya, *J. Org. Chem*. **2019**, *84*, 1972−1979.

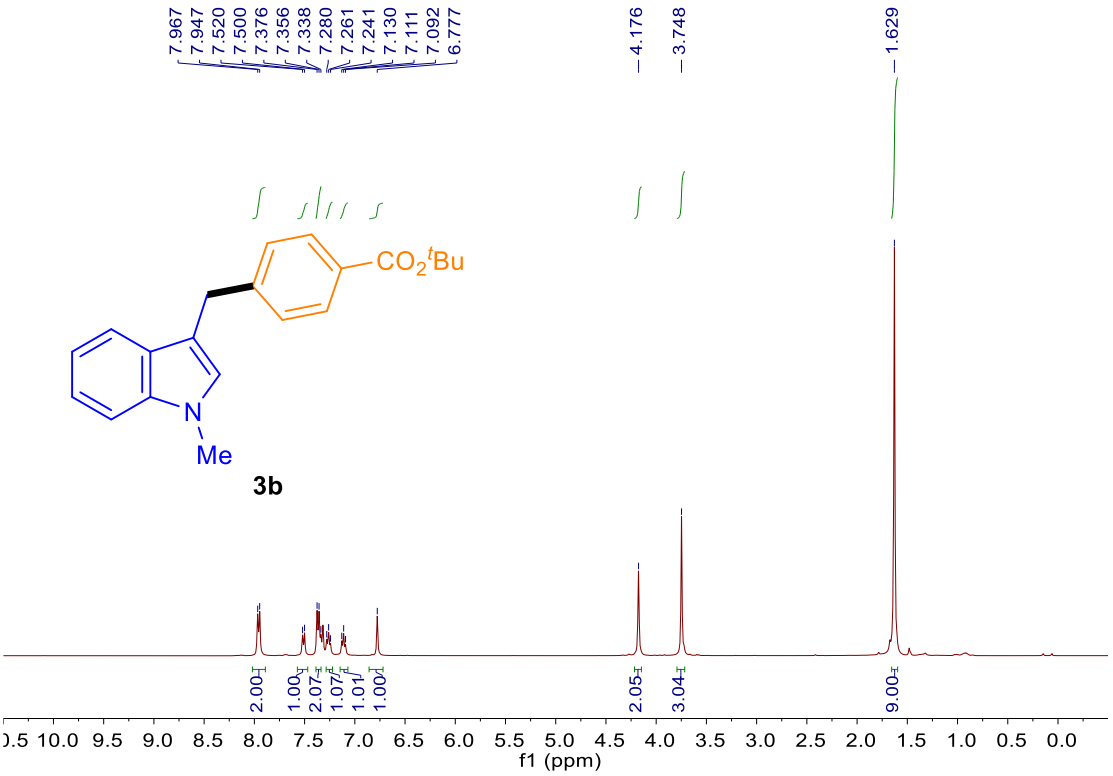
[4] C. C. Kofink, P. Knochel, *Org. Lett*. **2006**, *8*, 4121−4124.

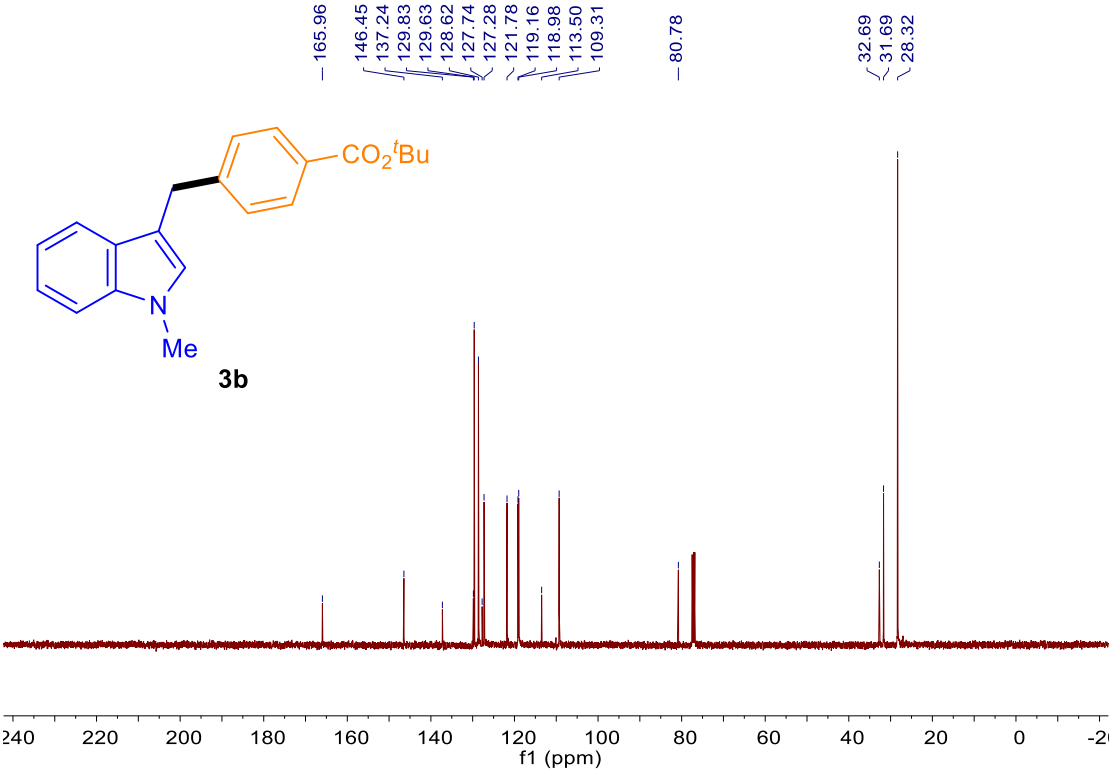
11. ^{1}H NMR, ^{13}C{^{1}H} NMR, ^{19}F NMR Spectra



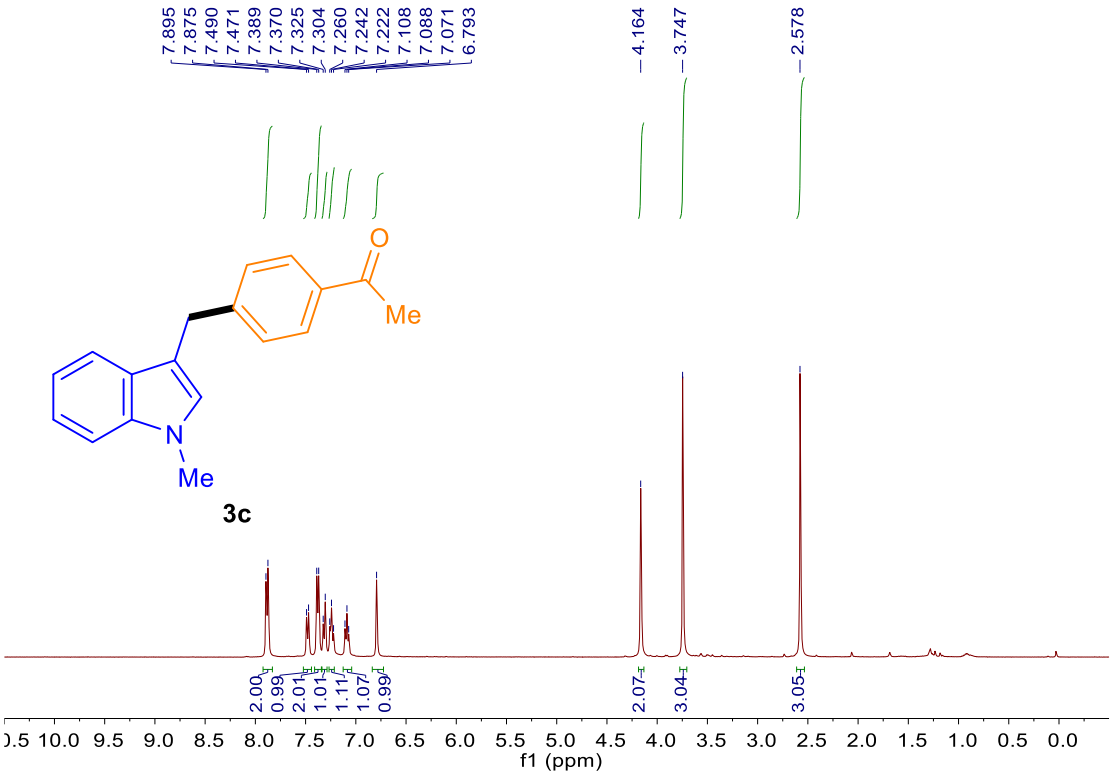


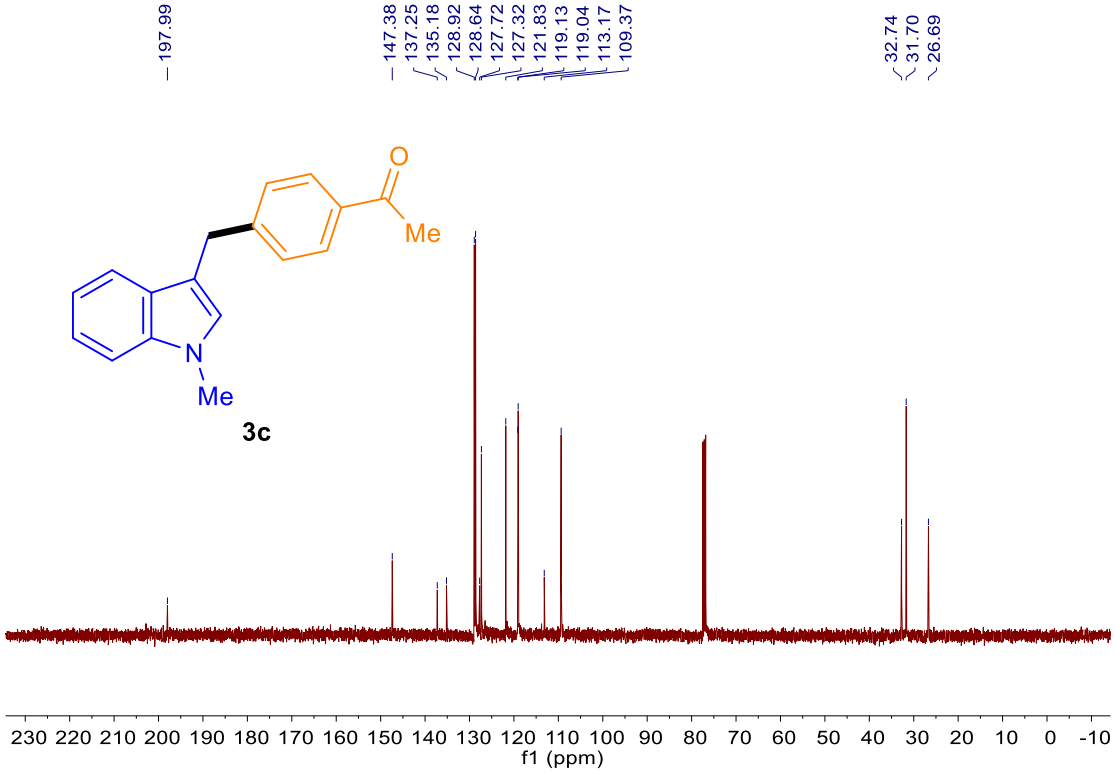
^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3a** ($CDCl_3$, rt).



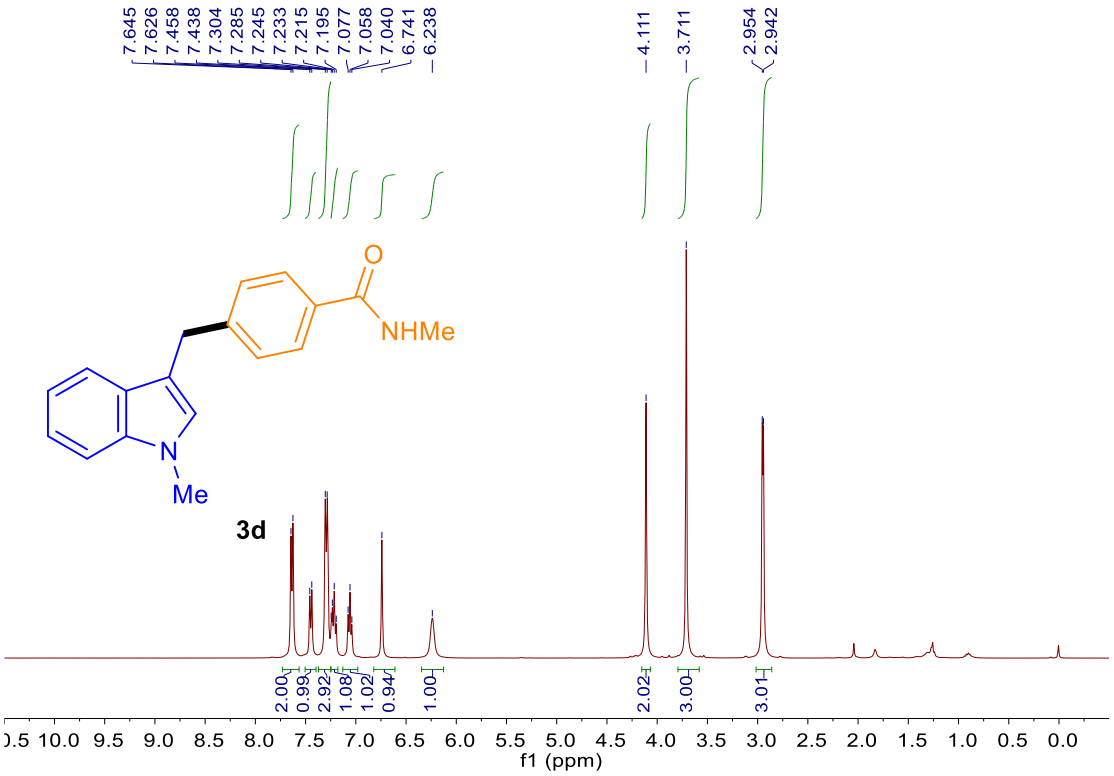


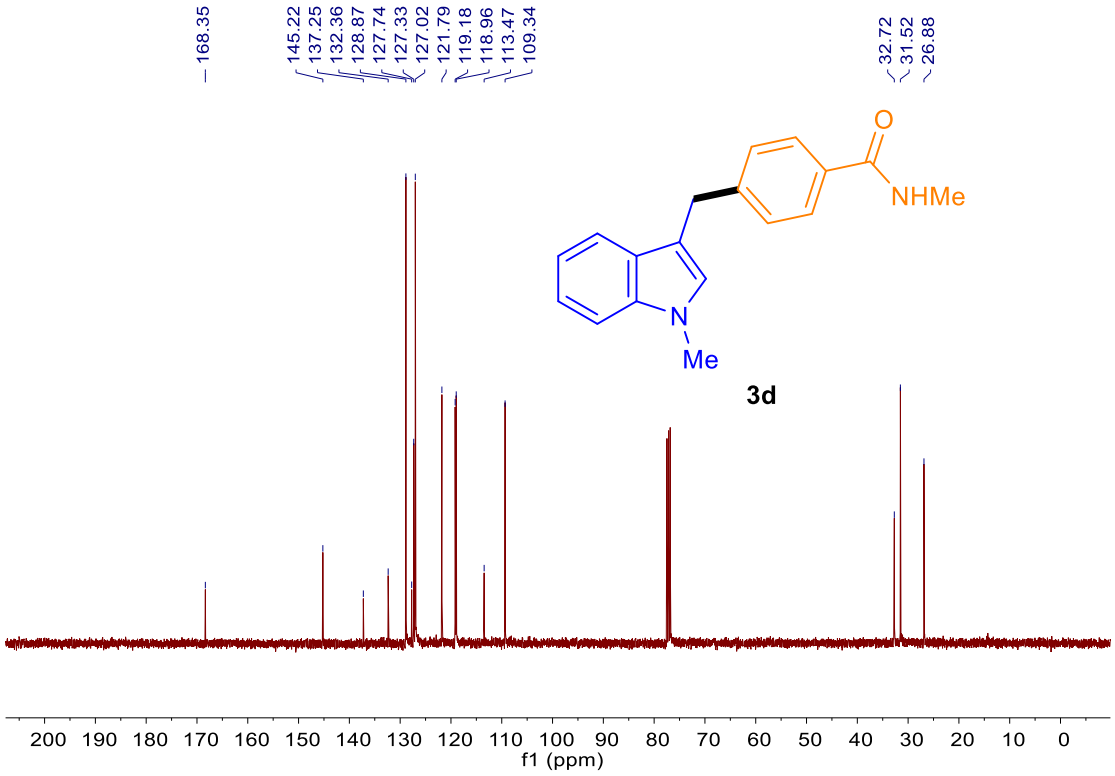
^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3b** ($CDCl_3$, rt).



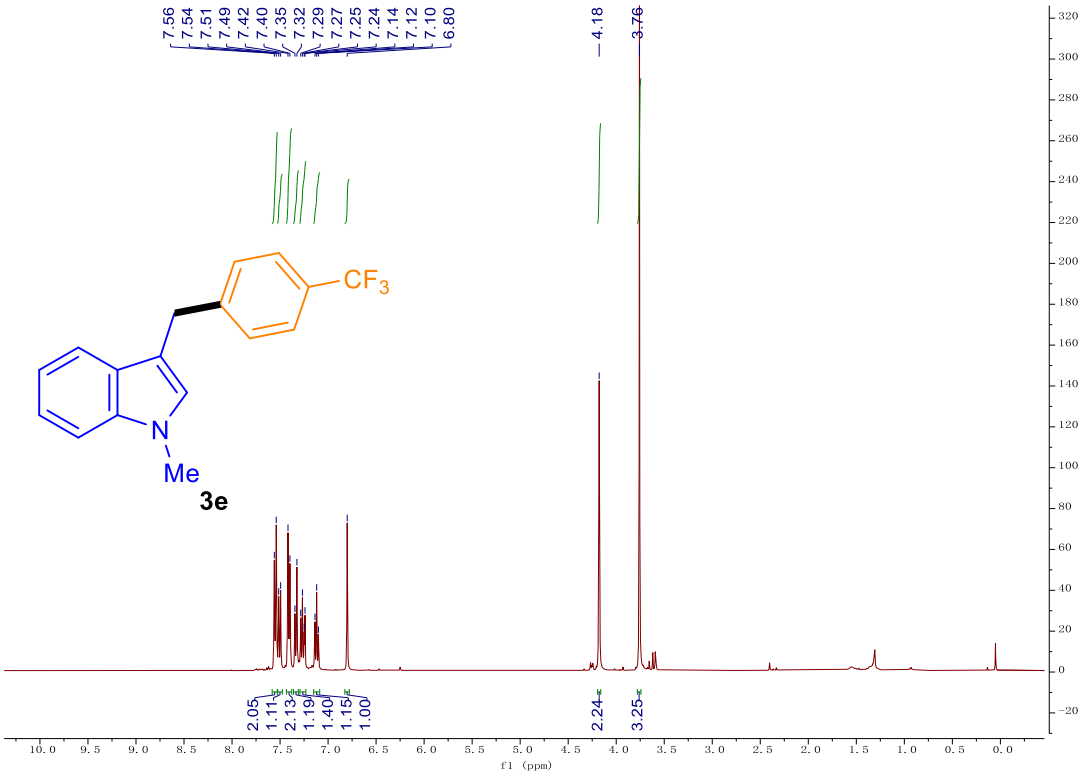


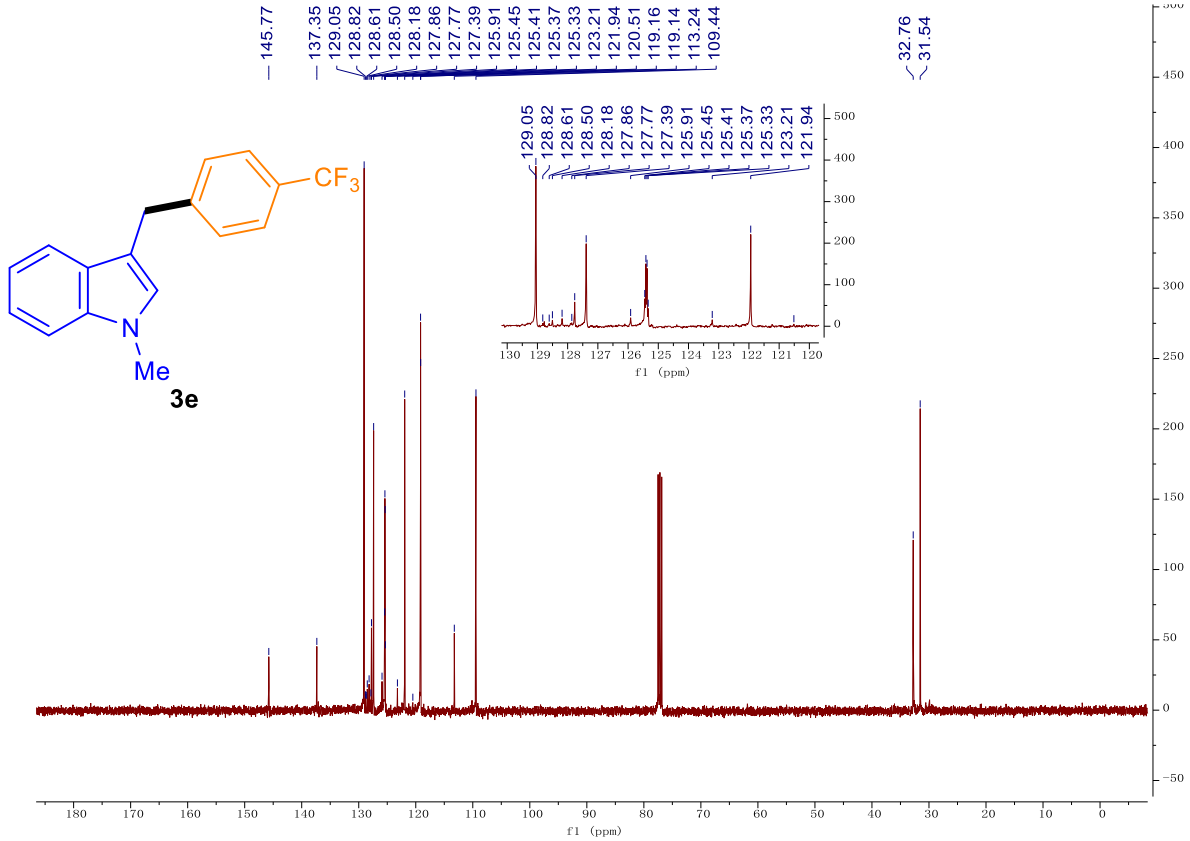
^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3c** ($CDCl_3$, rt).

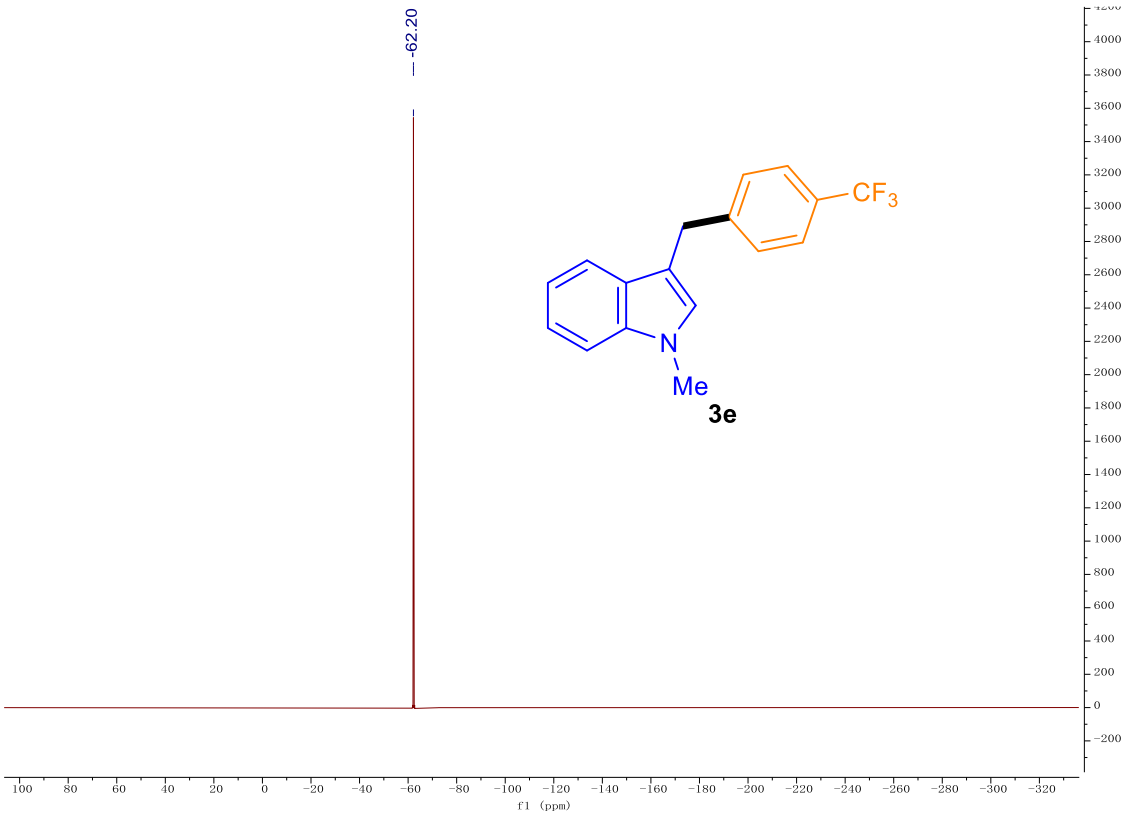




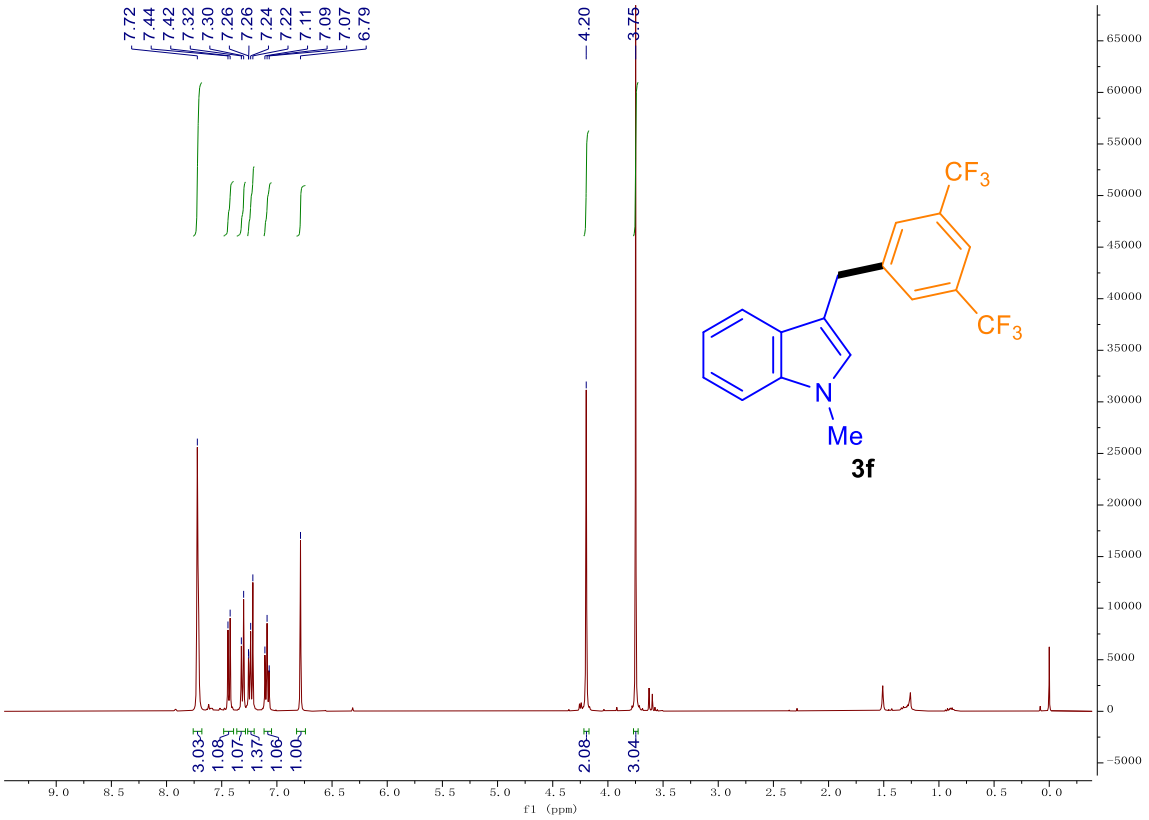
^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3d** ($CDCl_3$, rt).

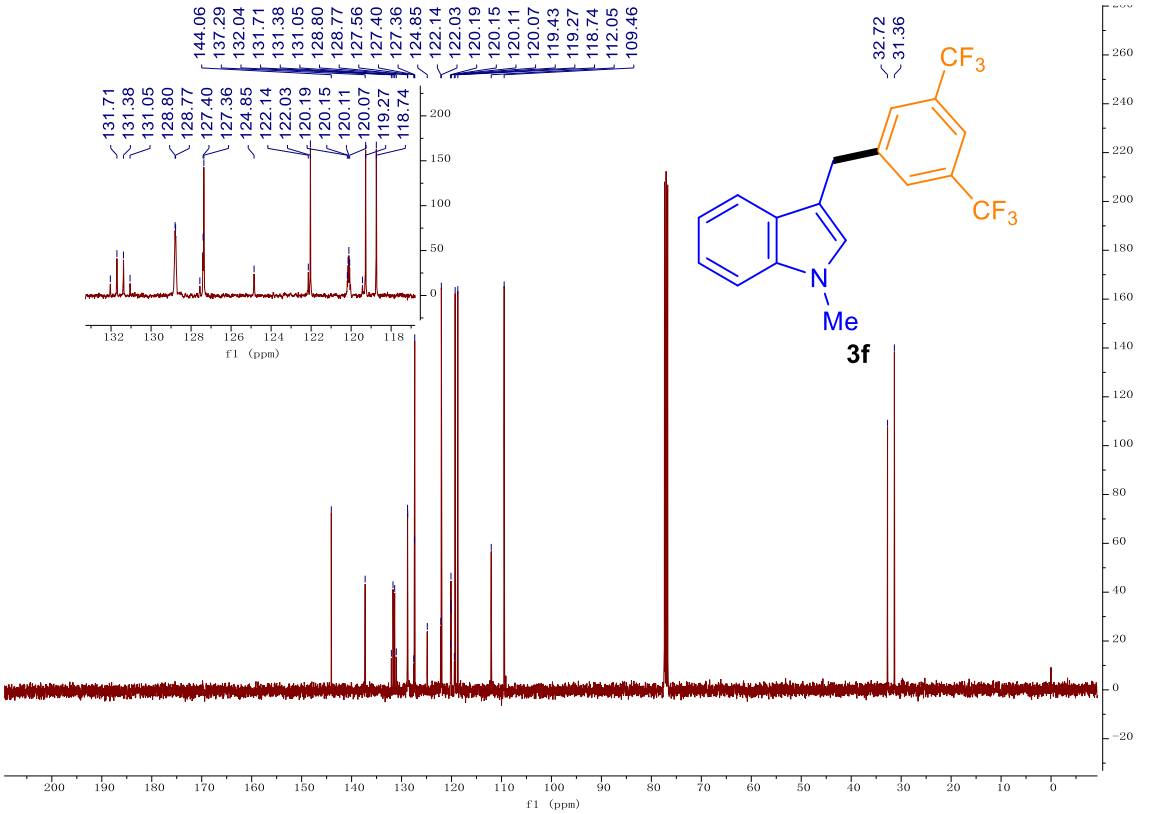

7.56
7.54
7.51
7.49
7.42
7.40
7.35
7.32
7.29
7.27
7.25
7.24
7.14
7.12
7.10
6.80
4.18
3.76
CF3
N
Me
3e
2.05
1.11
2.13
1.19
1.40
1.15
1.00
2.24
3.25
f1 (ppm)

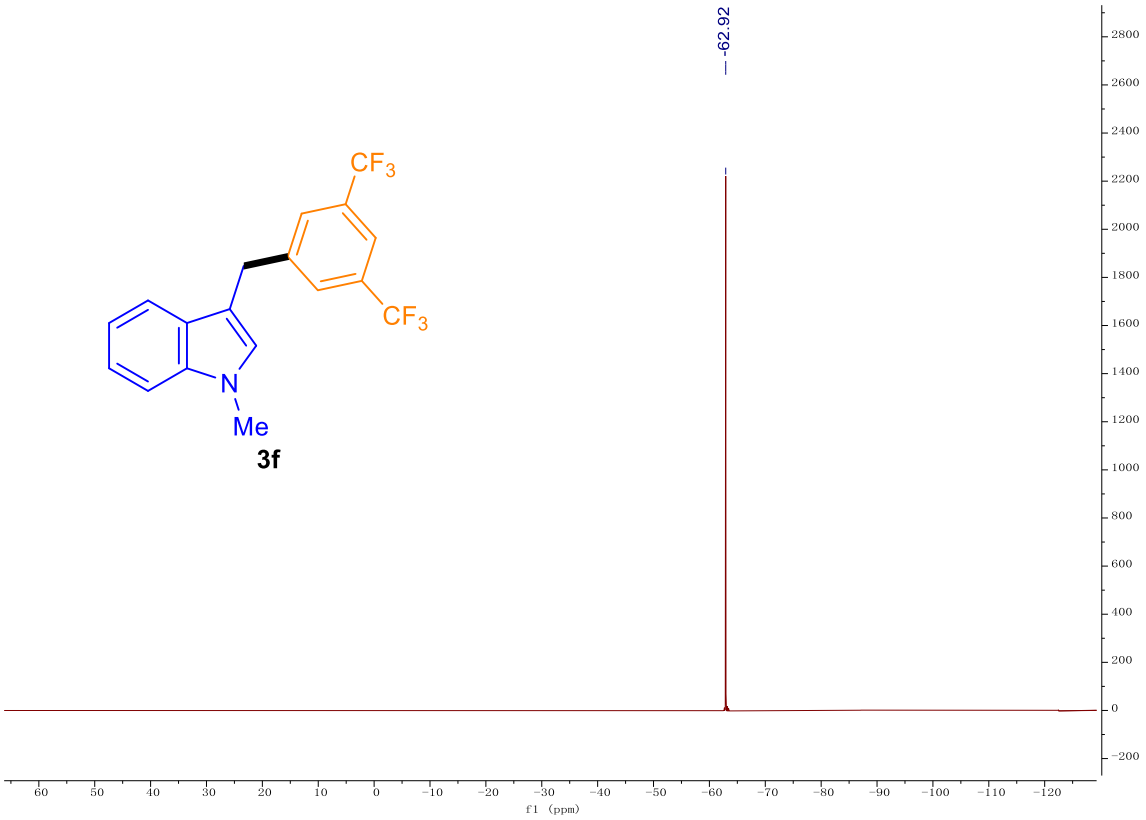

145.77
137.35
129.05
128.82
128.61
128.50
128.18
127.86
127.77
127.39
125.91
125.45
125.41
125.37
125.33
123.21
121.94
120.51
119.16
119.14
113.24
109.44
32.76
31.54
CF3
N
Me
3e
f1 (ppm)



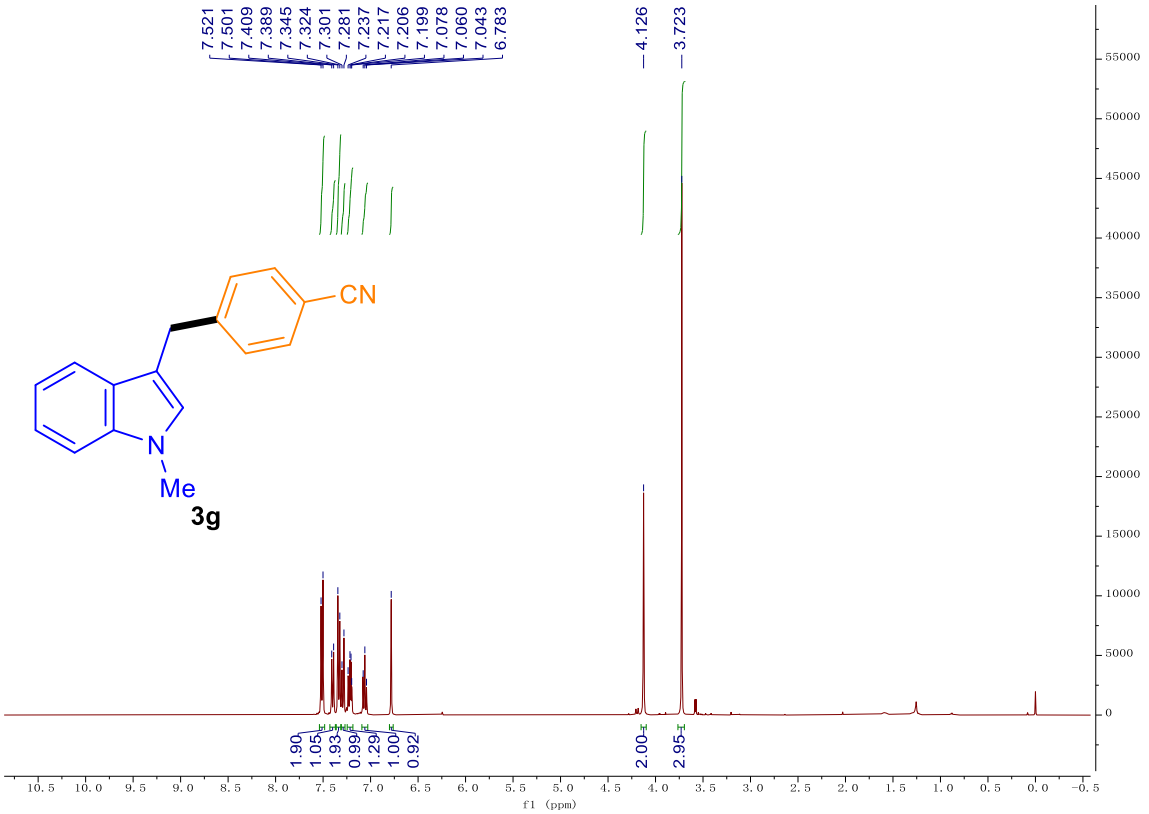
^{1}H NMR (400 MHz), ^{13}C{^{1}H} NMR (100 MHz) and ^{19}F NMR (376 MHz) spectra of **3e** ($CDCl_3$, rt).

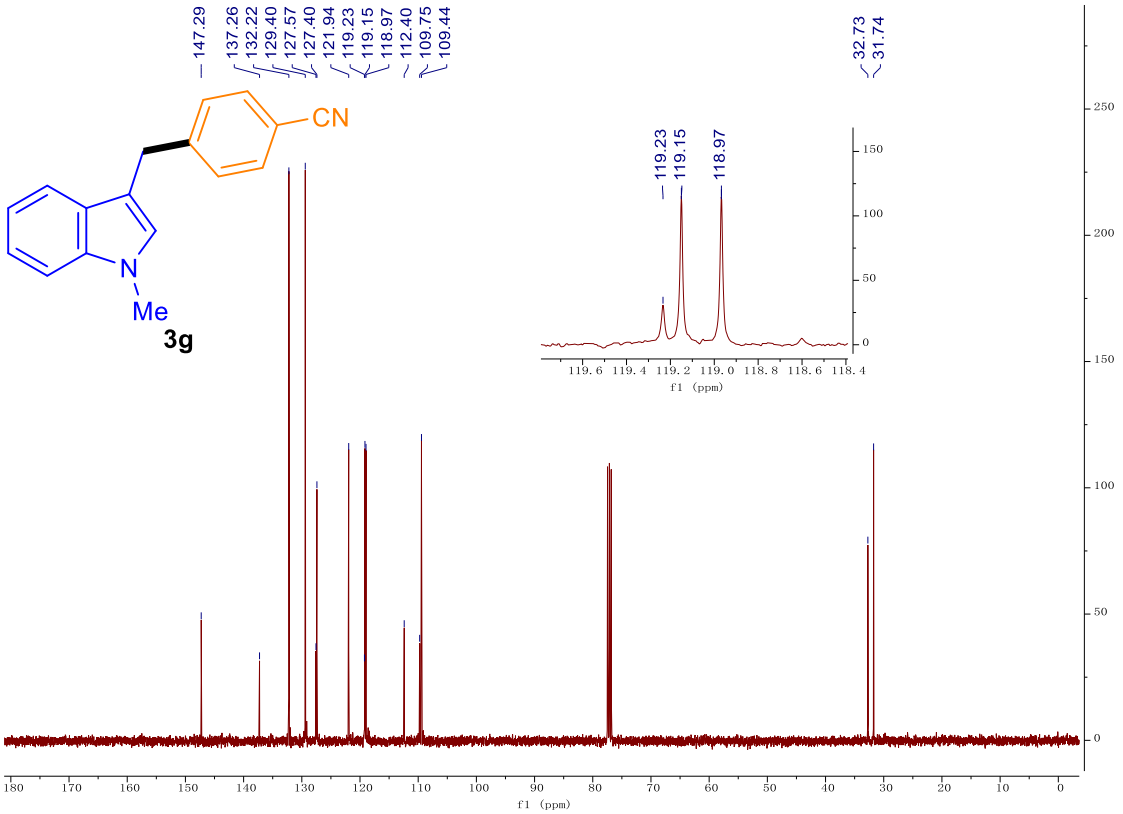

7.72
7.44
7.42
7.32
7.30
7.26
7.26
7.24
7.22
7.11
7.09
7.07
6.79
4.20
3.75
3.03
1.08
1.07
1.37
1.06
1.00
2.08
3.04
CF3
CF3
N
Me
3f
f1 (ppm)


144.06
137.29
132.04
131.71
131.38
131.05
128.80
128.77
127.56
127.40
127.36
124.85
122.14
122.03
120.19
120.15
120.11
120.07
119.43
119.27
118.74
112.05
109.46
32.72
31.36
CF3
CF3
N
Me
3f
f1 (ppm)

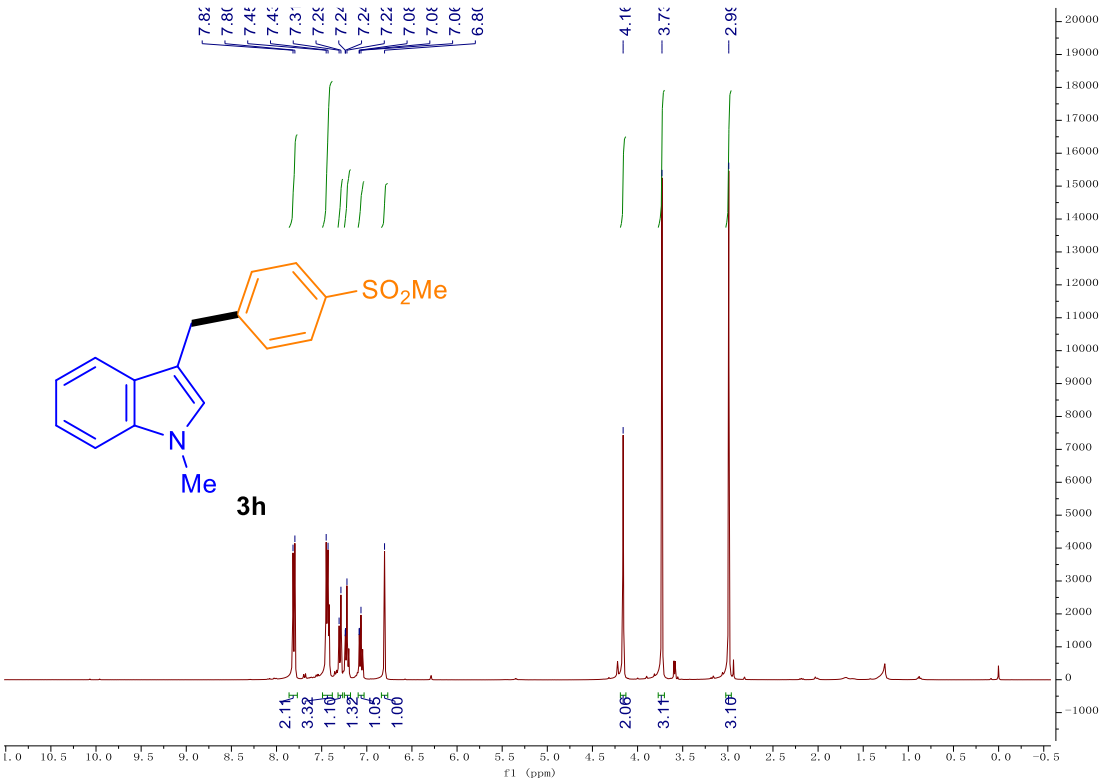


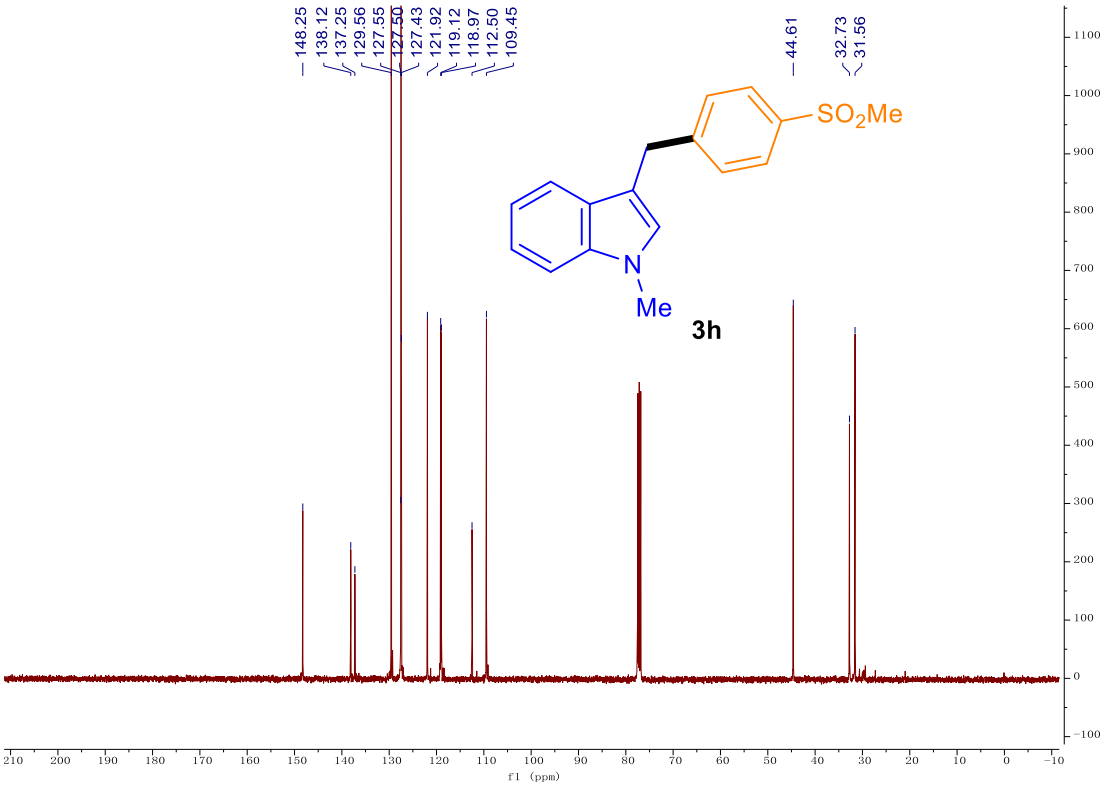
^{1}H NMR (400 MHz), ^{13}C{^{1}H} NMR (100 MHz) and ^{19}F NMR (376 MHz) spectra of **3f** ($CDCl_3$, rt).



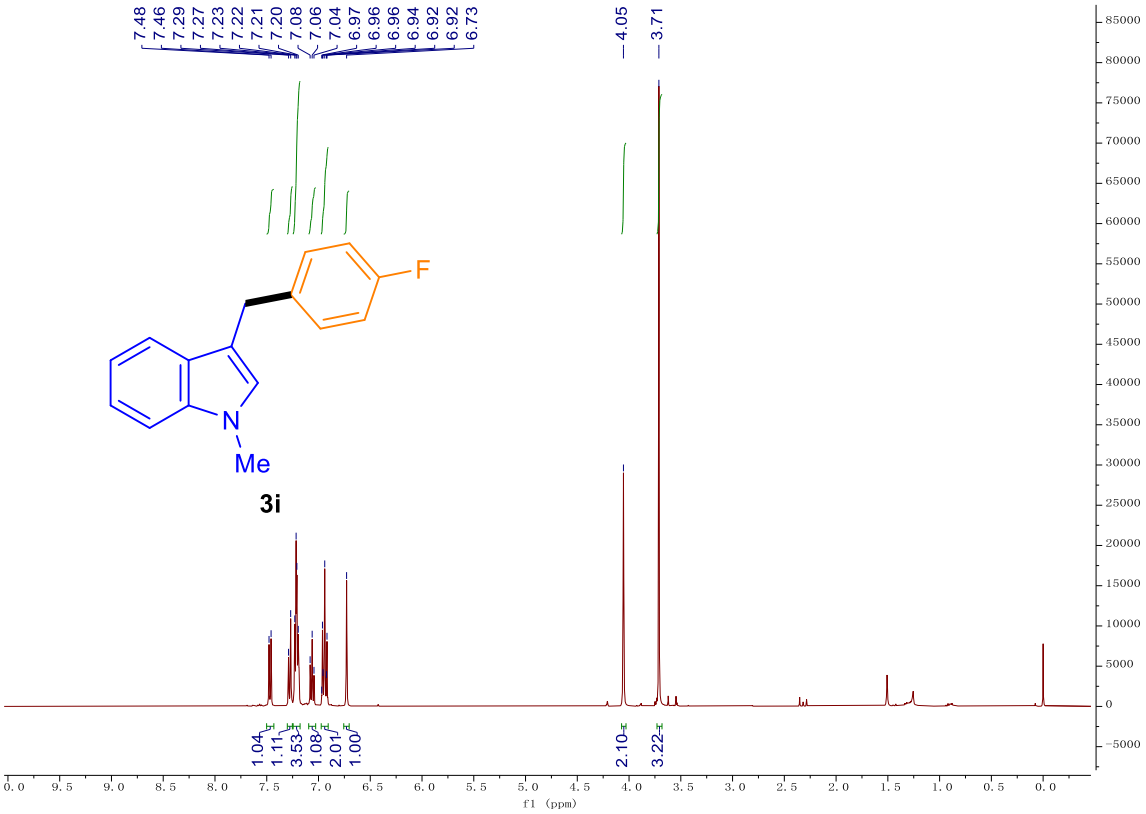


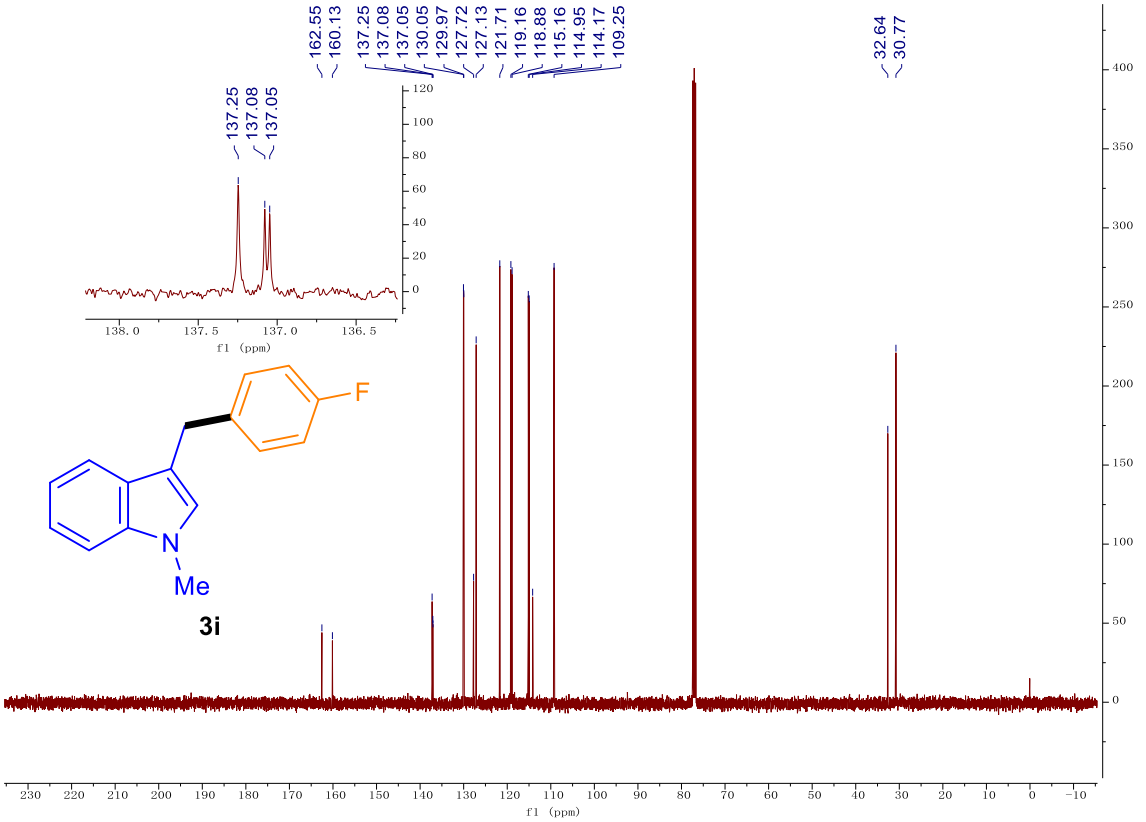
^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3g** ($CDCl_3$, rt).

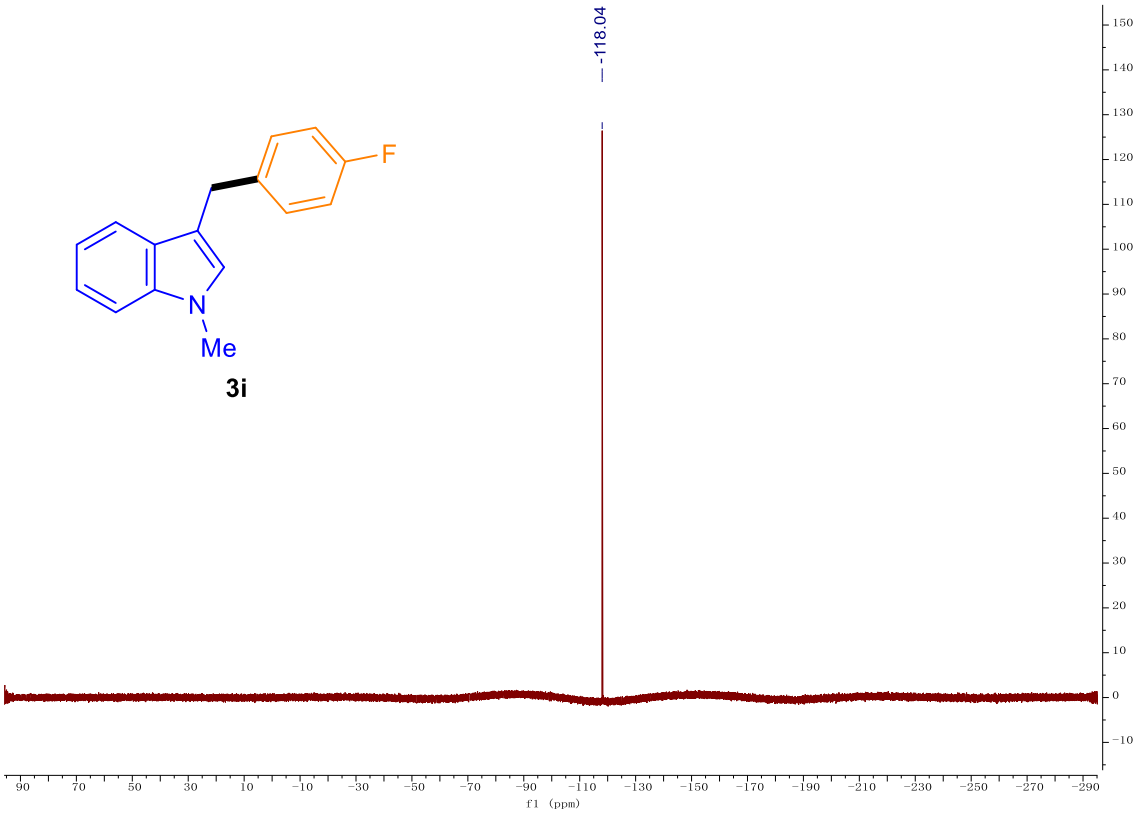




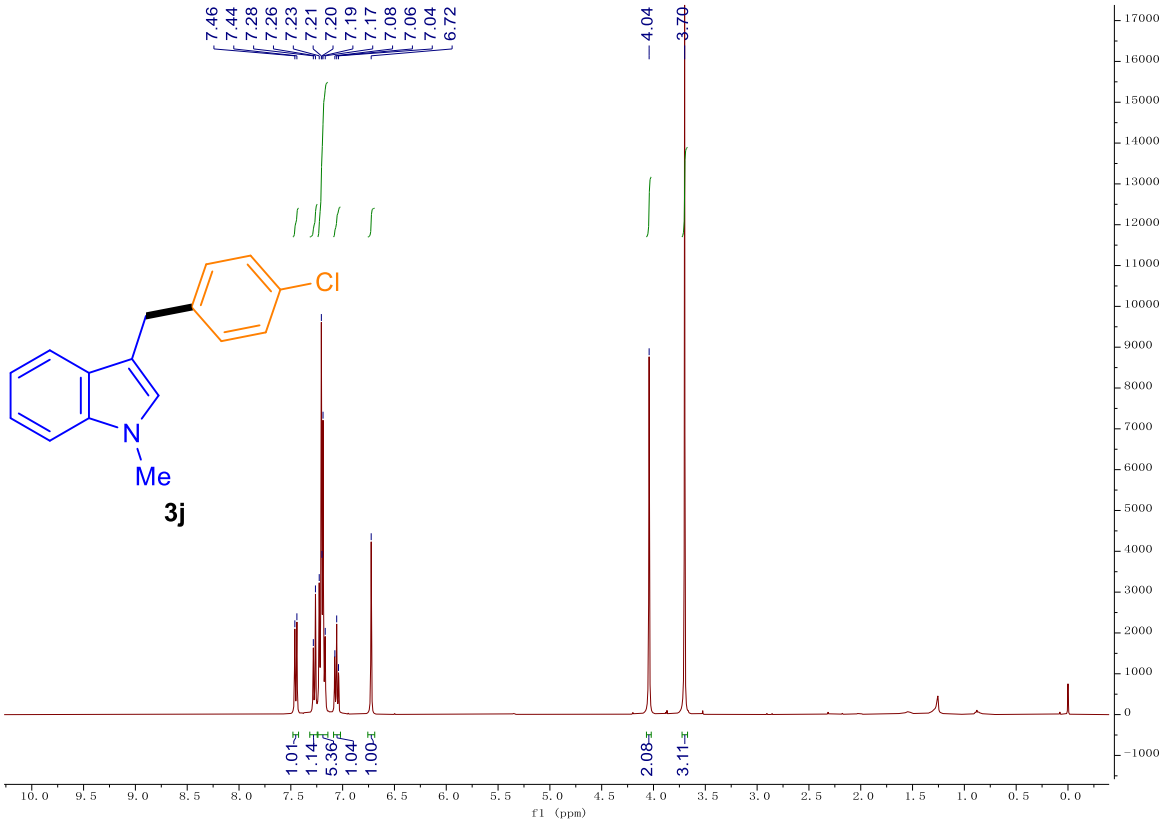
^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3h** ($CDCl_3$, rt).

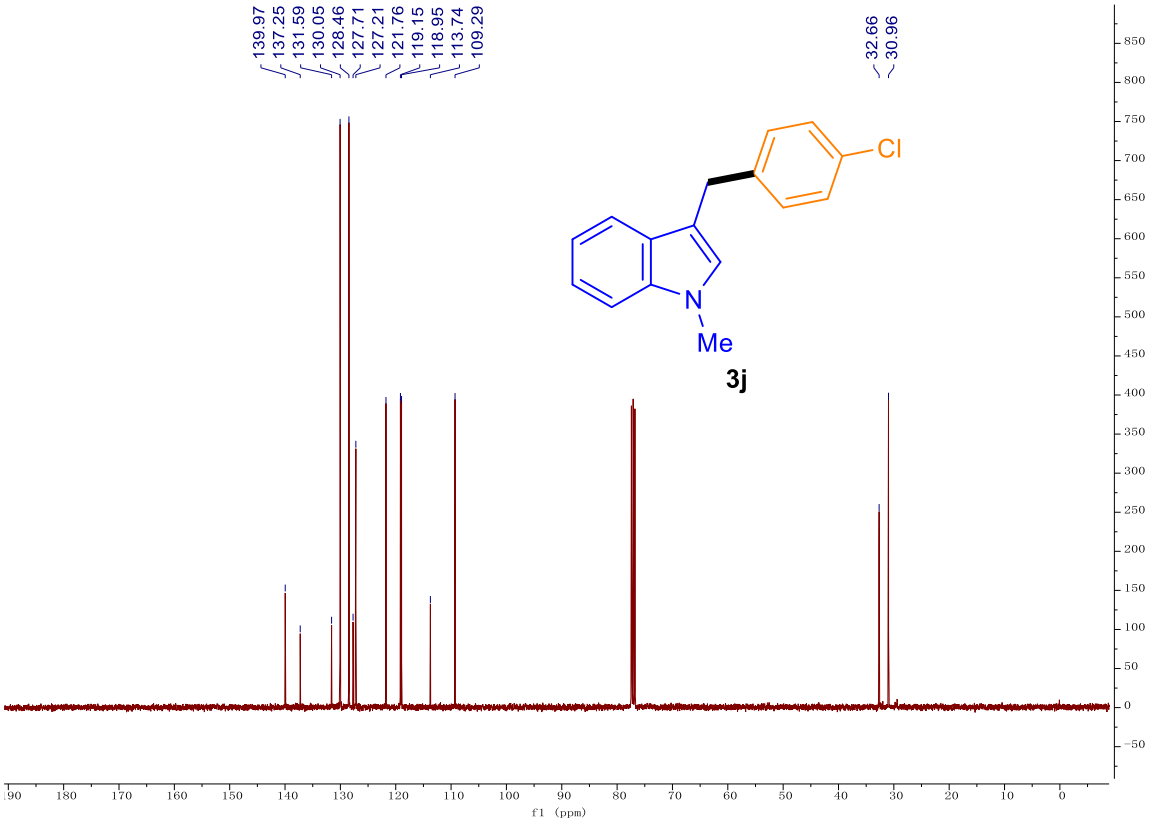

7.48
7.46
7.29
7.27
7.23
7.22
7.21
7.20
7.08
7.06
7.04
6.97
6.96
6.96
6.94
6.92
6.92
6.73
4.05
3.71
F
N
Me
3i
1.04
1.11
3.53
1.08
2.01
1.00
2.10
3.22
f1 (ppm)


162.55
160.13
137.25
137.08
137.05
130.05
129.97
127.72
127.13
121.71
119.16
118.88
115.16
114.95
114.17
109.25
32.64
30.77
137.25
137.08
137.05
f1 (ppm)
F
N
Me
3i
f1 (ppm)

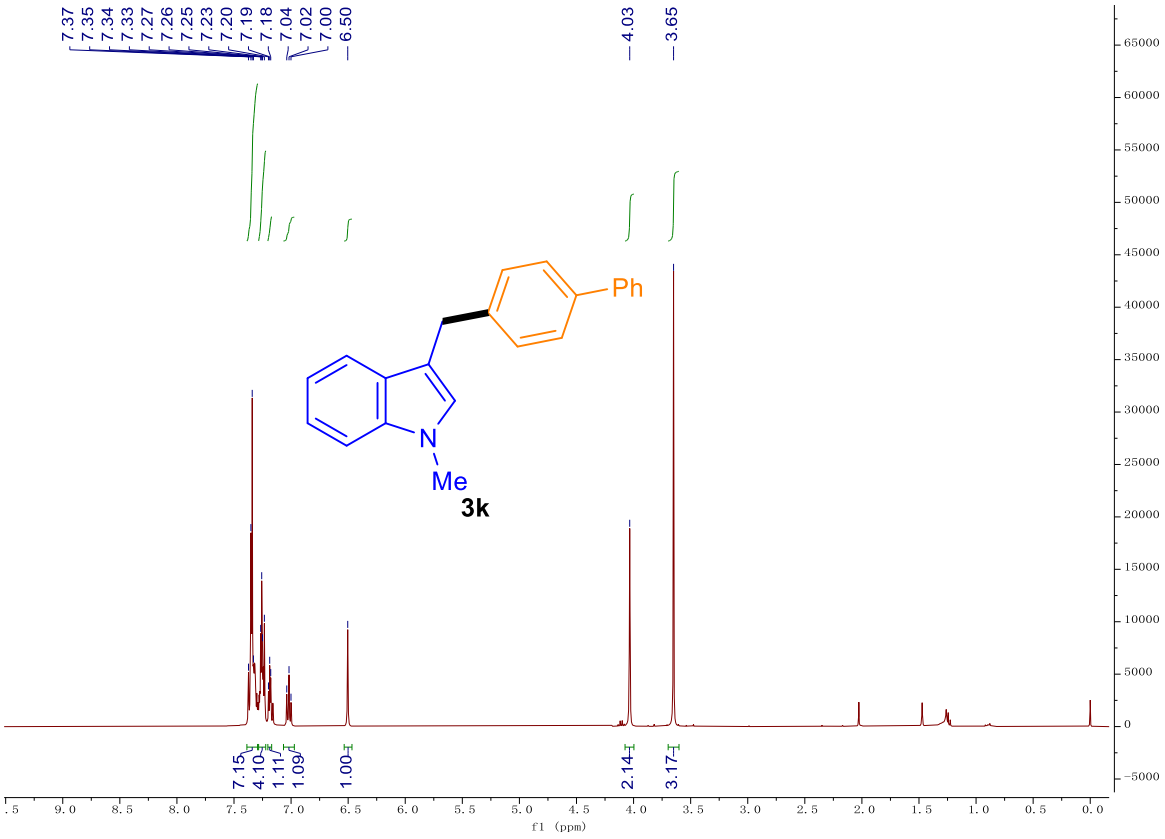


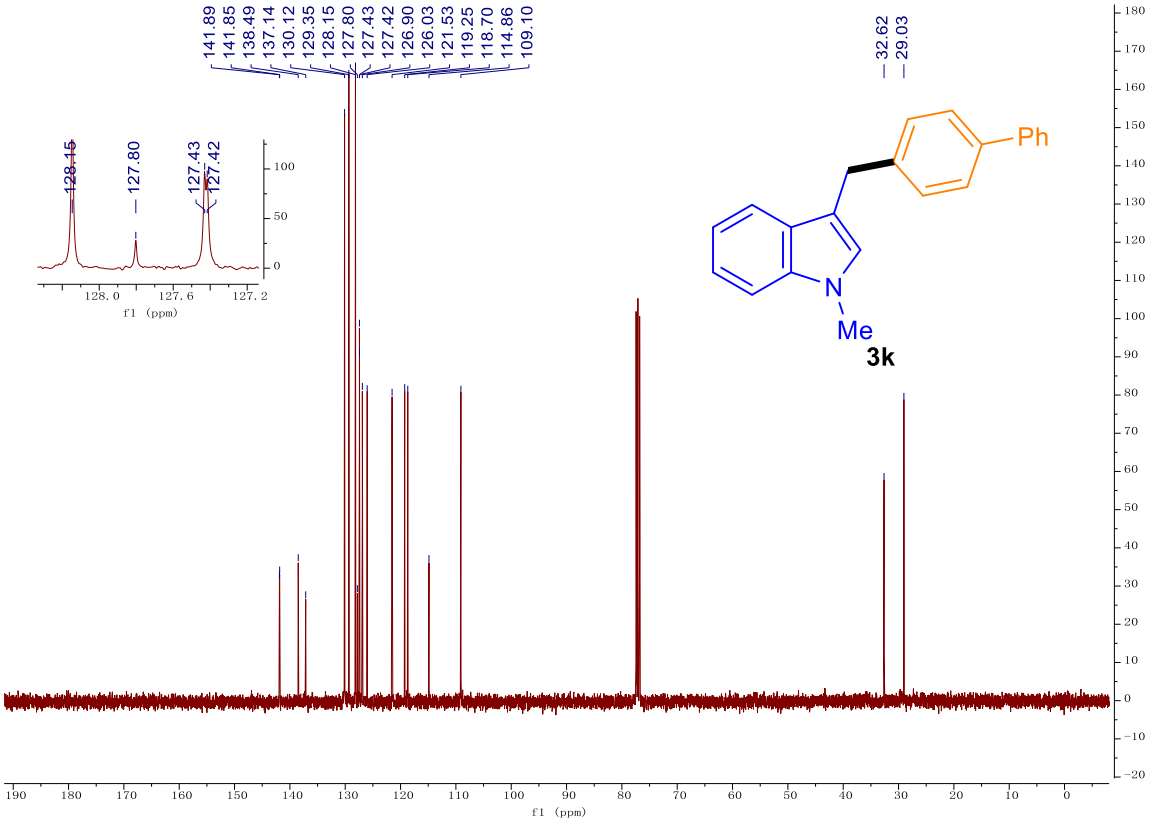
^{1}H NMR (400 MHz), ^{13}C{^{1}H} NMR (100 MHz) and ^{19}F NMR (376 MHz) spectra of **3i** ($CDCl_3$, rt).



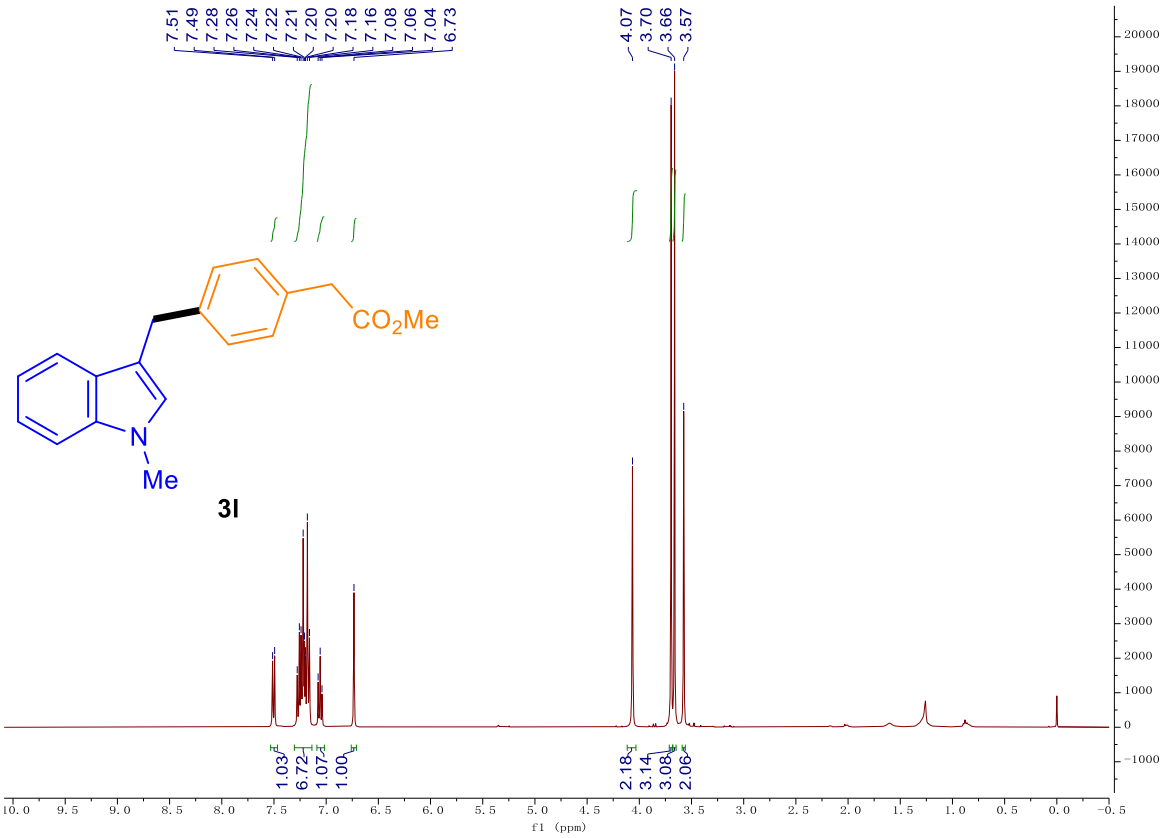


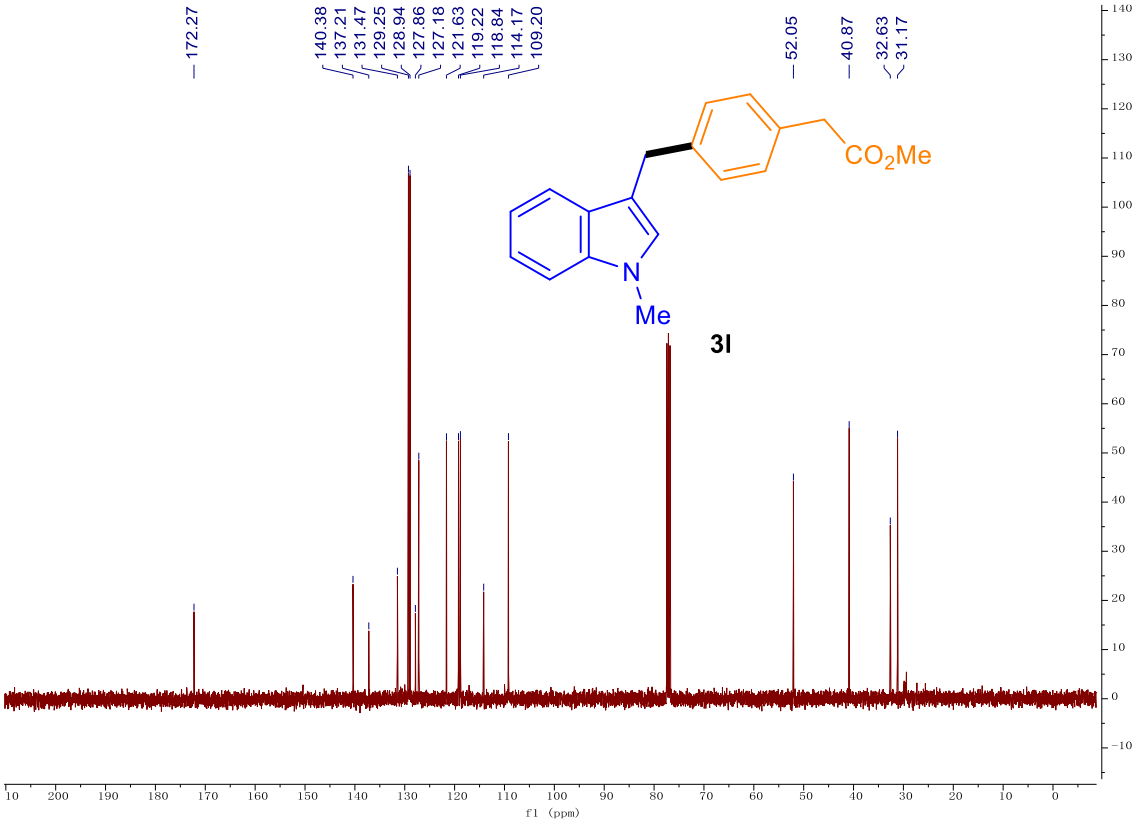
^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3j** ($CDCl_3$, rt).



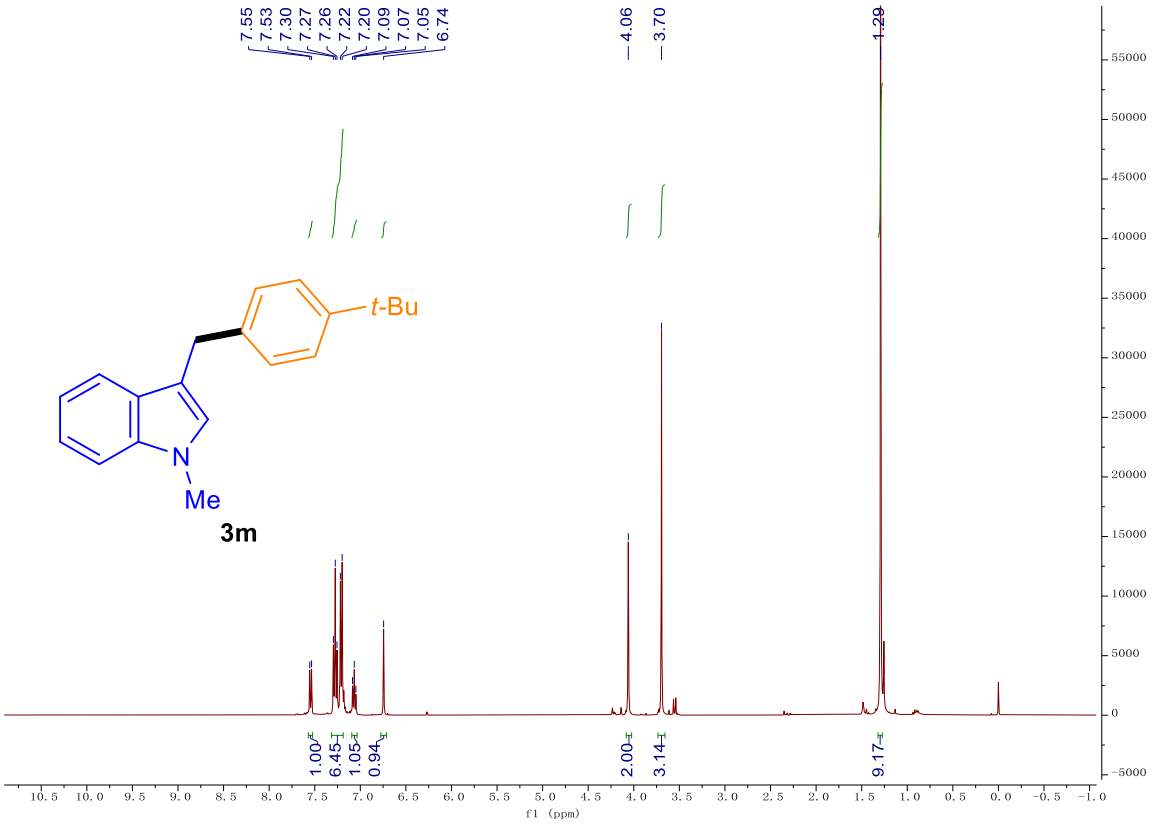


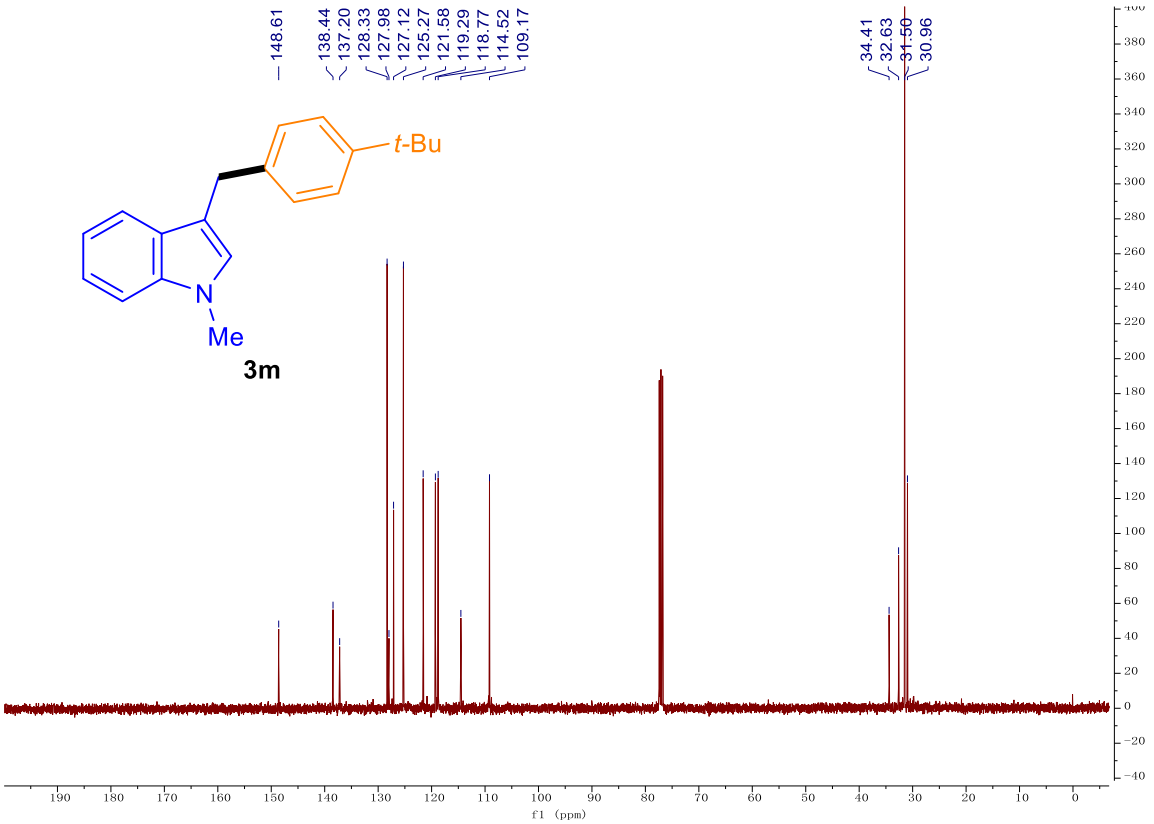
^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3k** ($CDCl_3$, rt).



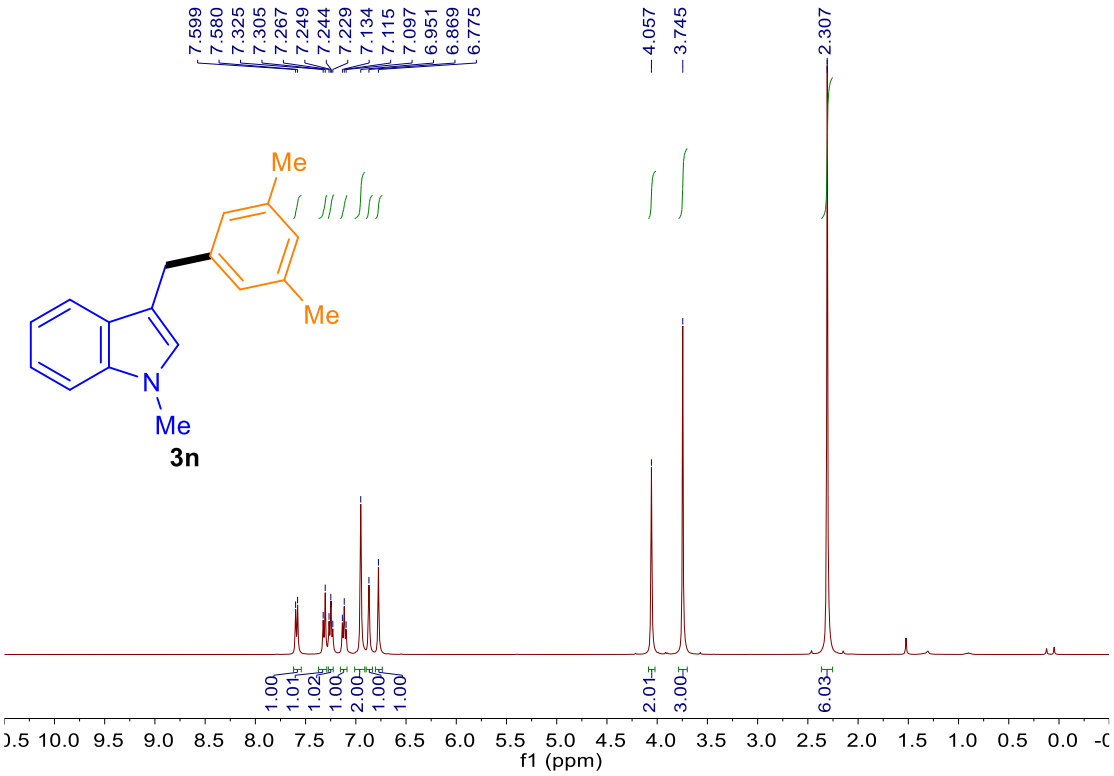


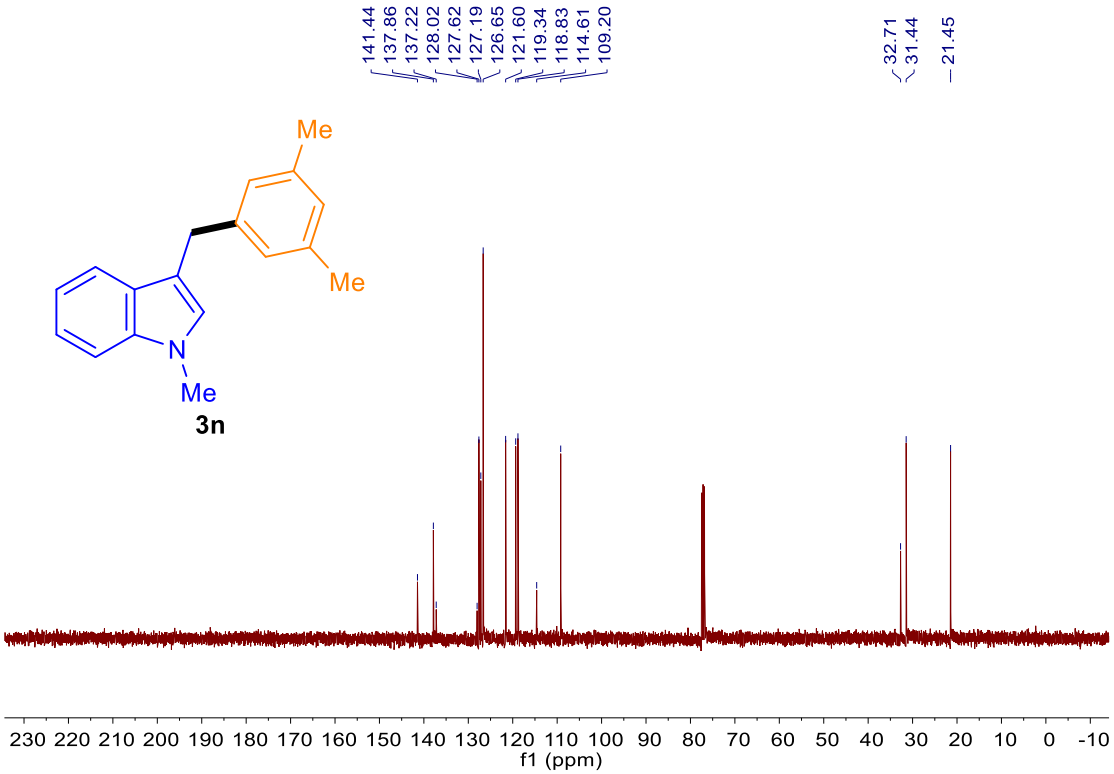
^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3l** ($CDCl_3$, rt).



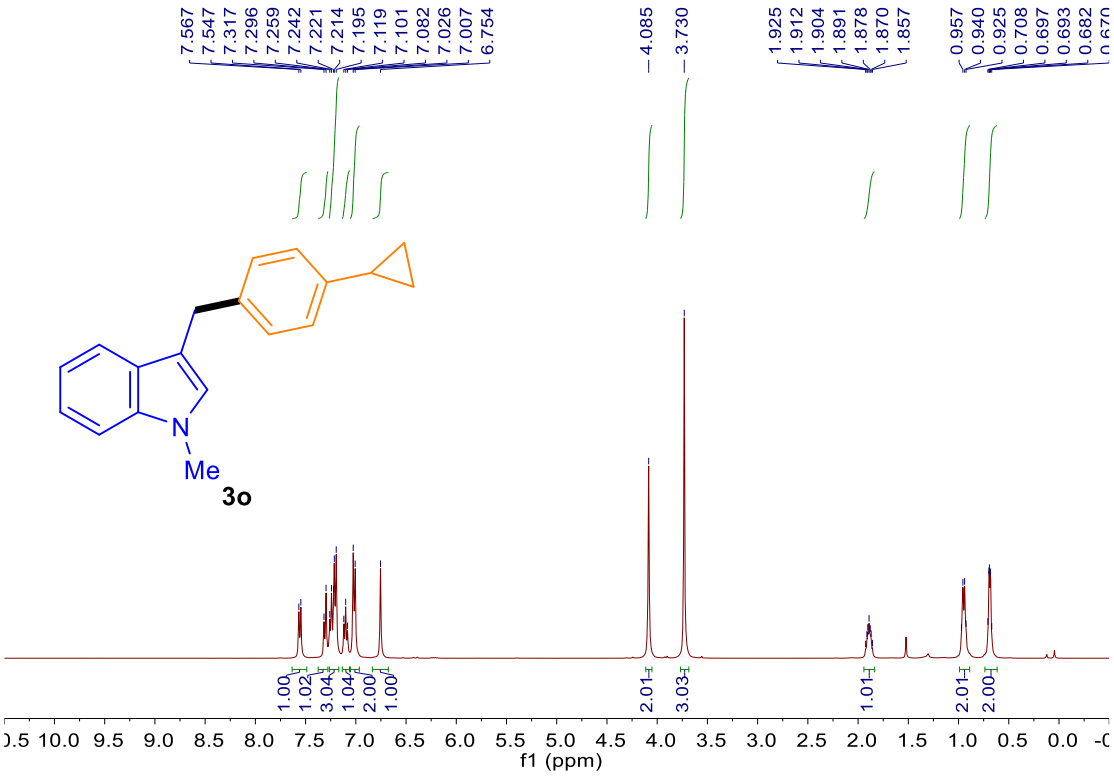


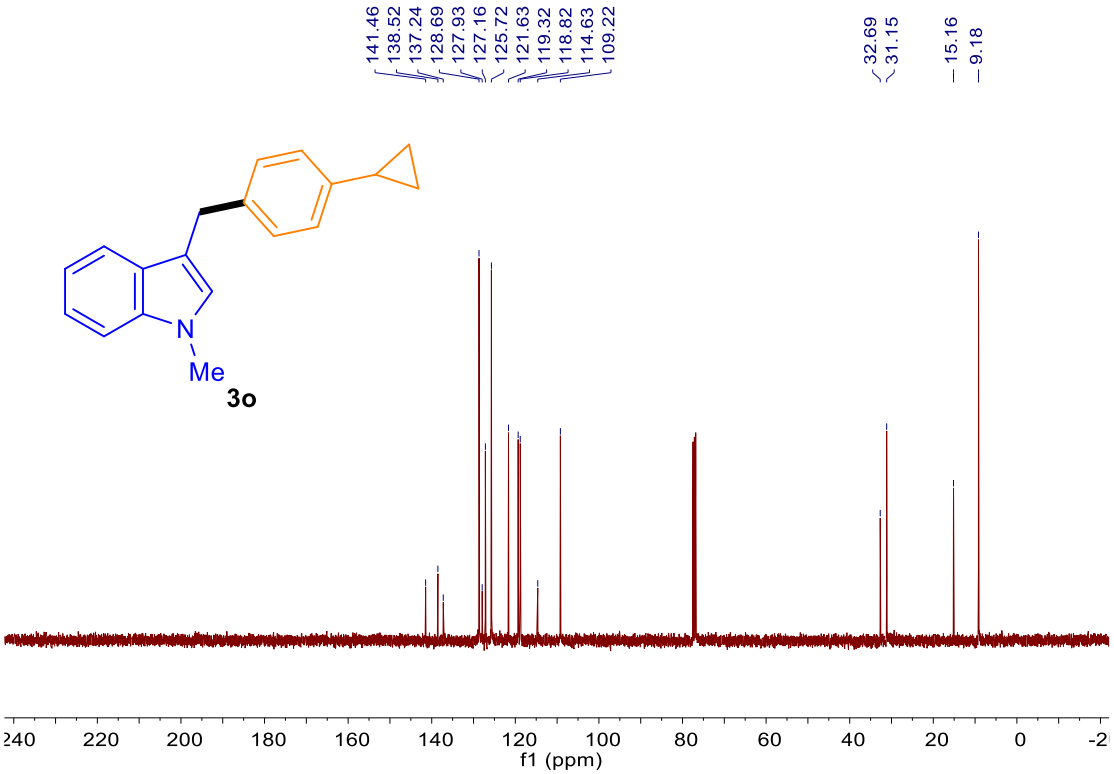
^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3m** ($CDCl_3$, rt).



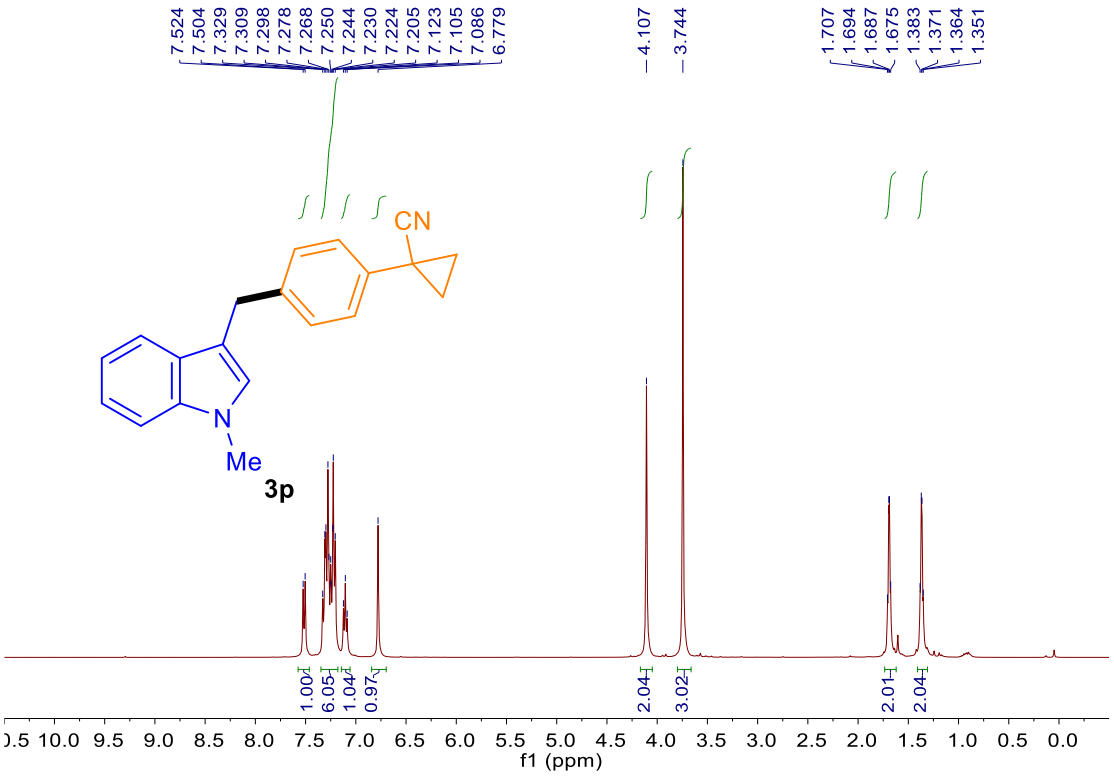


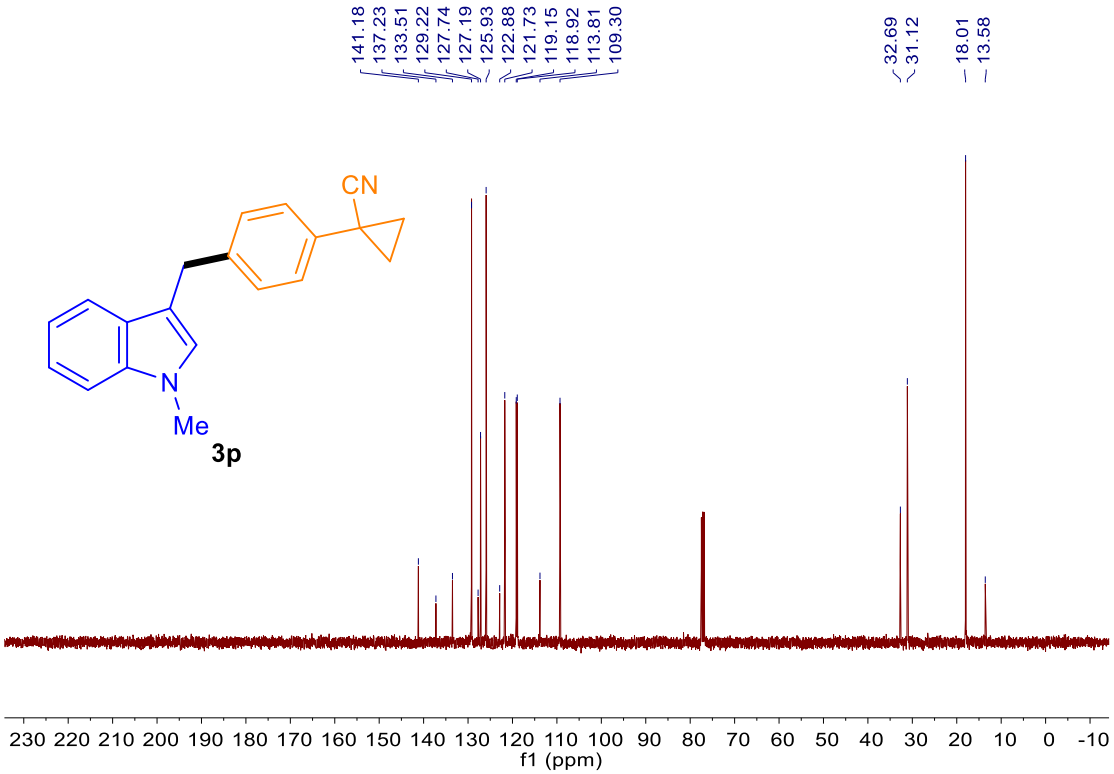
^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3n** ($CDCl_3$, rt).



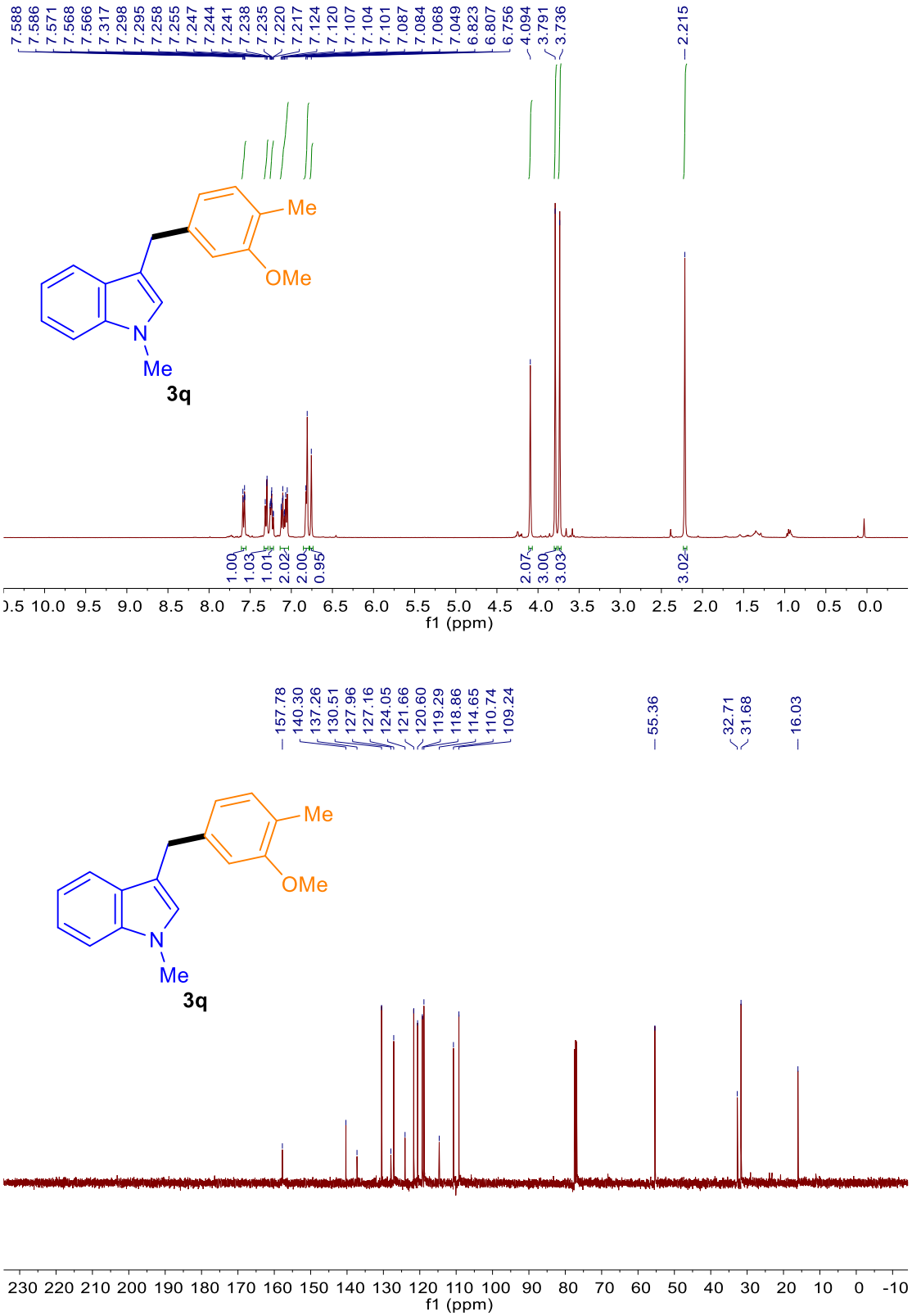


^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3o** ($CDCl_3$, rt).

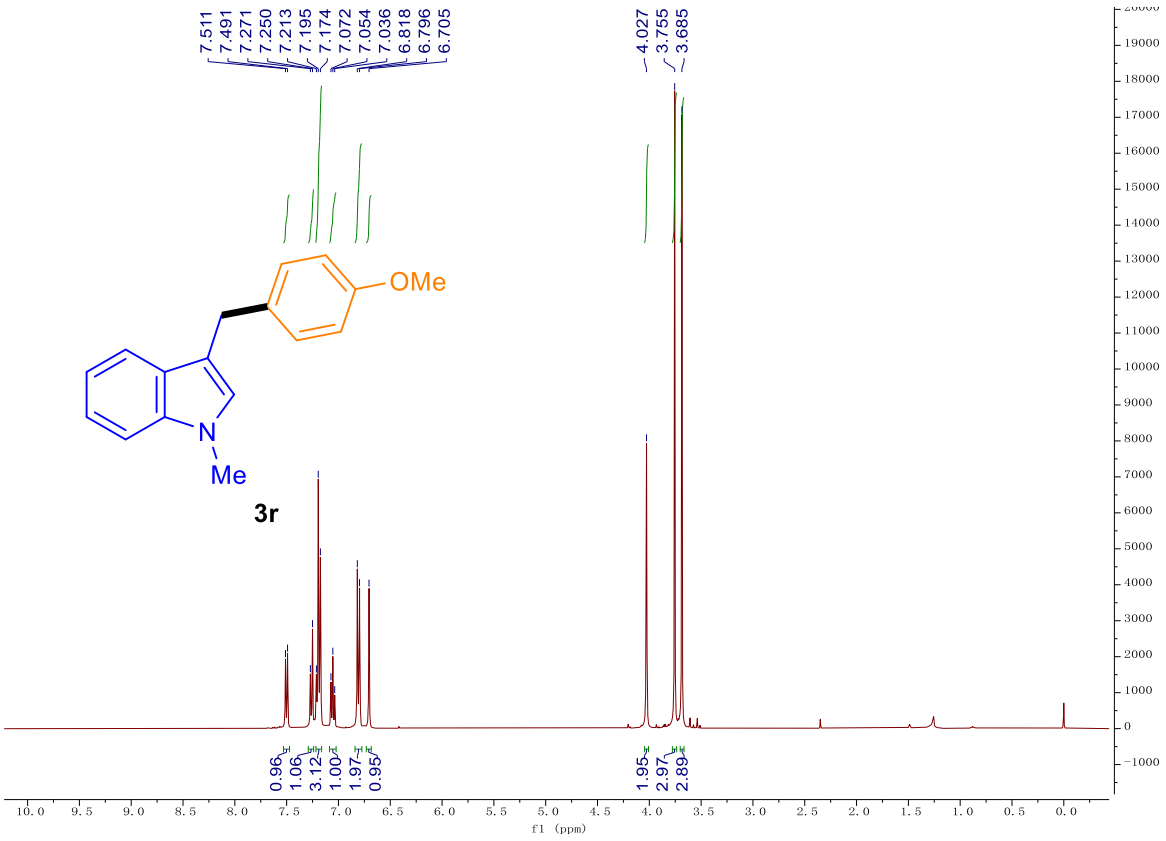


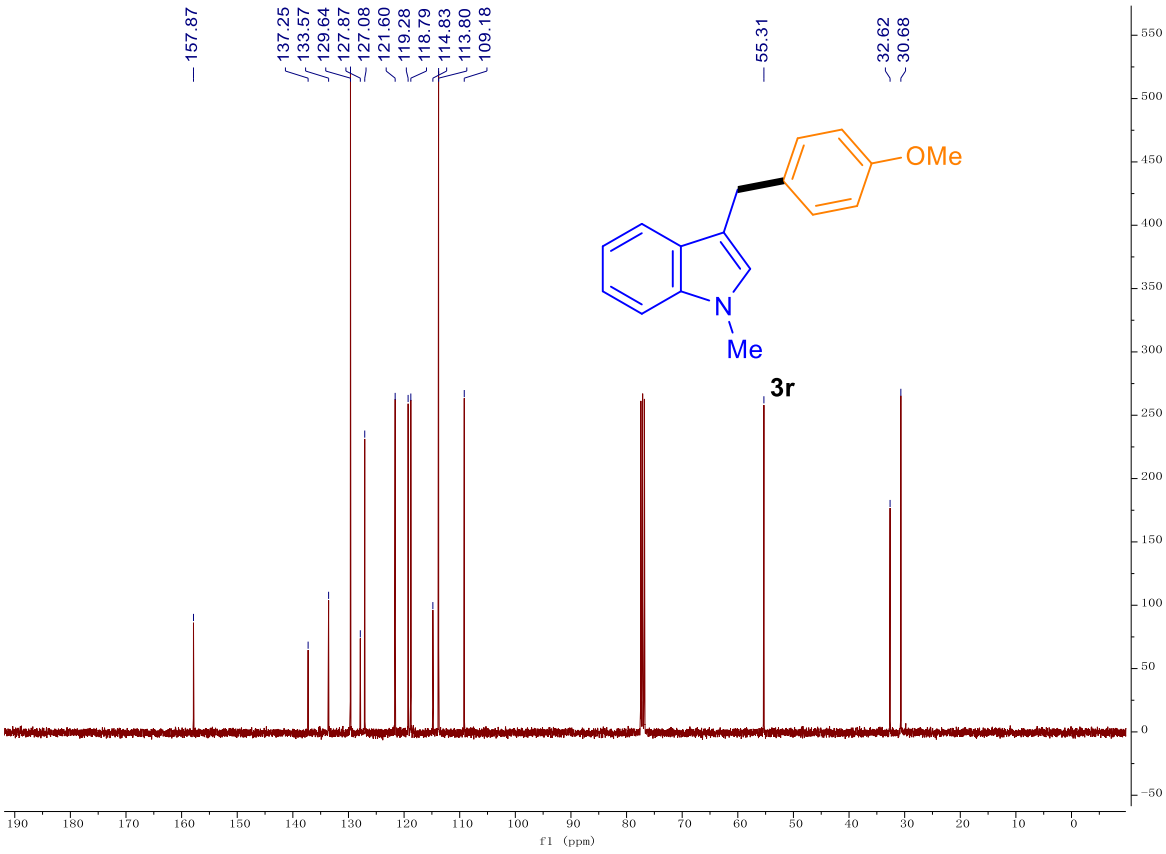


^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3p** ($CDCl_3$, rt).

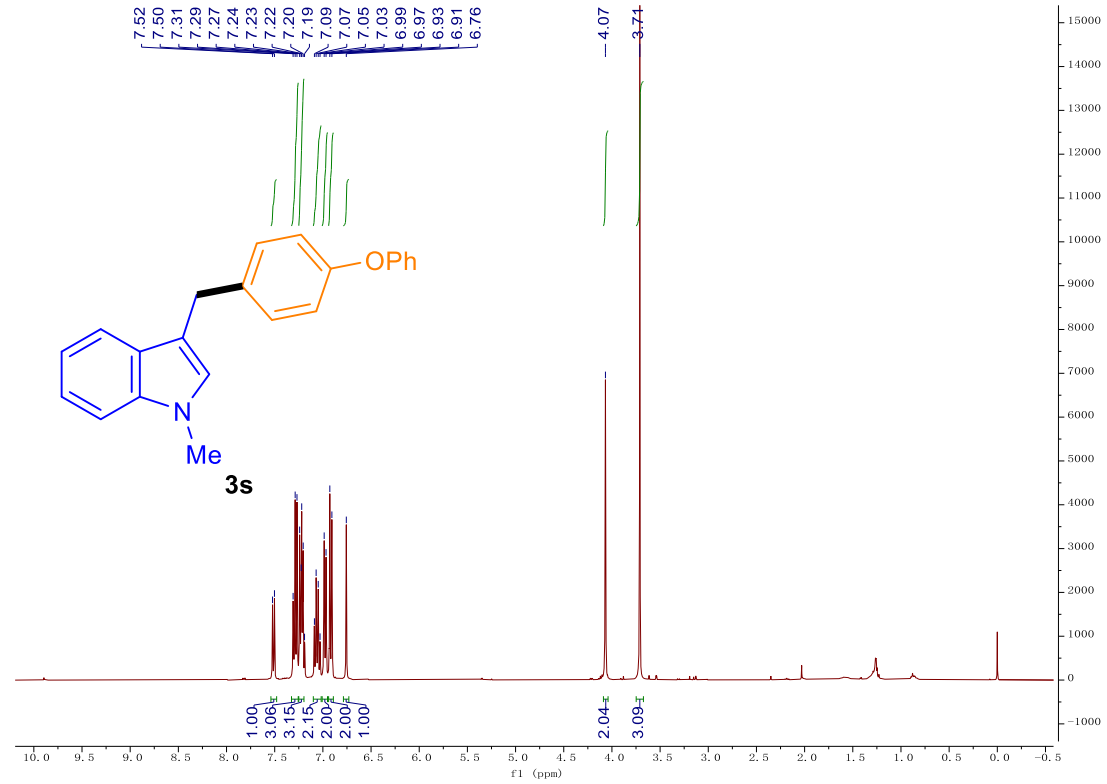


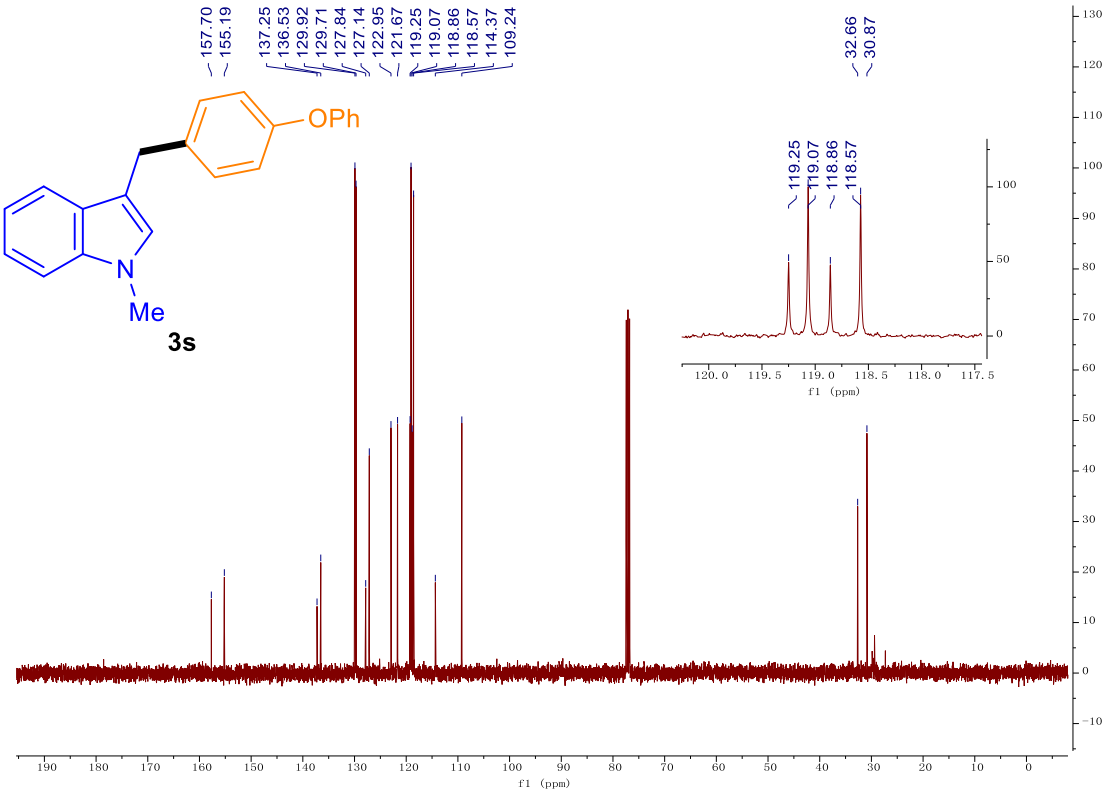
^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3q** ($CDCl_3$, rt).



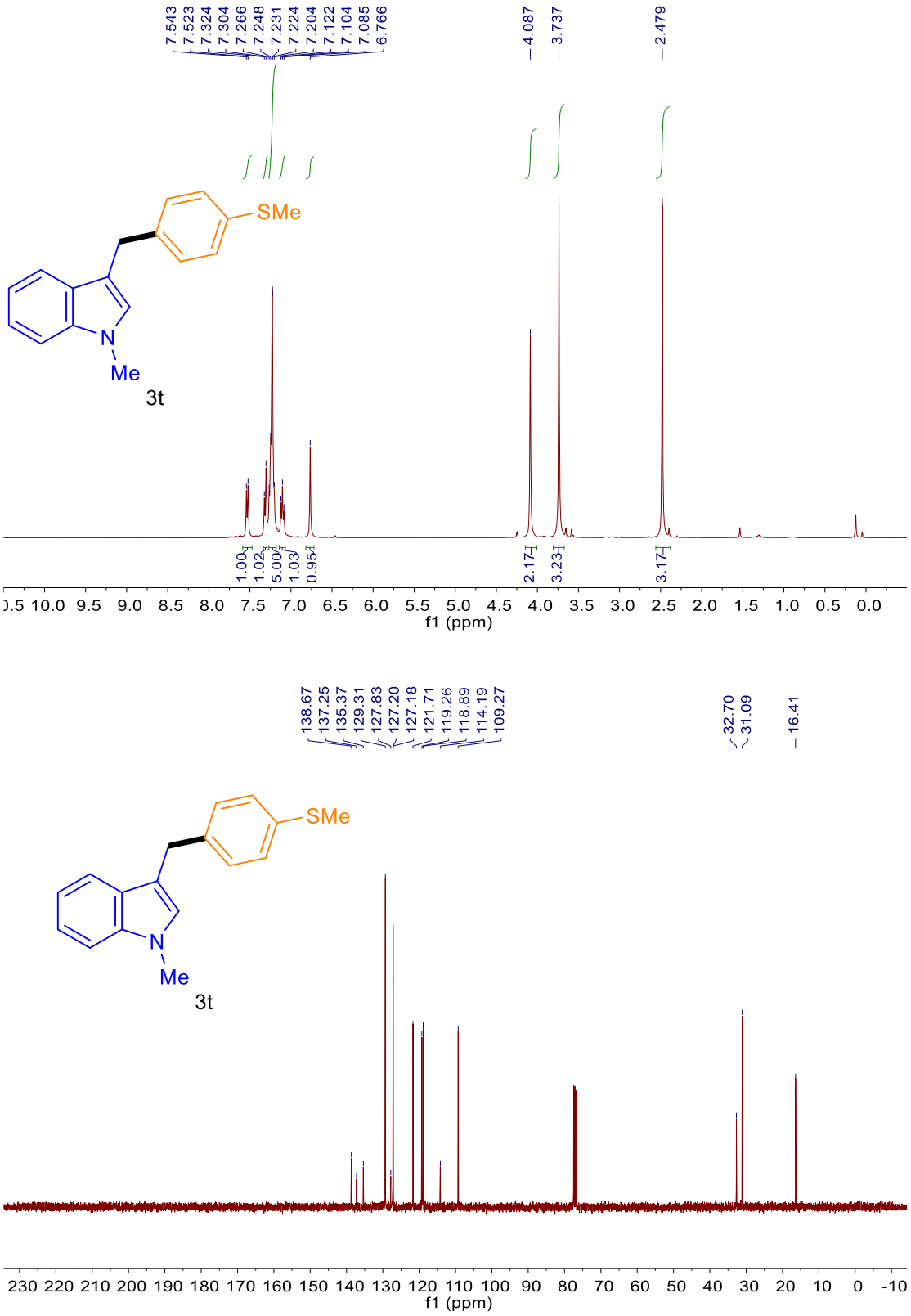


^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3r** ($CDCl_3$, rt).

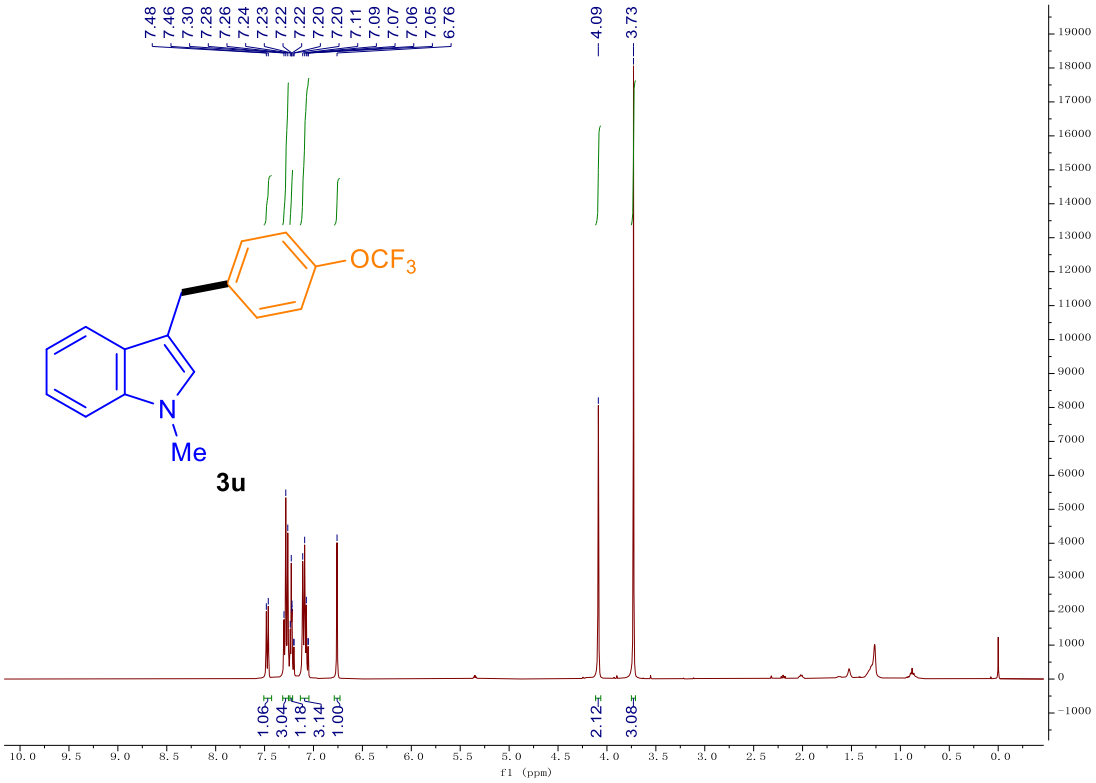


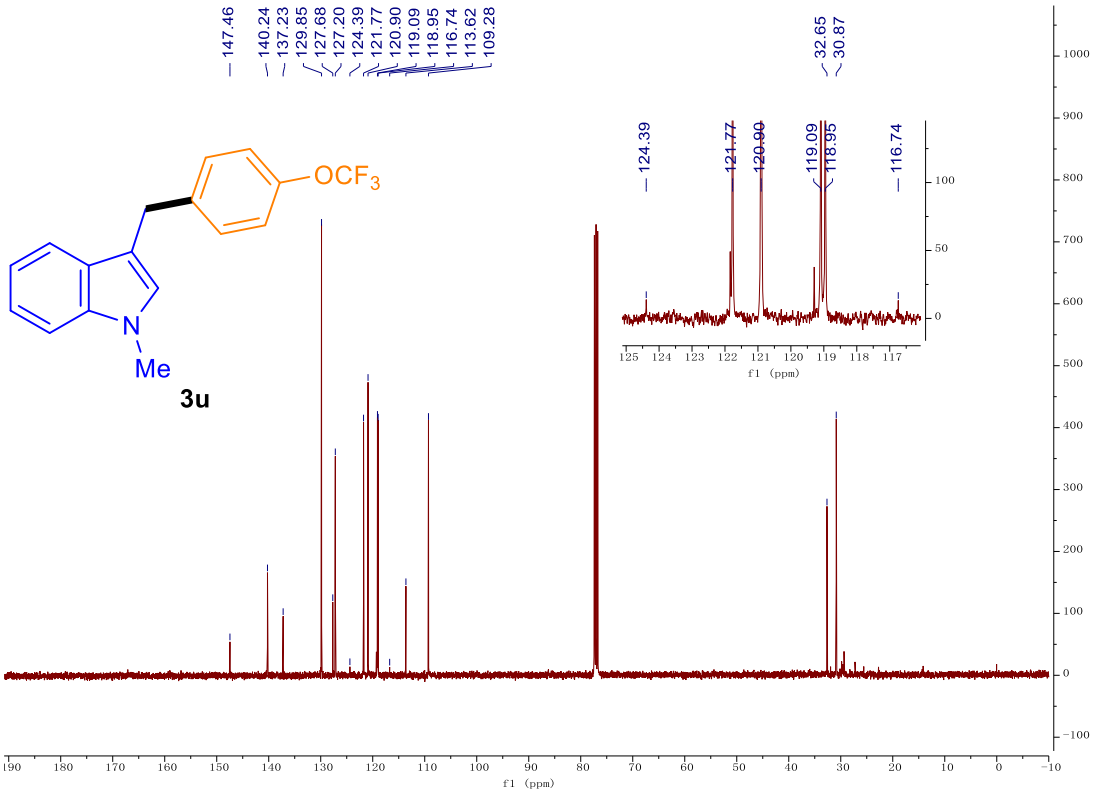


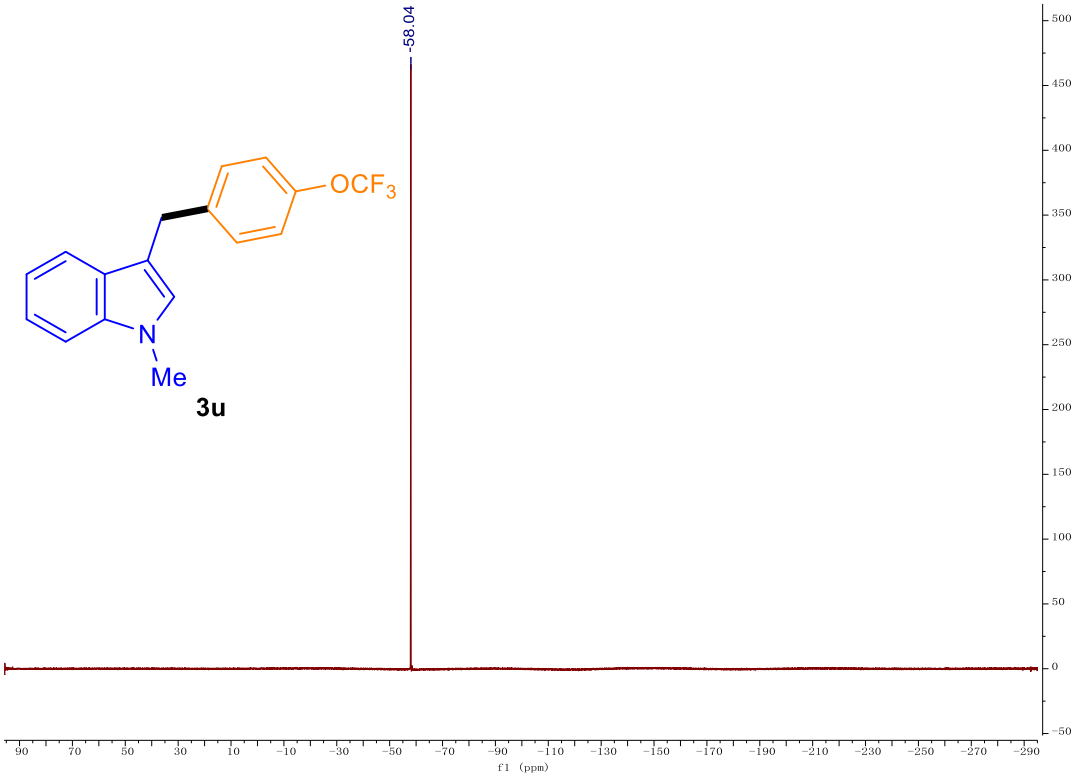
^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3s** ($CDCl_3$, rt).



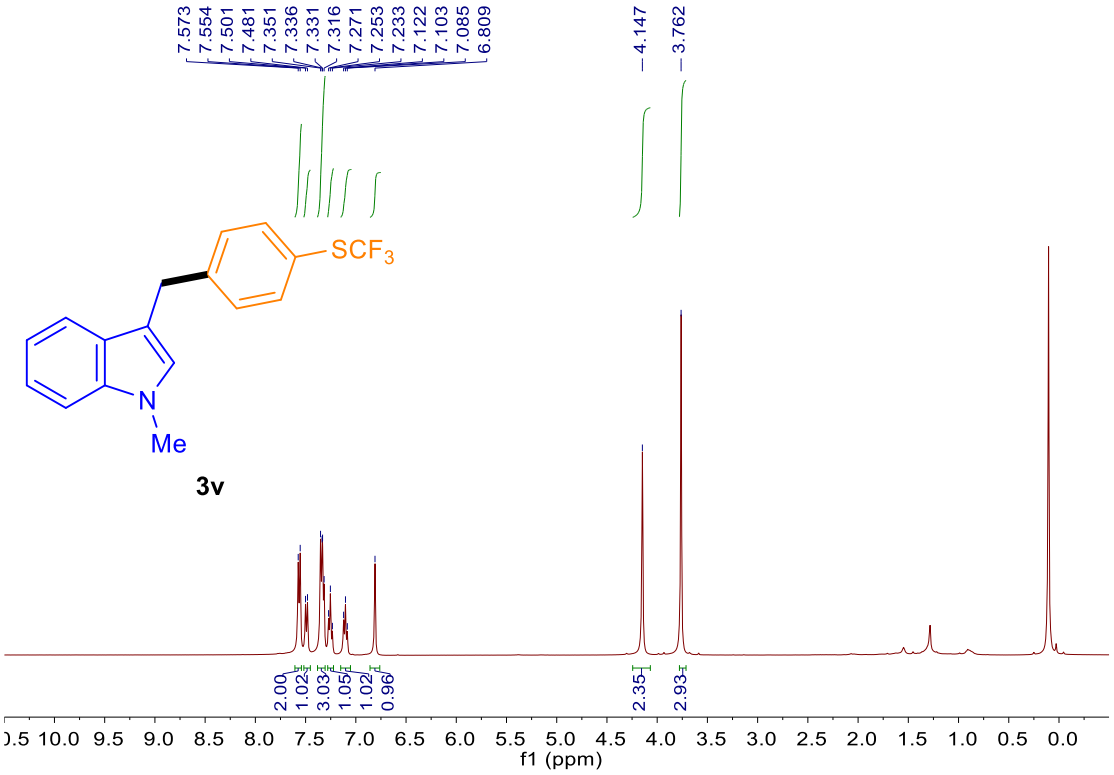
^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3t** ($CDCl_3$, rt).

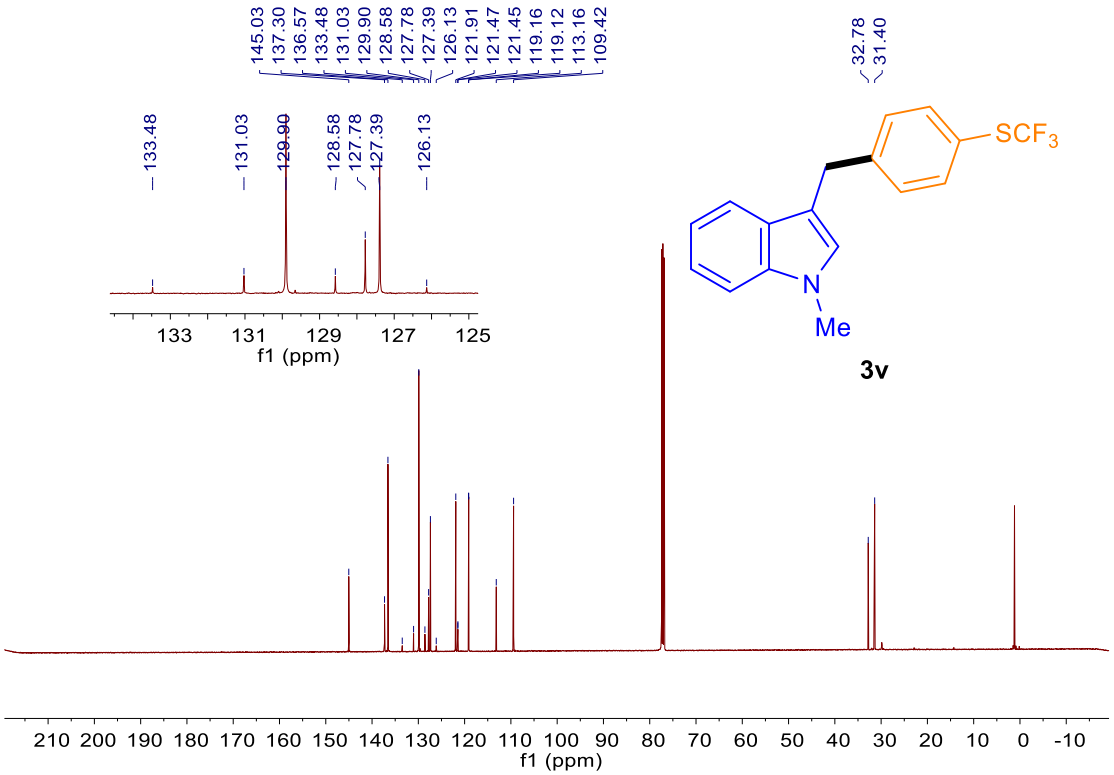

7.48
7.46
7.30
7.28
7.26
7.24
7.23
7.22
7.22
7.20
7.20
7.11
7.09
7.07
7.06
7.05
6.76
4.09
3.73
OCF3
N
Me
3u
1.06
3.04
1.18
3.14
1.00
2.12
3.08
f1 (ppm)

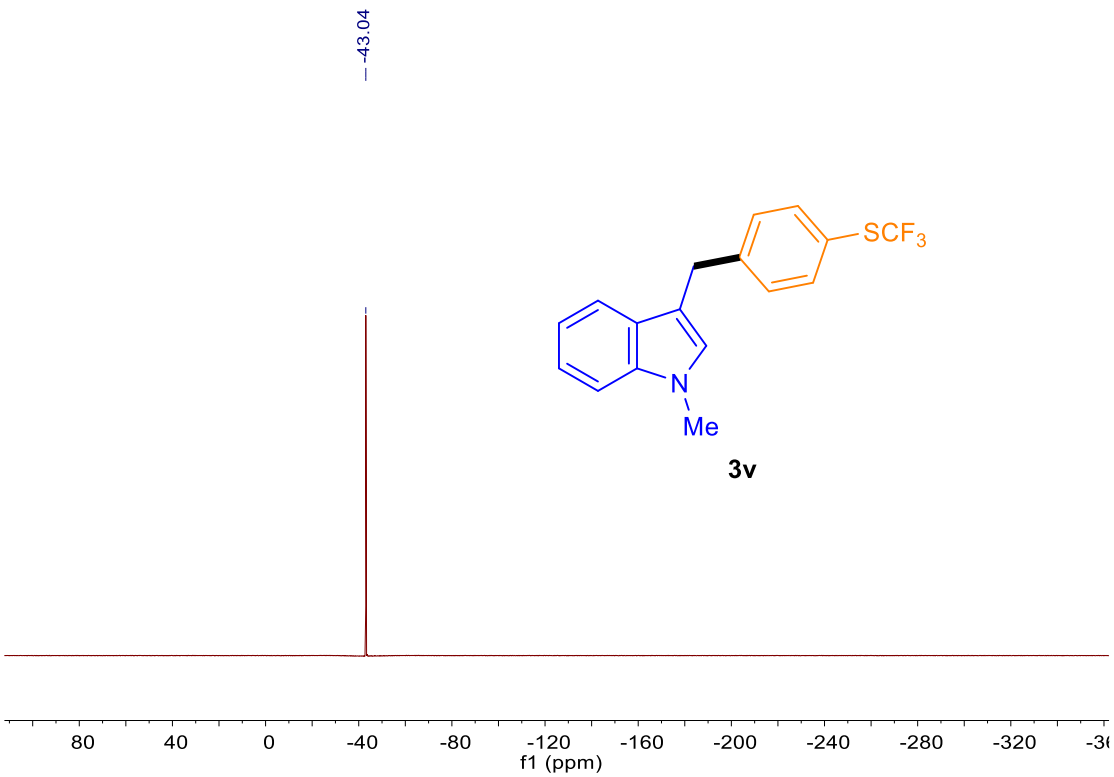

147.46
140.24
137.23
129.85
127.68
127.20
124.39
121.77
120.90
119.09
118.95
116.74
113.62
109.28
32.65
30.87
OCF3
N
Me
3u
f1 (ppm)



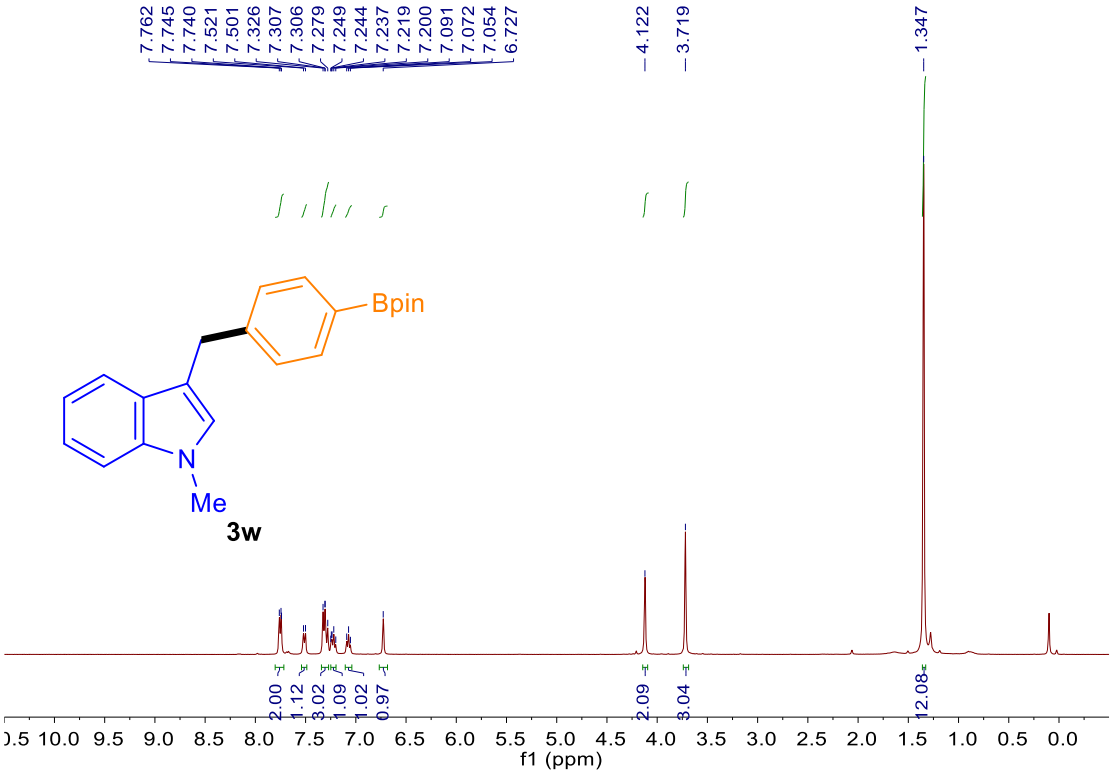
^{1}H NMR (400 MHz), ^{13}C{^{1}H} NMR (100 MHz) and ^{19}F NMR (376 MHz) spectra of **3u** ($CDCl_3$, rt).

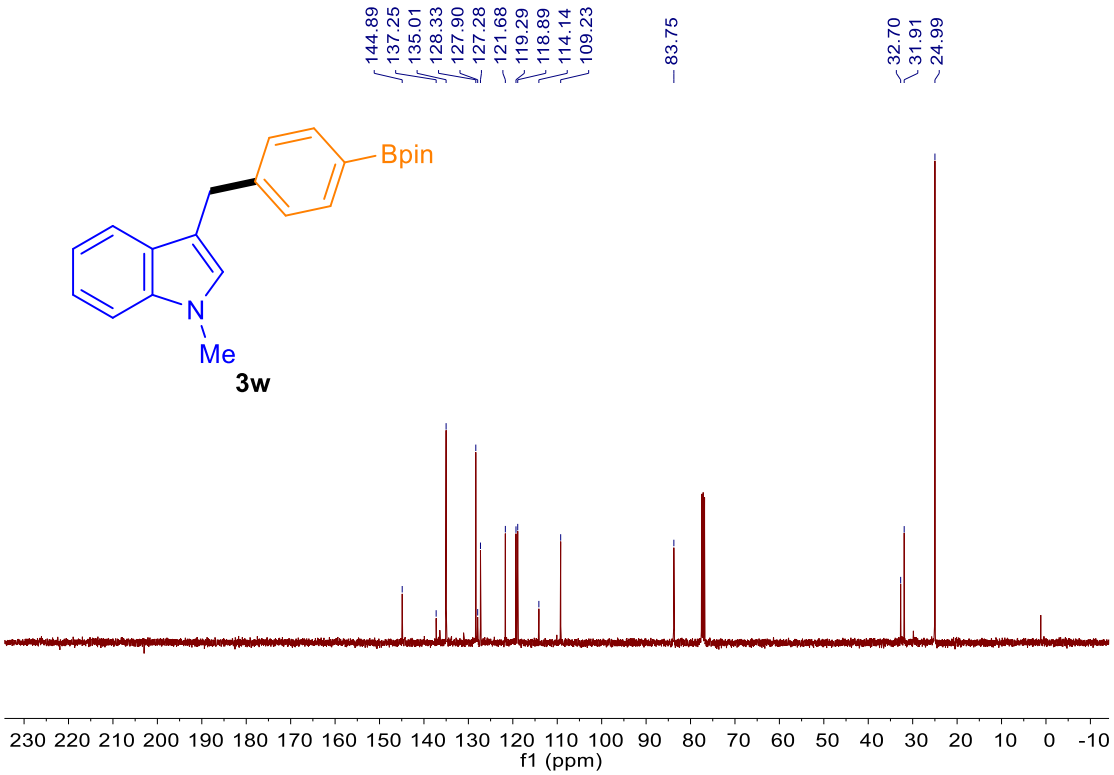

7.573
7.554
7.501
7.481
7.351
7.336
7.331
7.316
7.271
7.253
7.233
7.122
7.103
7.085
6.809
4.147
3.762
SCF3
N
Me
3v
2.00
1.02
3.03
1.05
1.02
0.96
2.35
2.93
f1 (ppm)


145.03
137.30
136.57
133.48
131.03
129.90
128.58
127.78
127.39
126.13
121.91
121.47
121.45
119.16
119.12
113.16
109.42
32.78
31.40
133.48
131.03
129.90
128.58
127.78
127.39
126.13
133
131
129
127
125
f1 (ppm)
SCF3
N
Me
3v
f1 (ppm)

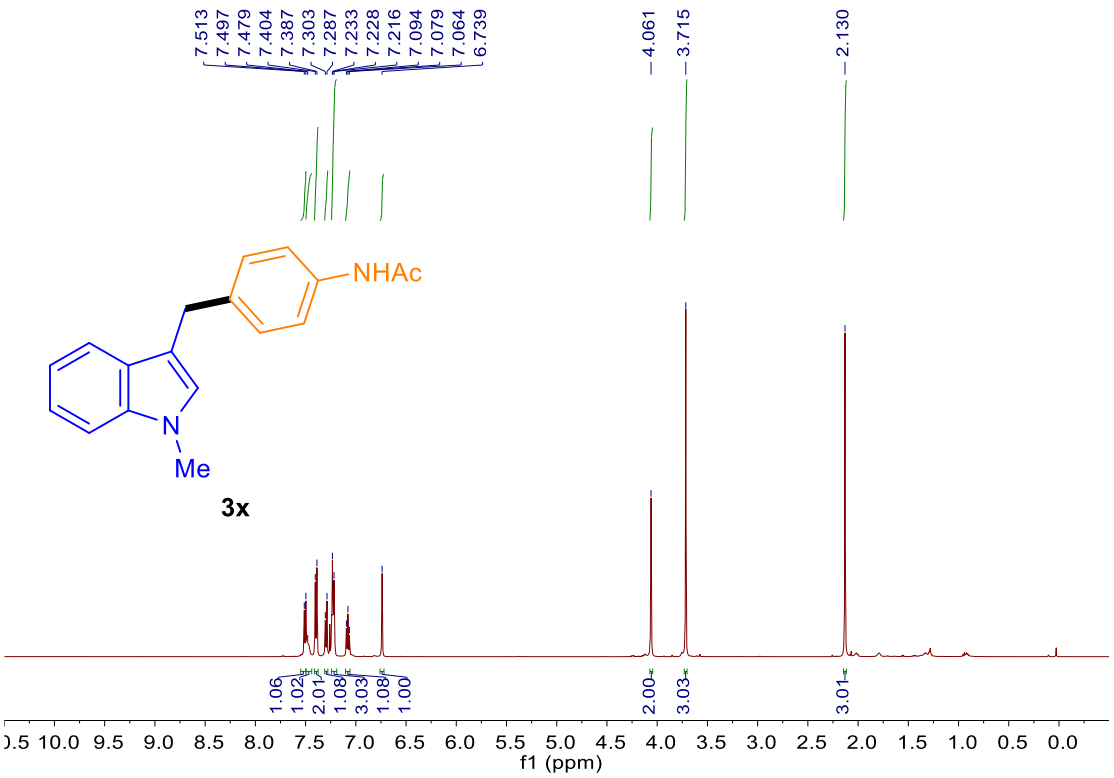


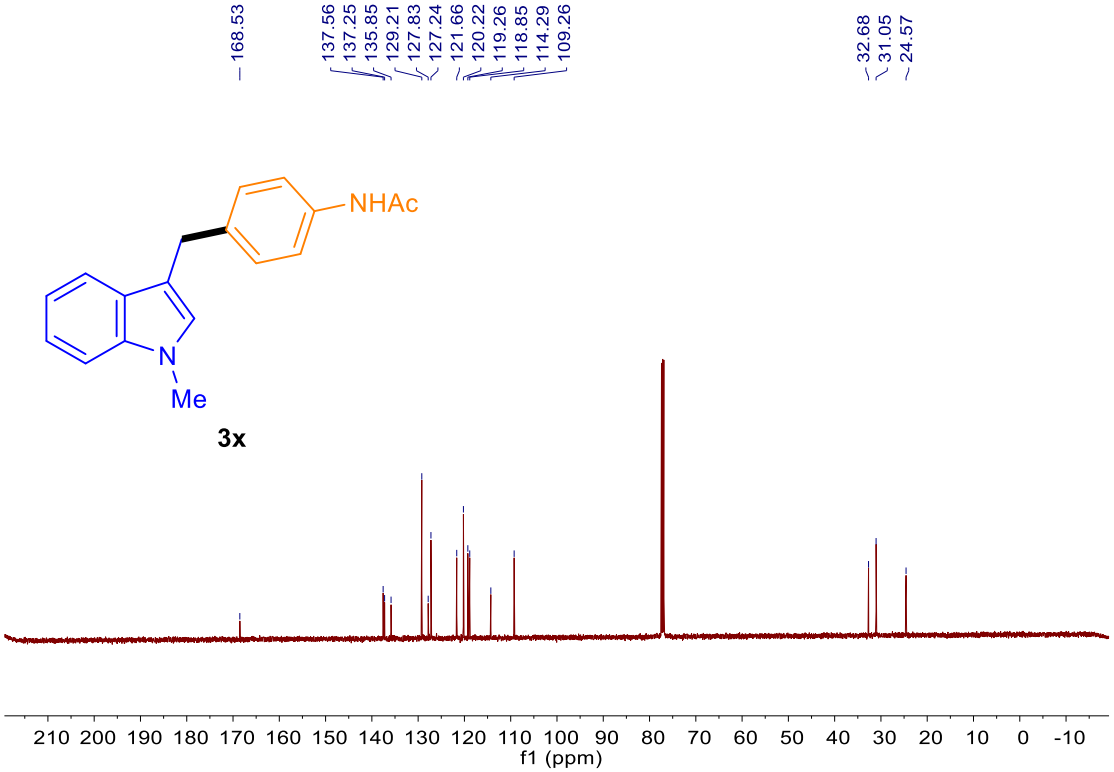
^{1}H NMR (400 MHz), ^{13}C{^{1}H} NMR (125 MHz) and ^{19}F NMR (376 MHz) spectra of **3v** ($CDCl_3$, rt).



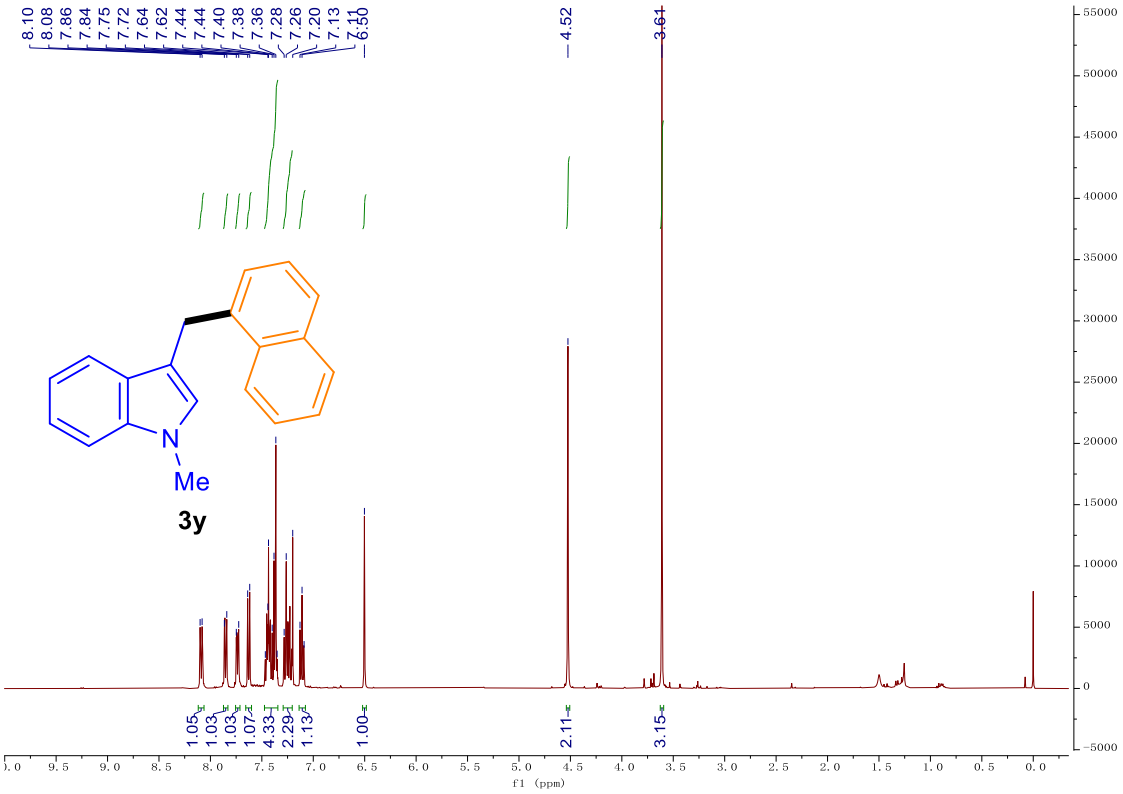


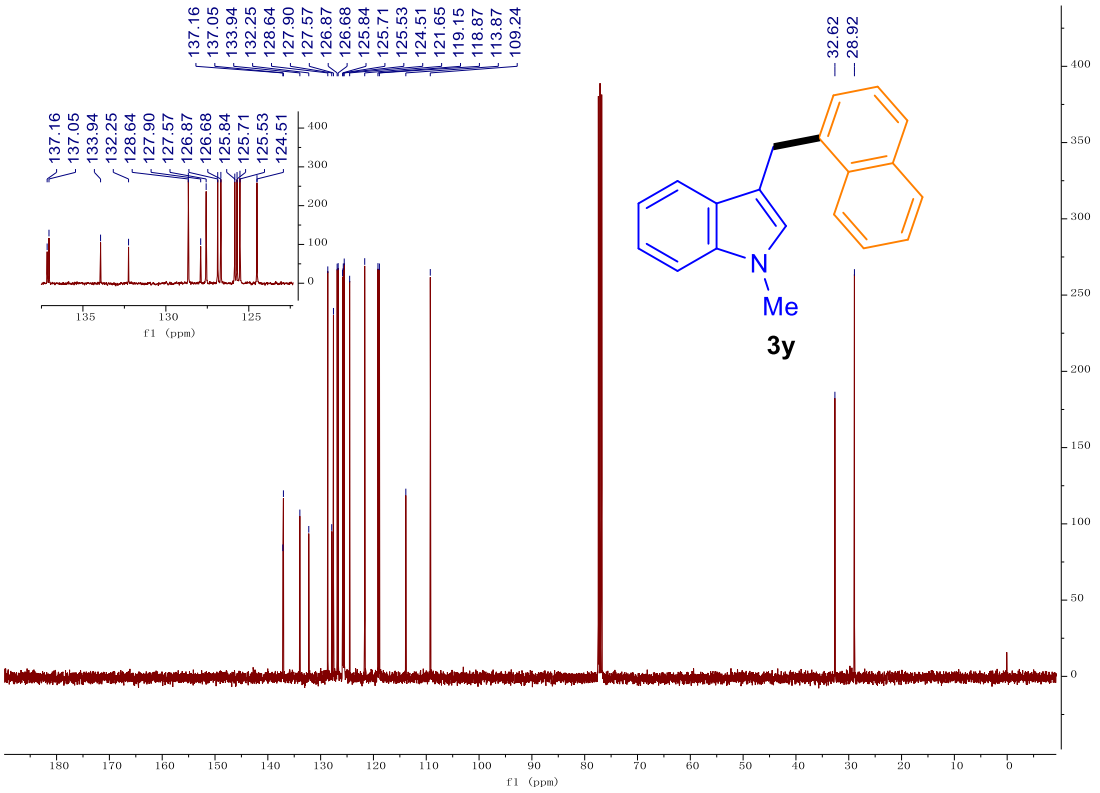
^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3w** ($CDCl_3$, rt).



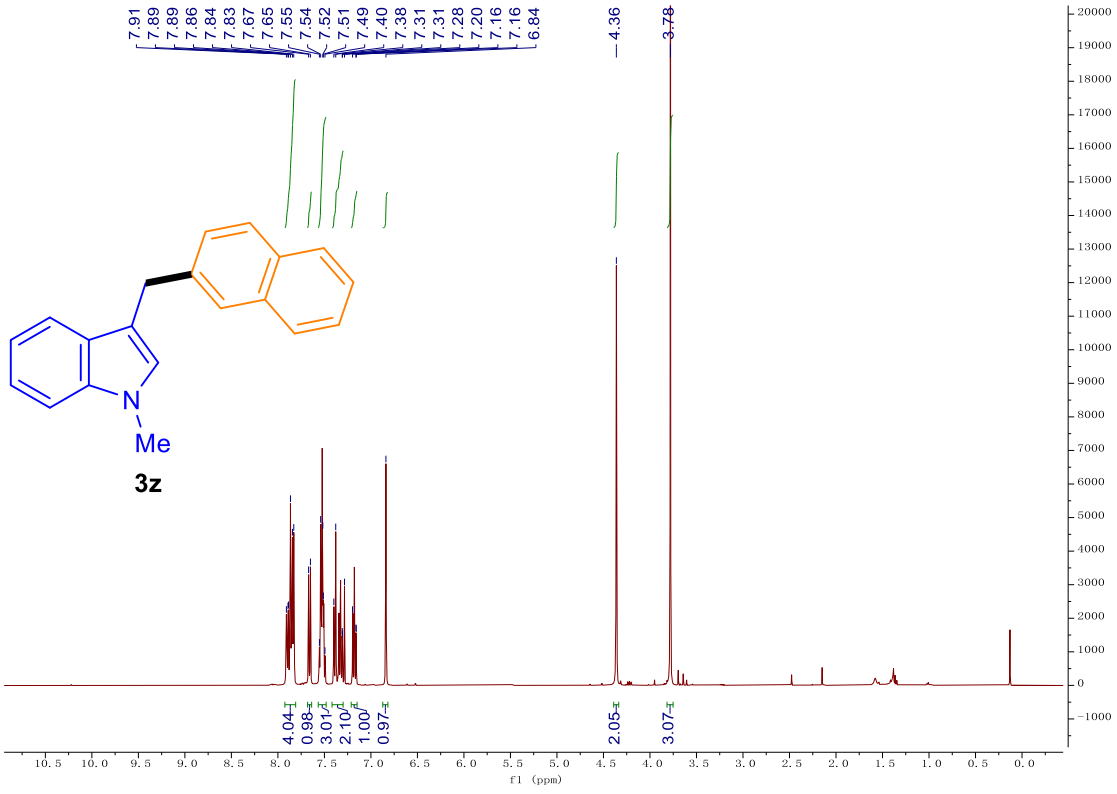


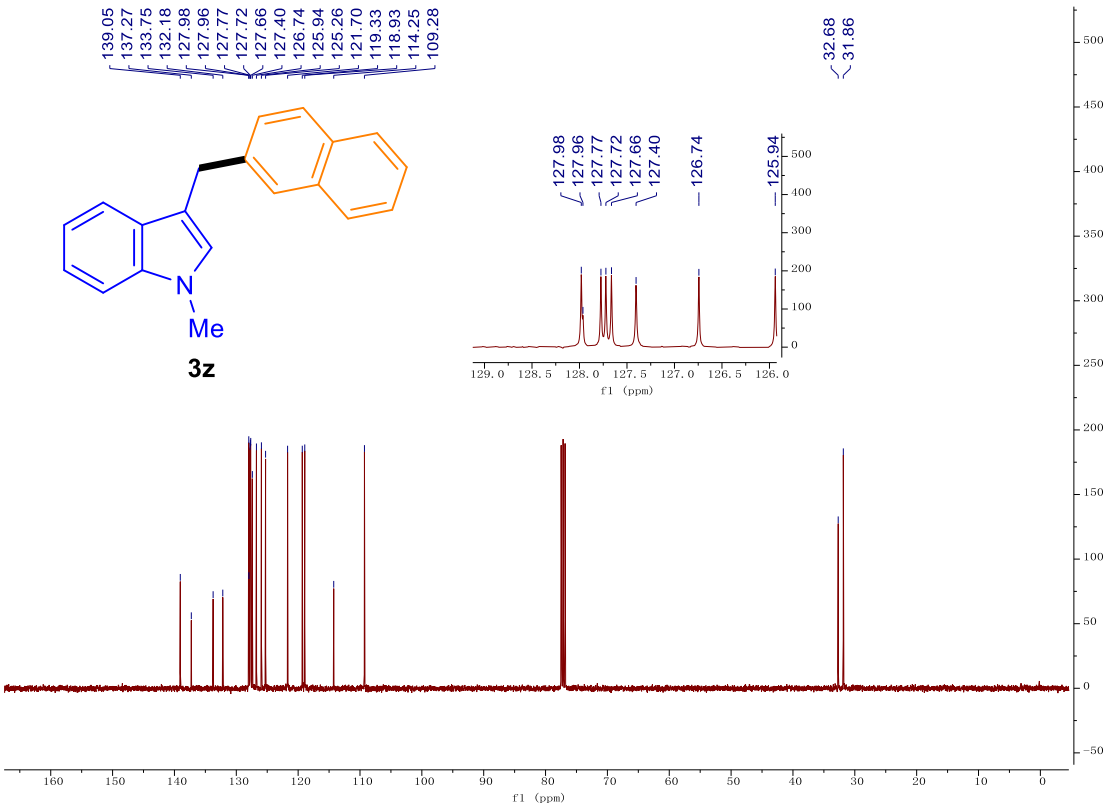
^{1}H NMR (500 MHz) and ^{13}C{^{1}H} NMR (125 MHz) spectra of **3x** ($CDCl_3$, rt).



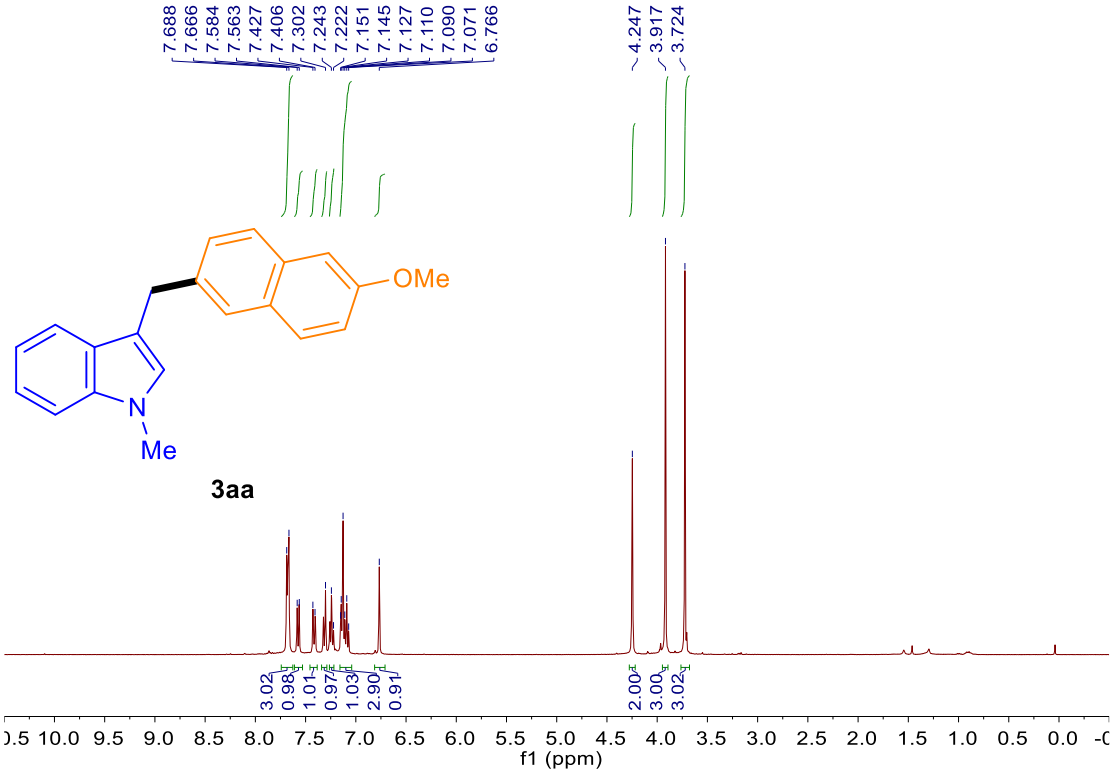


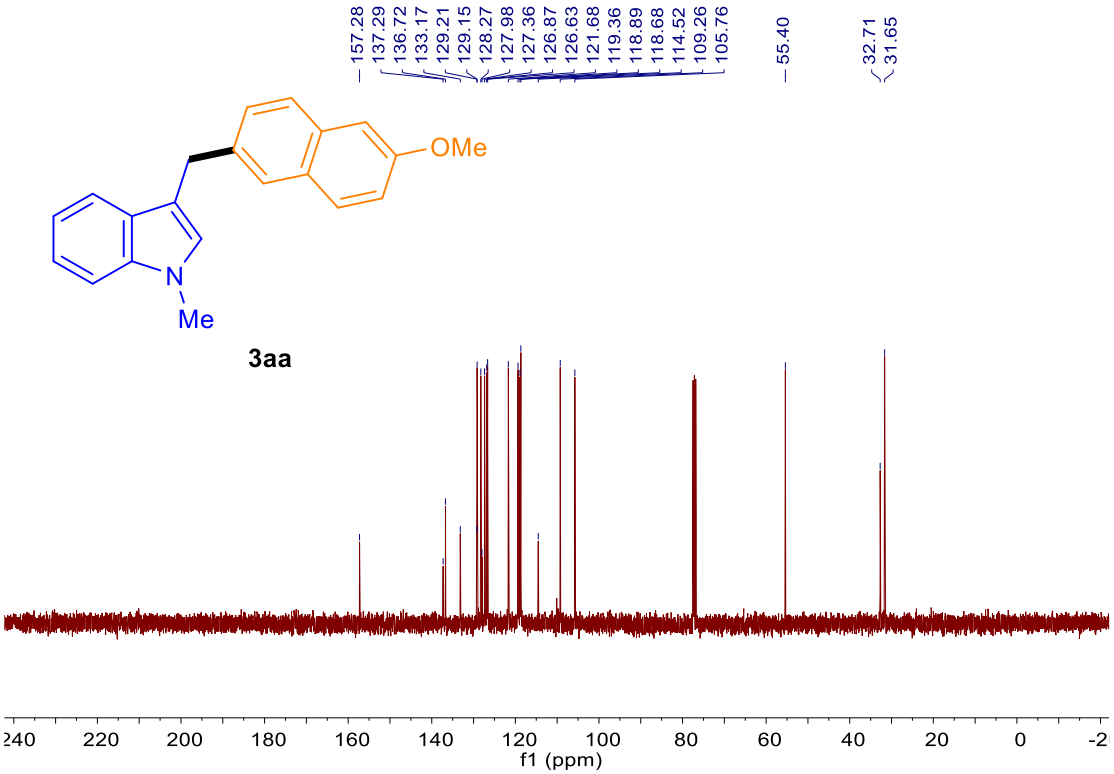
^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3y** ($CDCl_3$, rt).



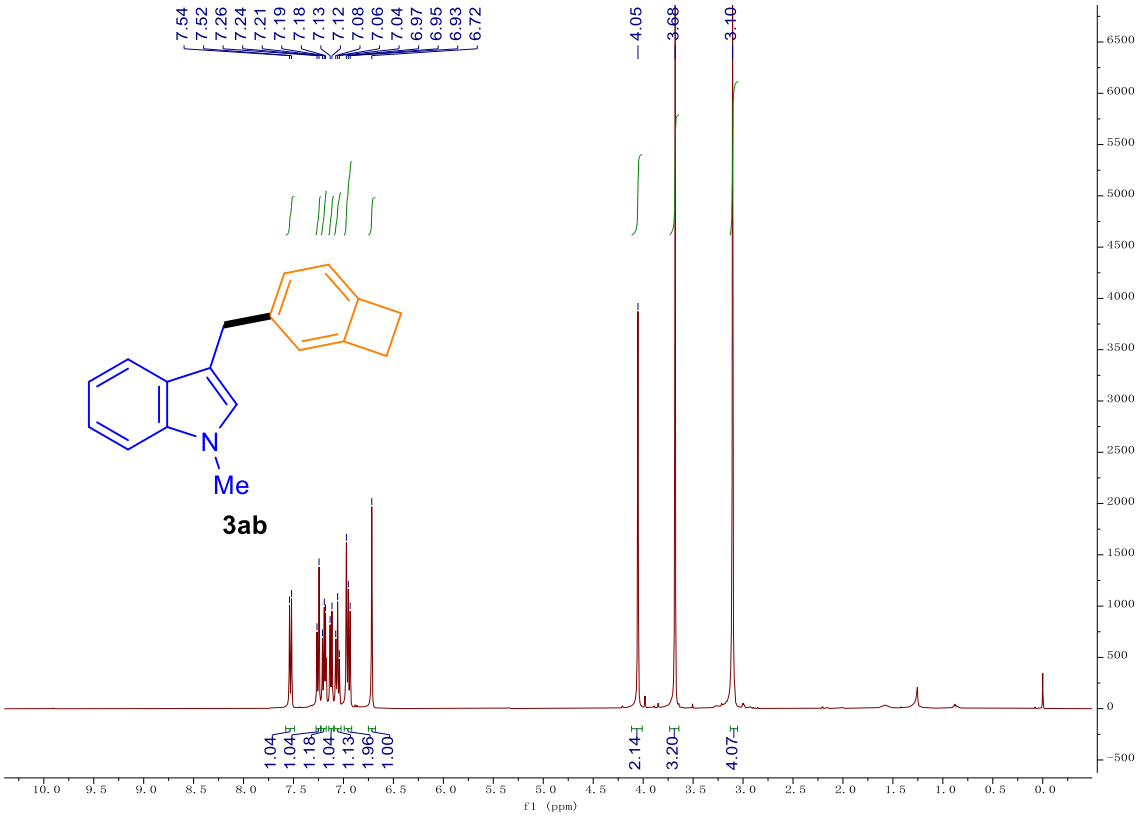


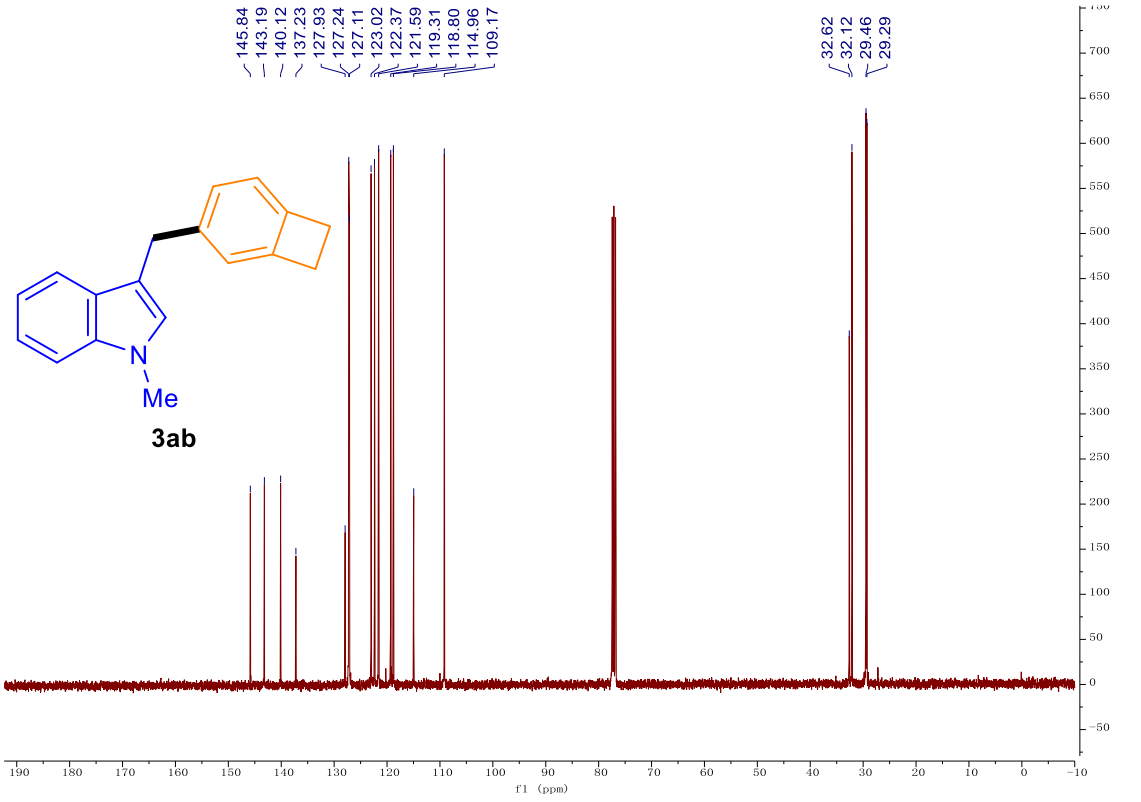
^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3z** ($CDCl_3$, rt).



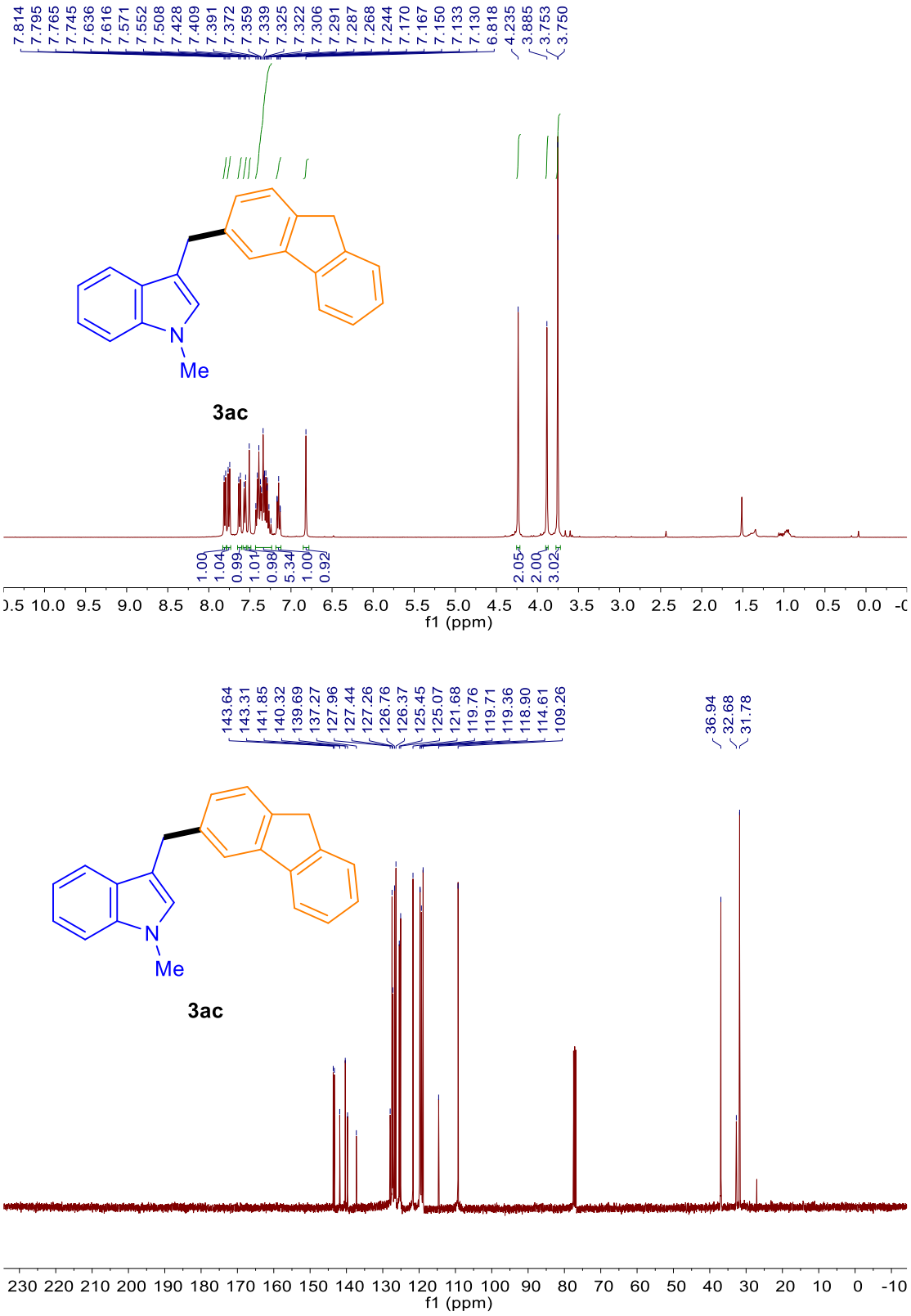


^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3aa** ($CDCl_3$, rt).

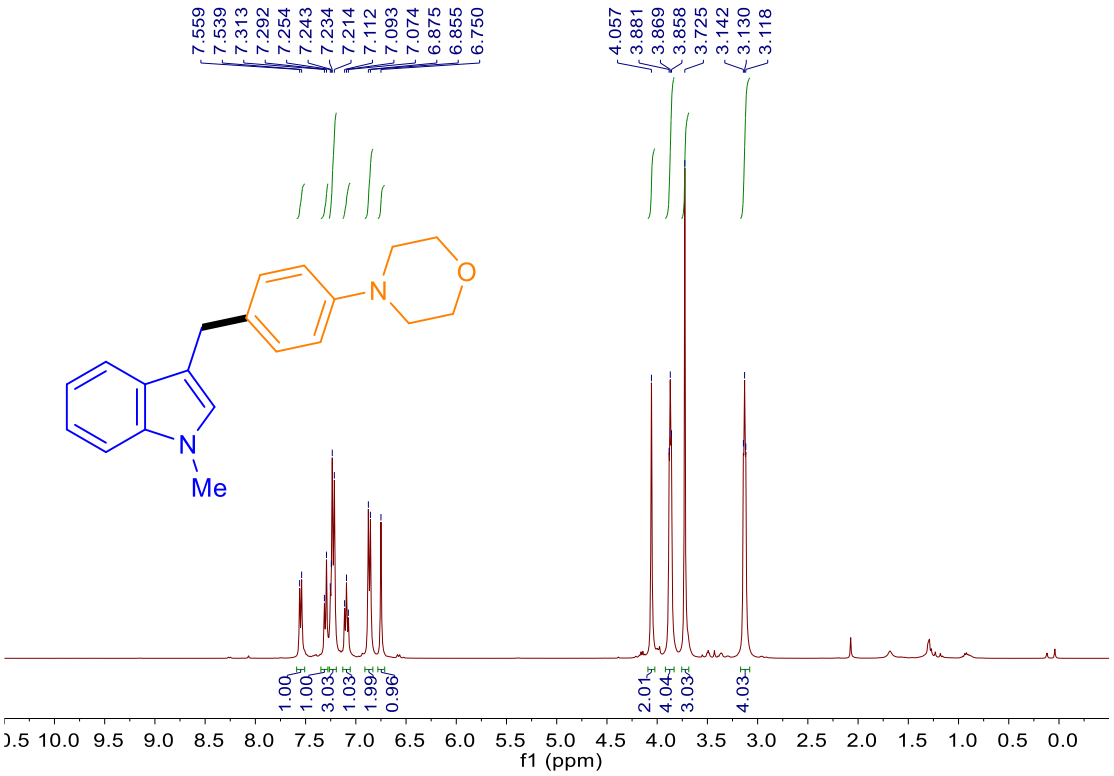


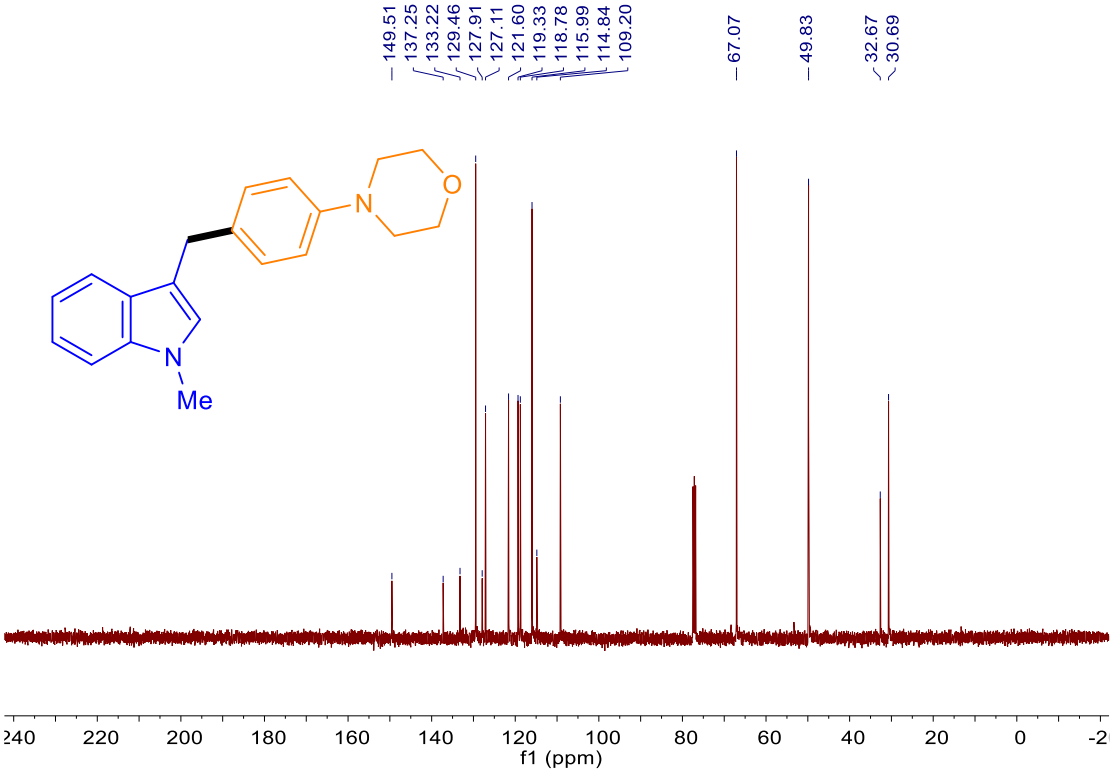


^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3ab** ($CDCl_3$, rt).

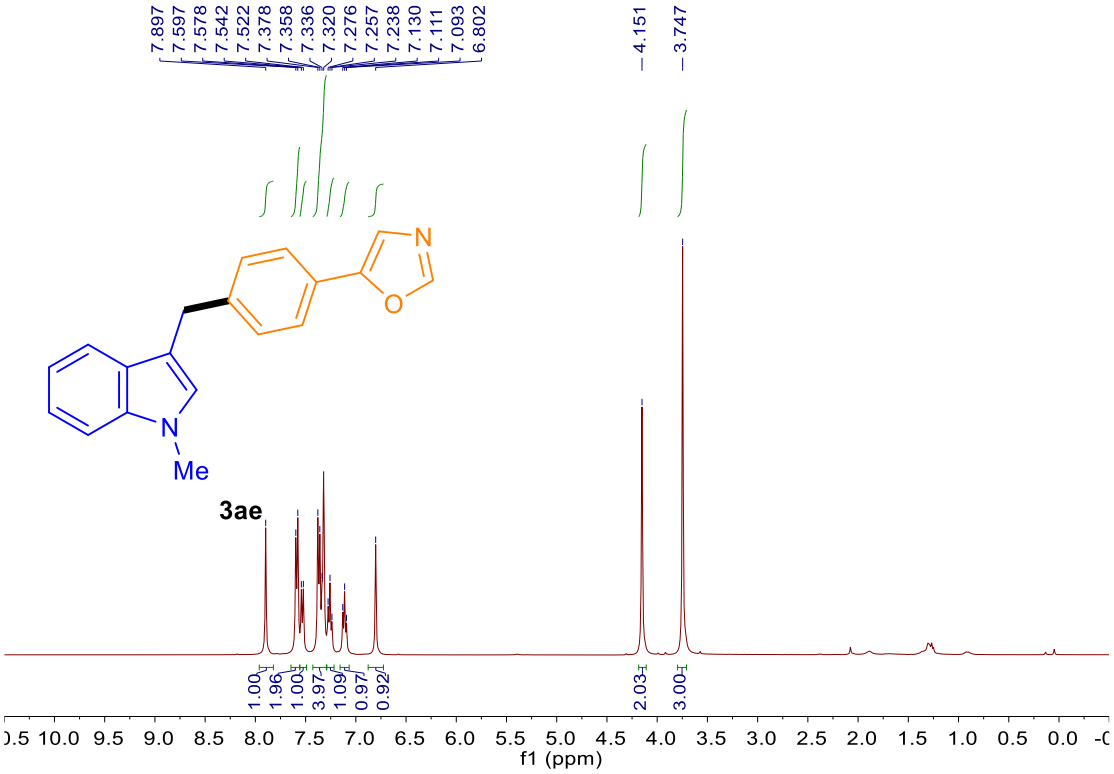


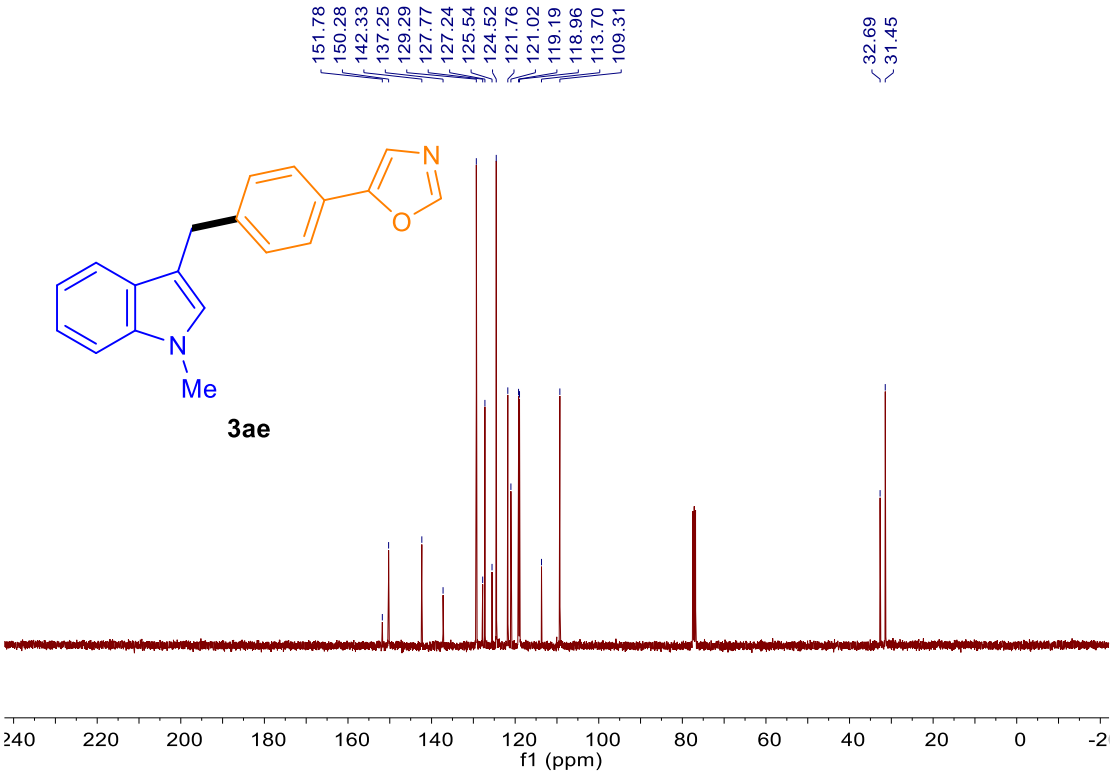
^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3ac** ($CDCl_3$, rt).



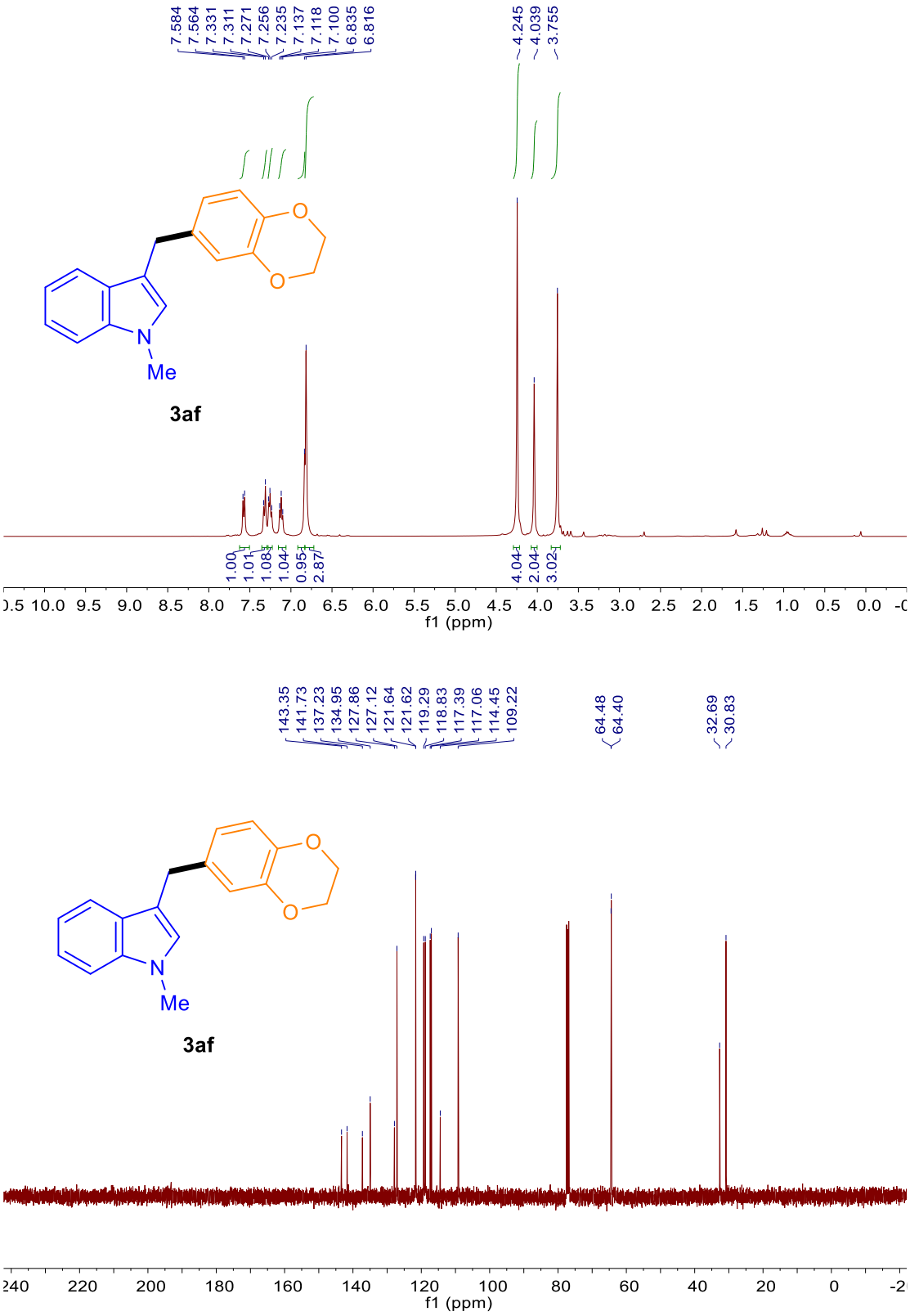


^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3ad** ($CDCl_3$, rt).

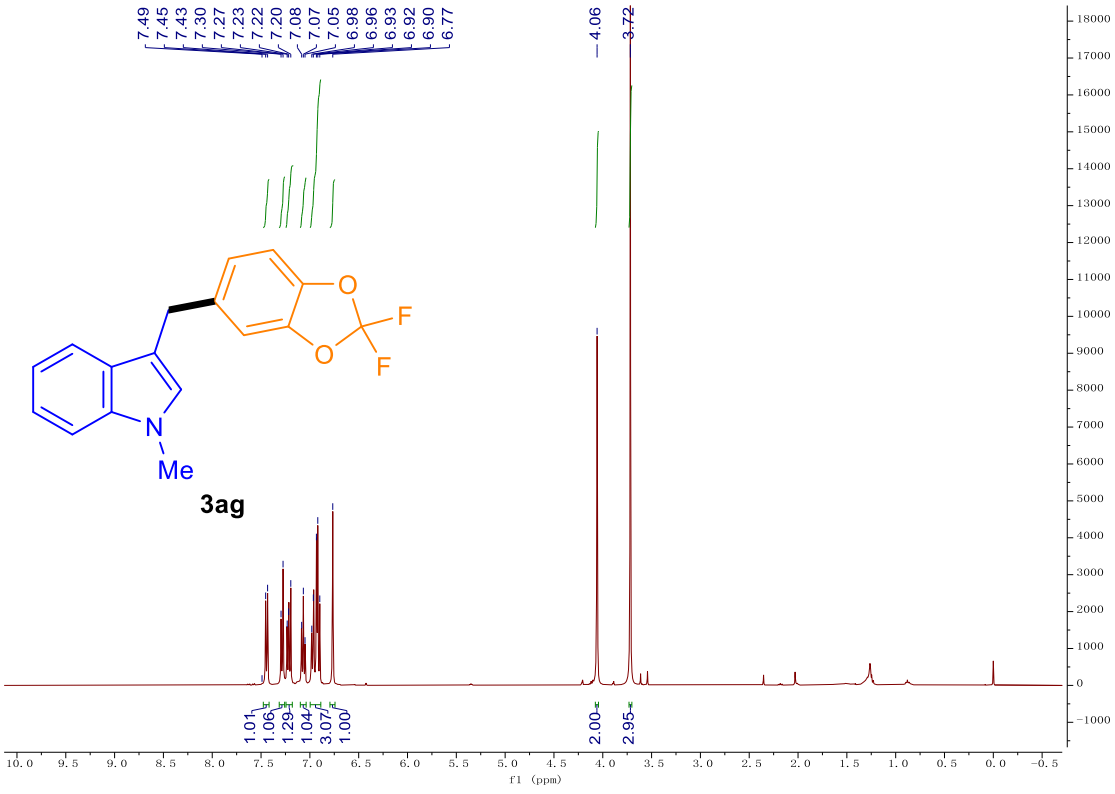


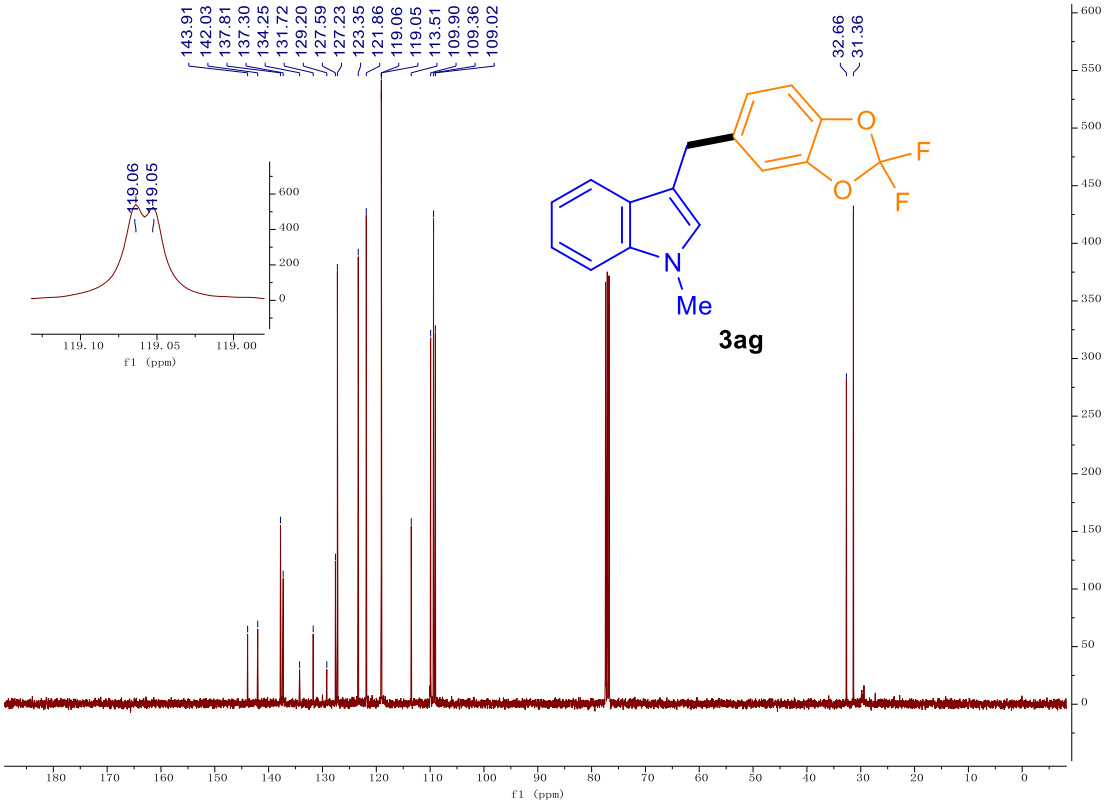


^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3ae** ($CDCl_3$, rt).

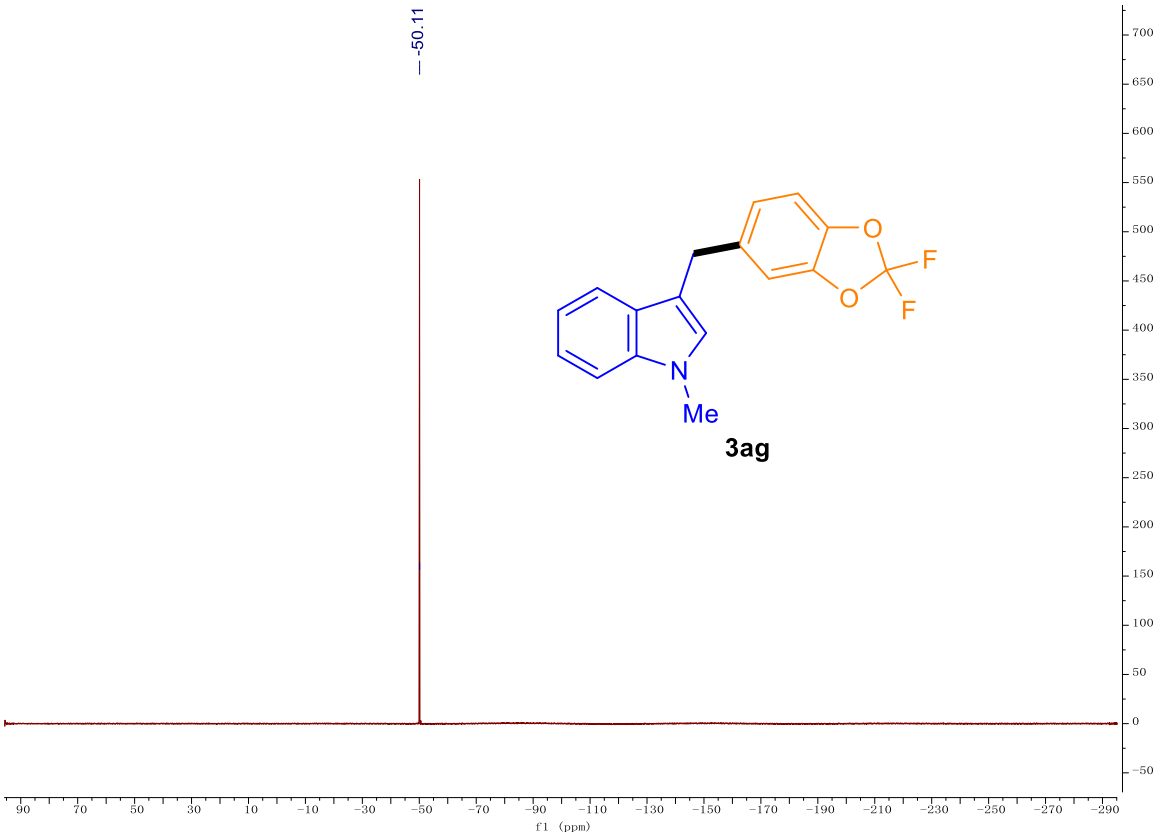


^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3af** ($CDCl_3$, rt).

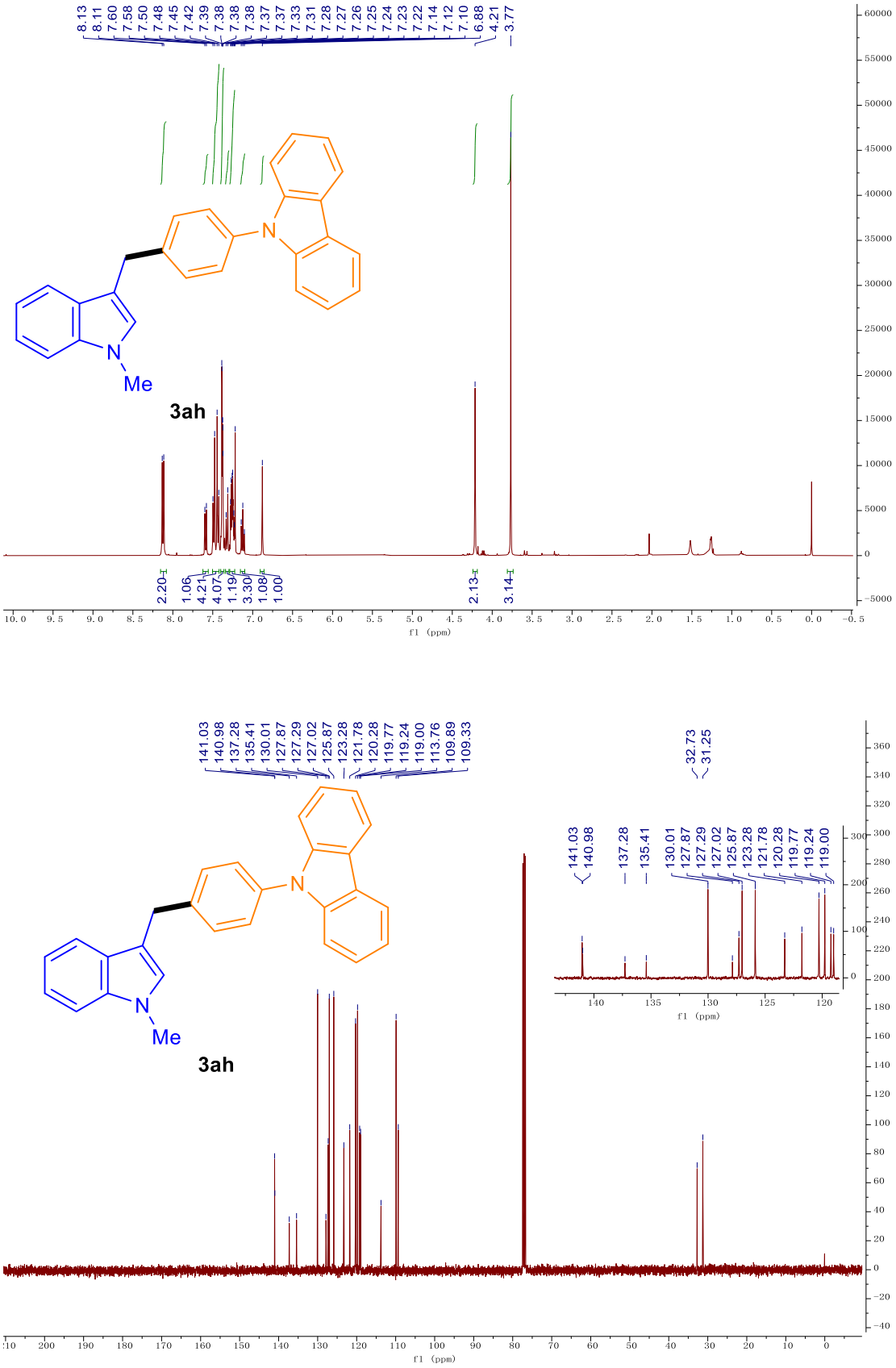




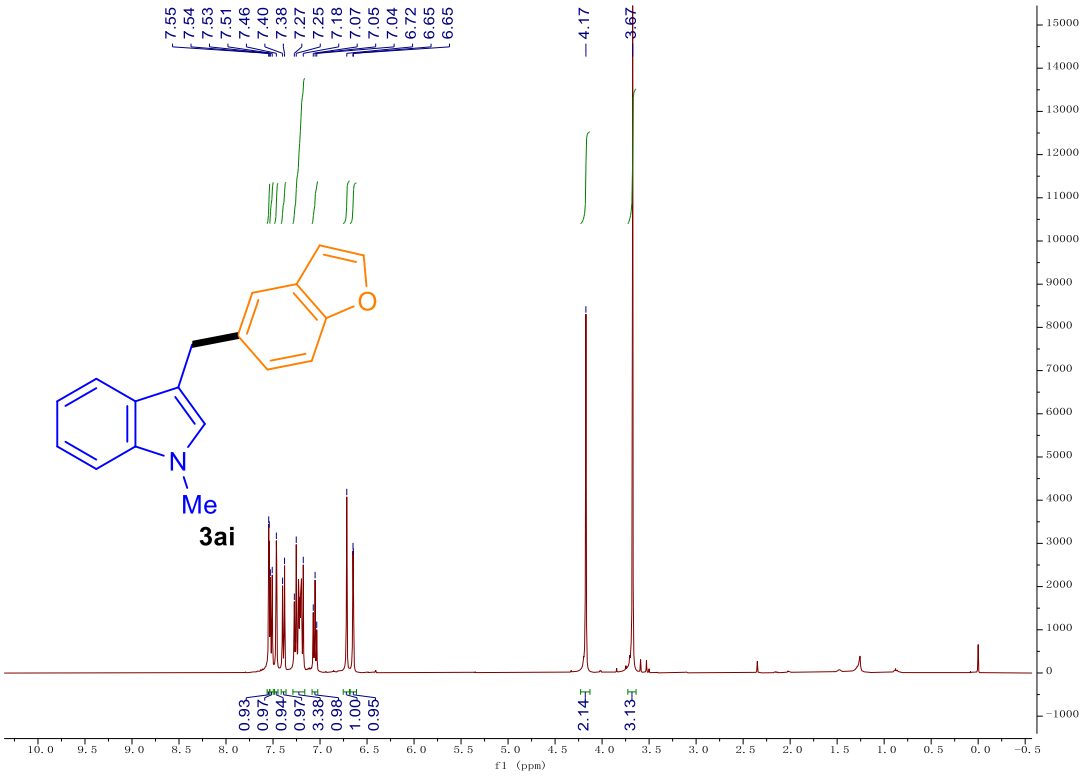
^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3ag** ($CDCl_3$, rt).

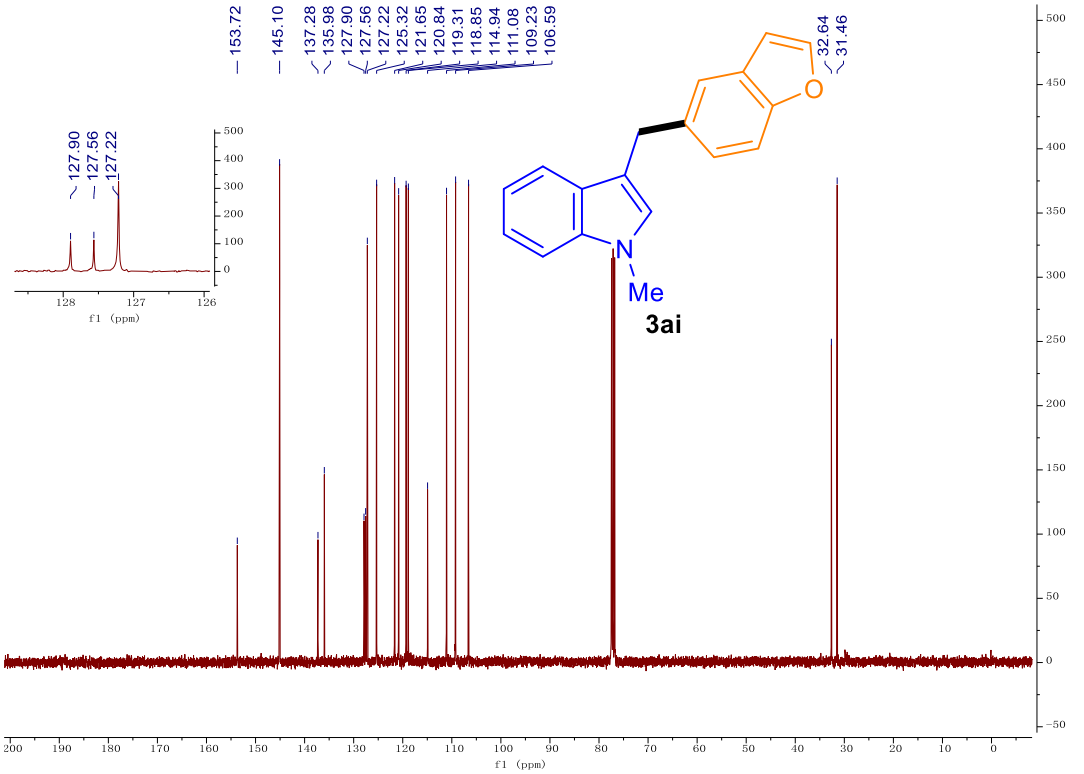


^{1}H NMR (400 MHz), ^{13}C{^{1}H} NMR (100 MHz) and ^{19}F NMR (376 MHz) spectra of **3ag** ($CDCl_3$, rt).

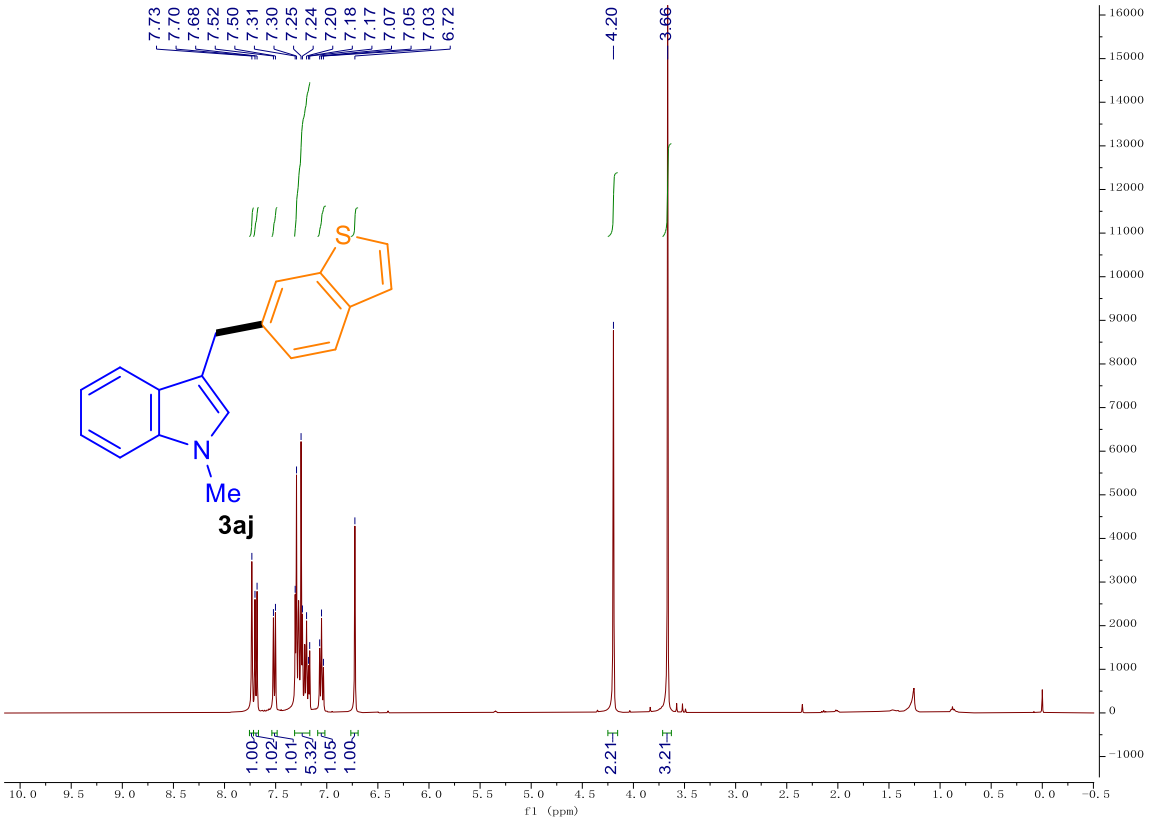


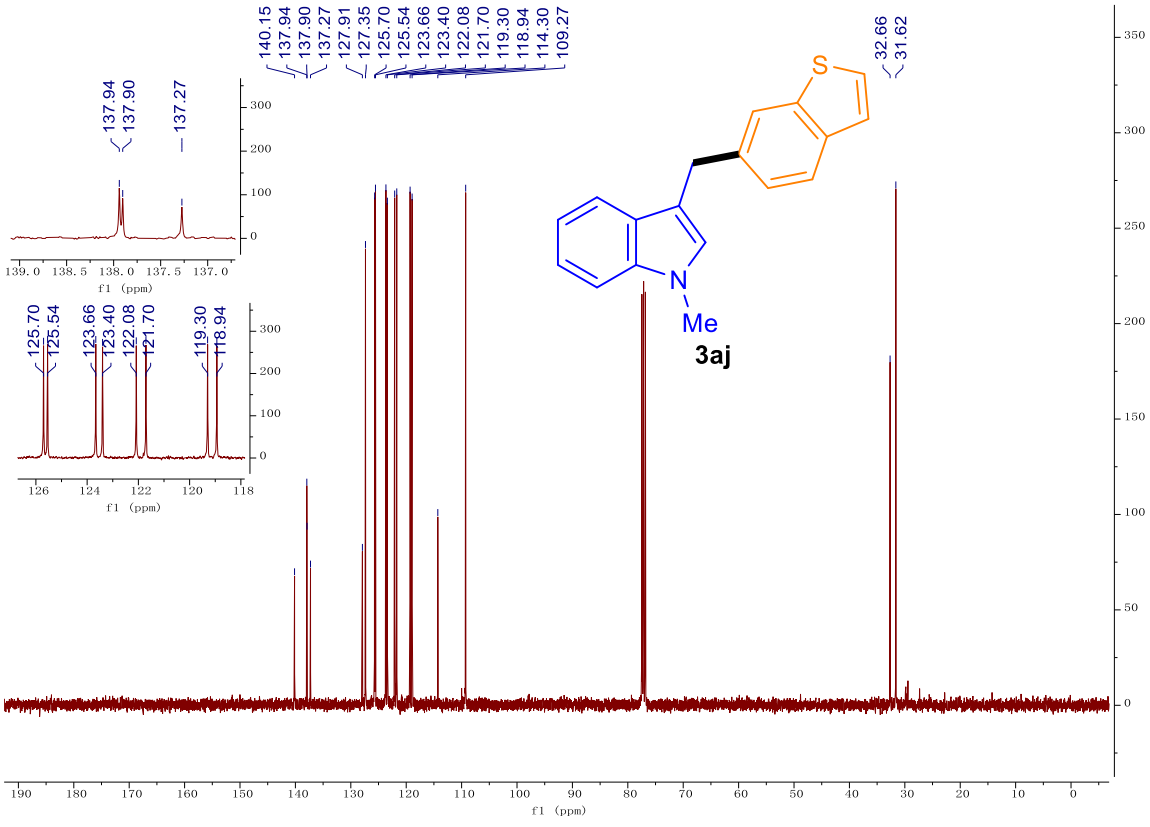
^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3ah** ($CDCl_3$, rt).



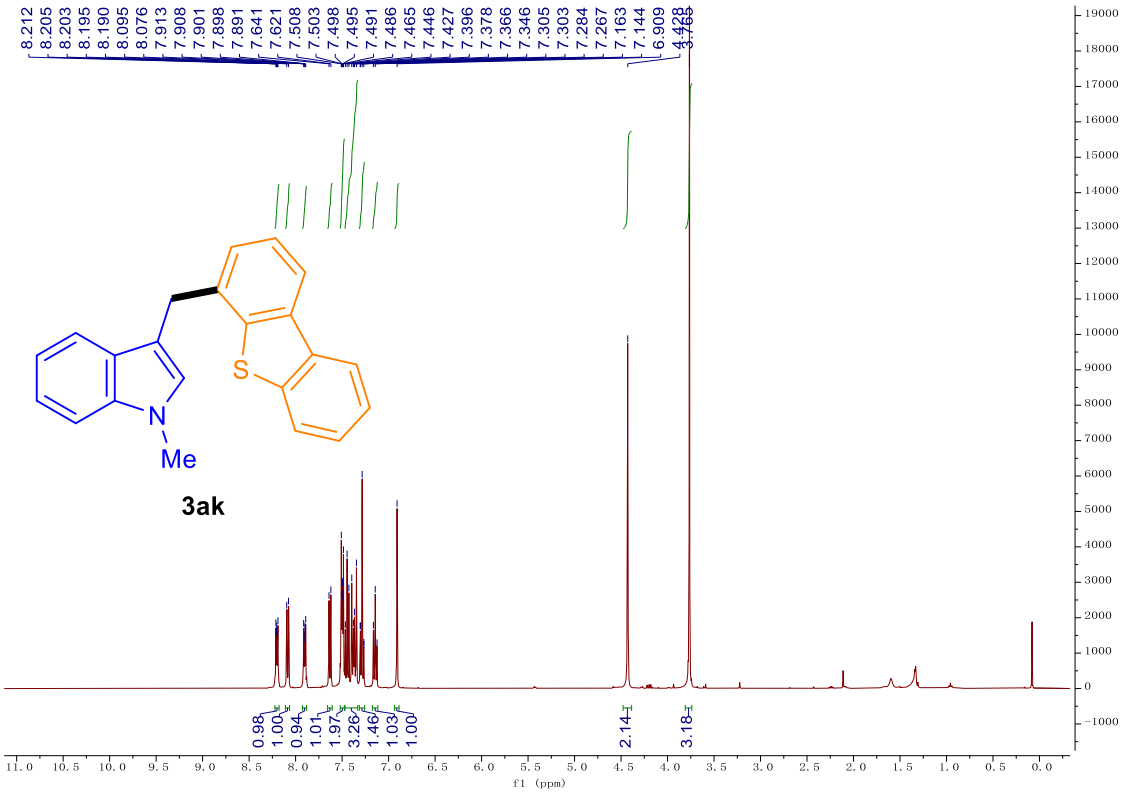


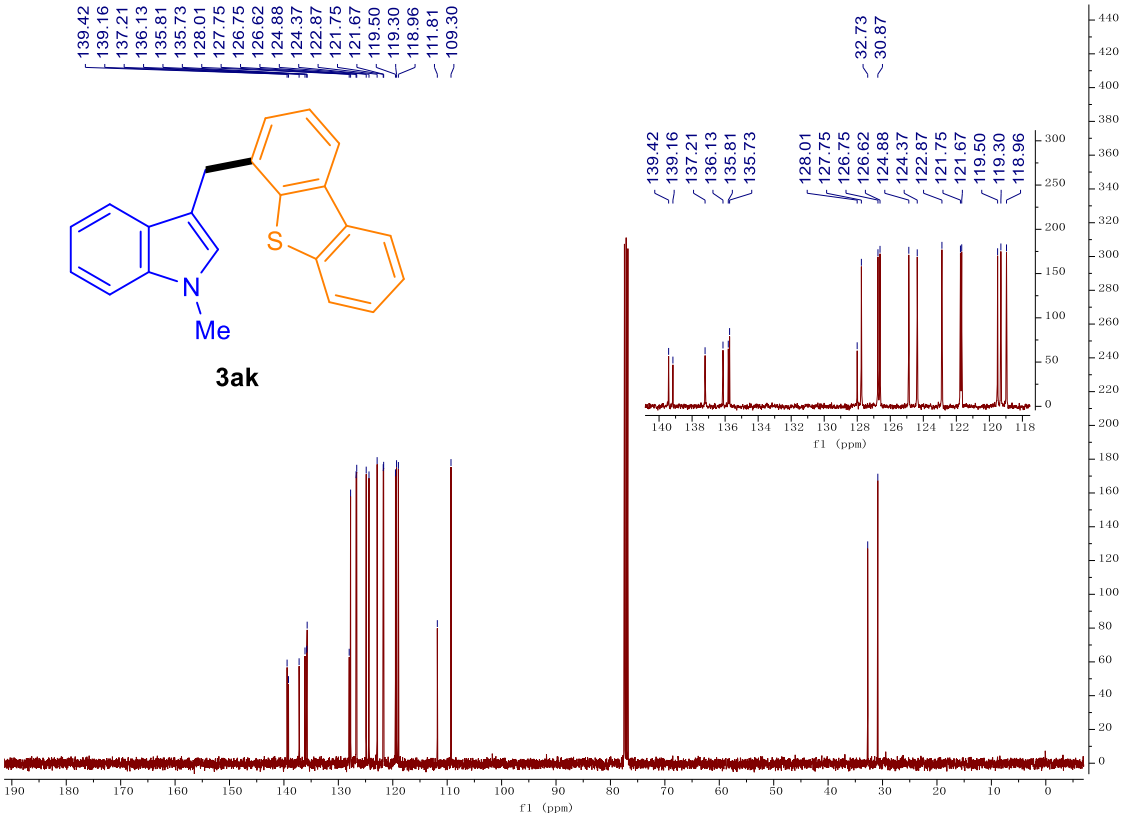
^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3ai** ($CDCl_3$, rt).



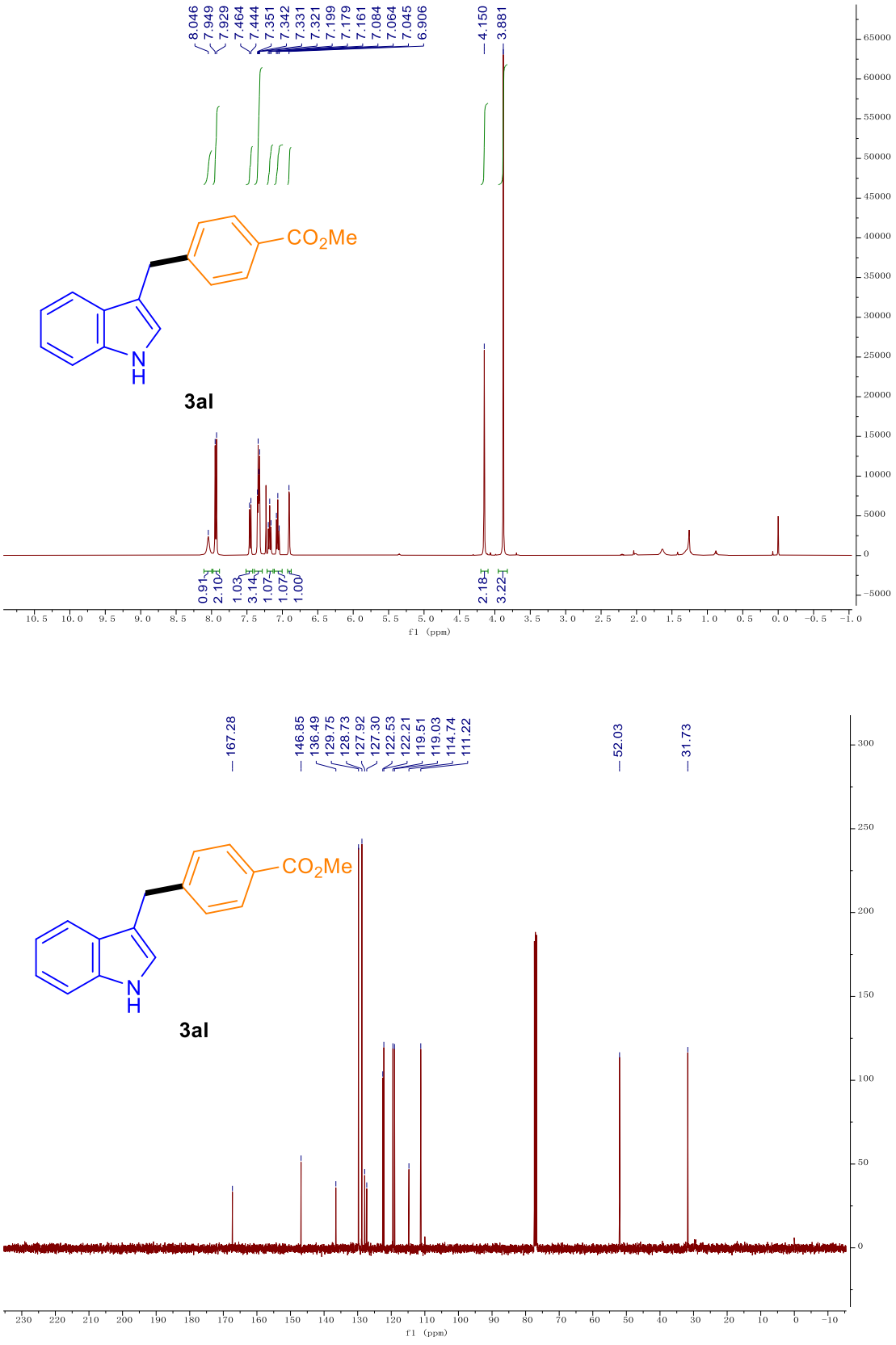


^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3aj** ($CDCl_3$, rt).

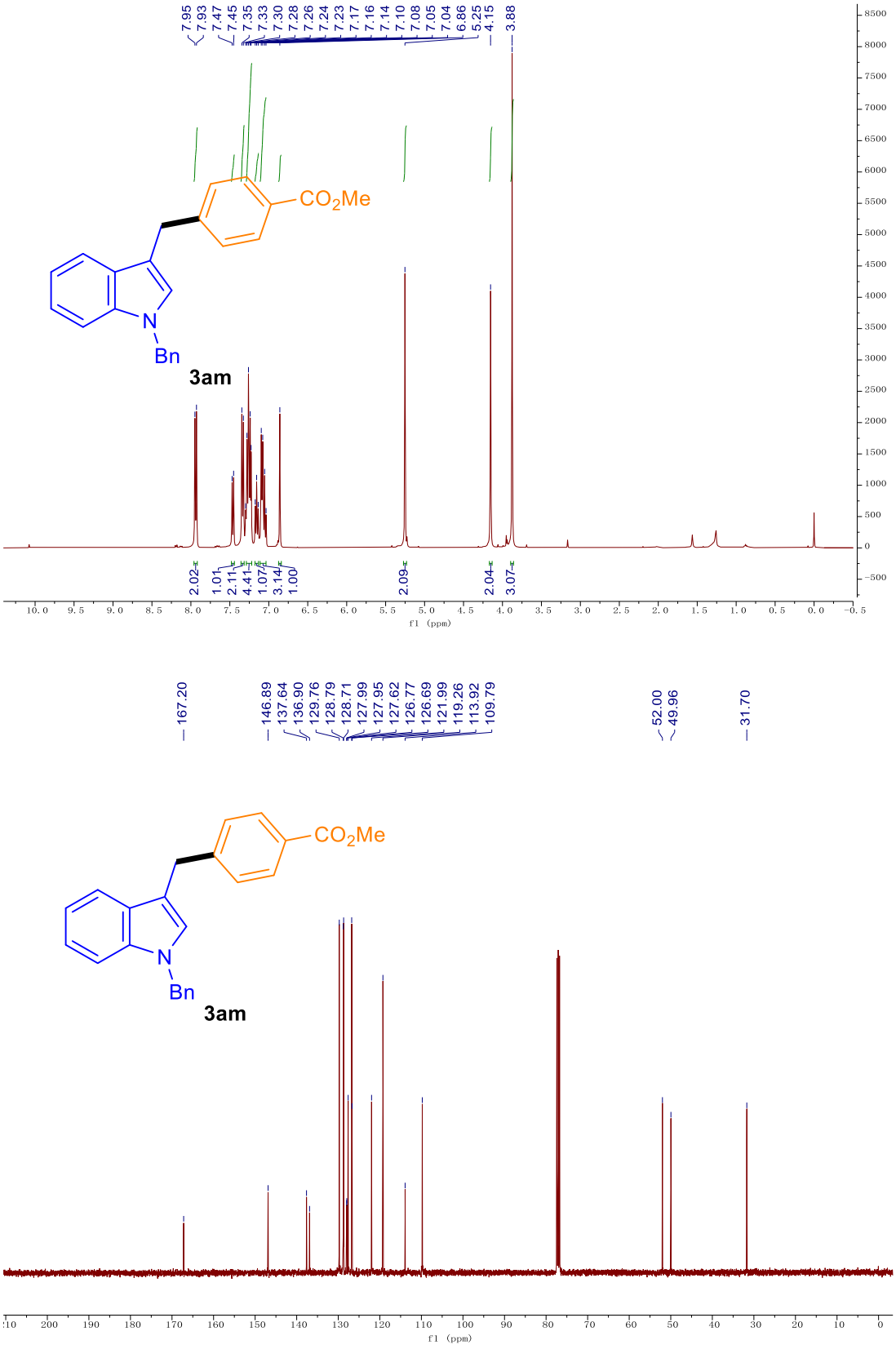




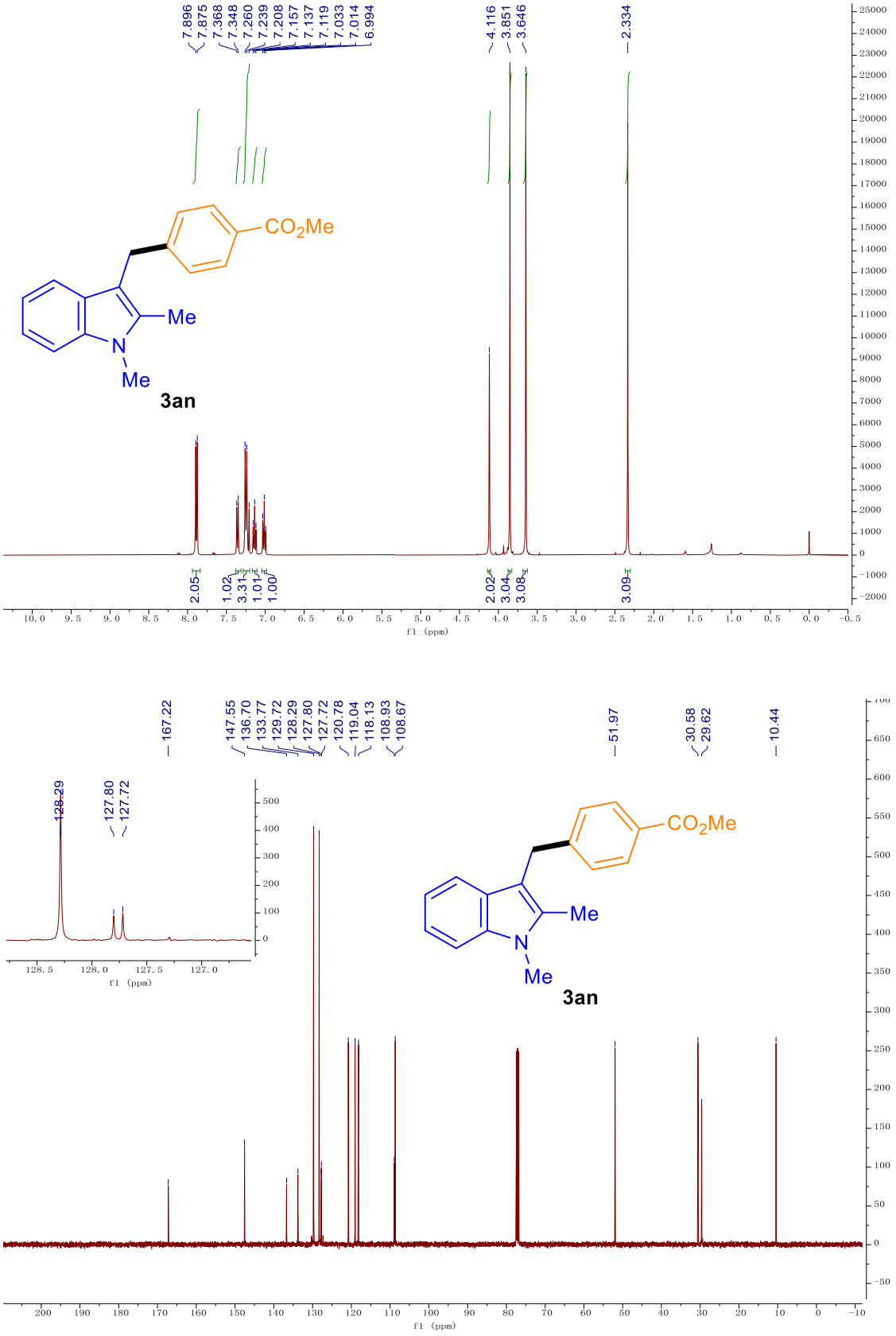
^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3ak** ($CDCl_3$, rt).



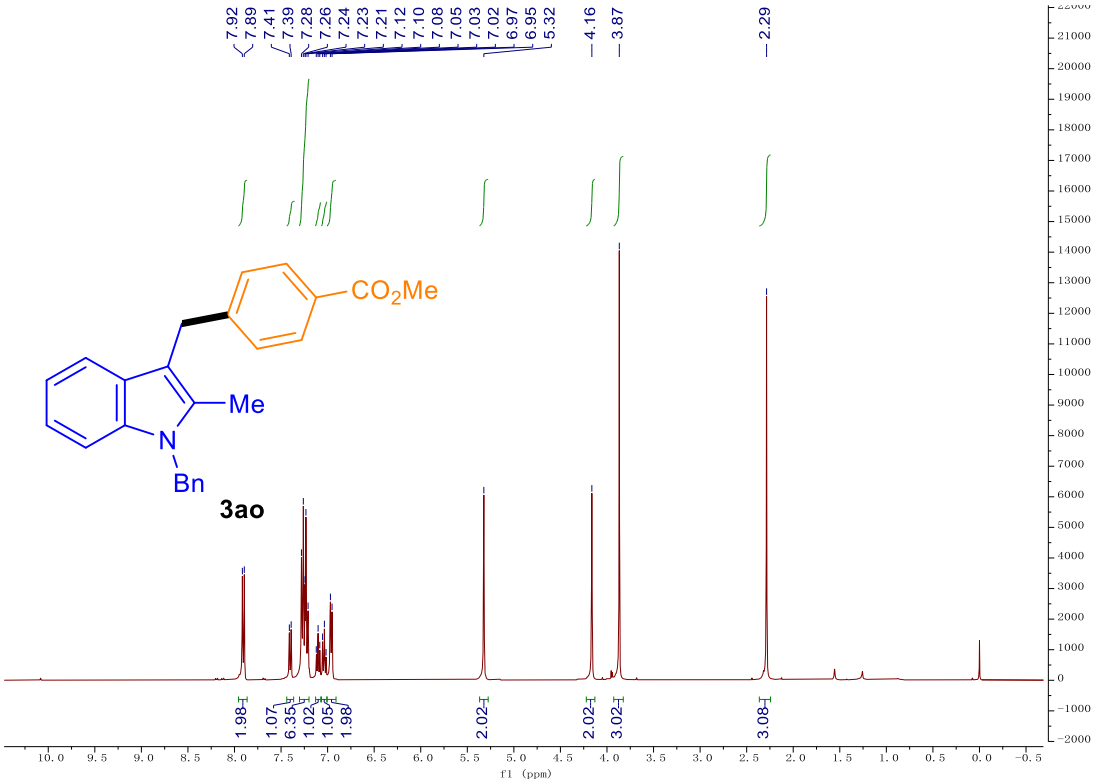
^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3al** ($CDCl_3$, rt).

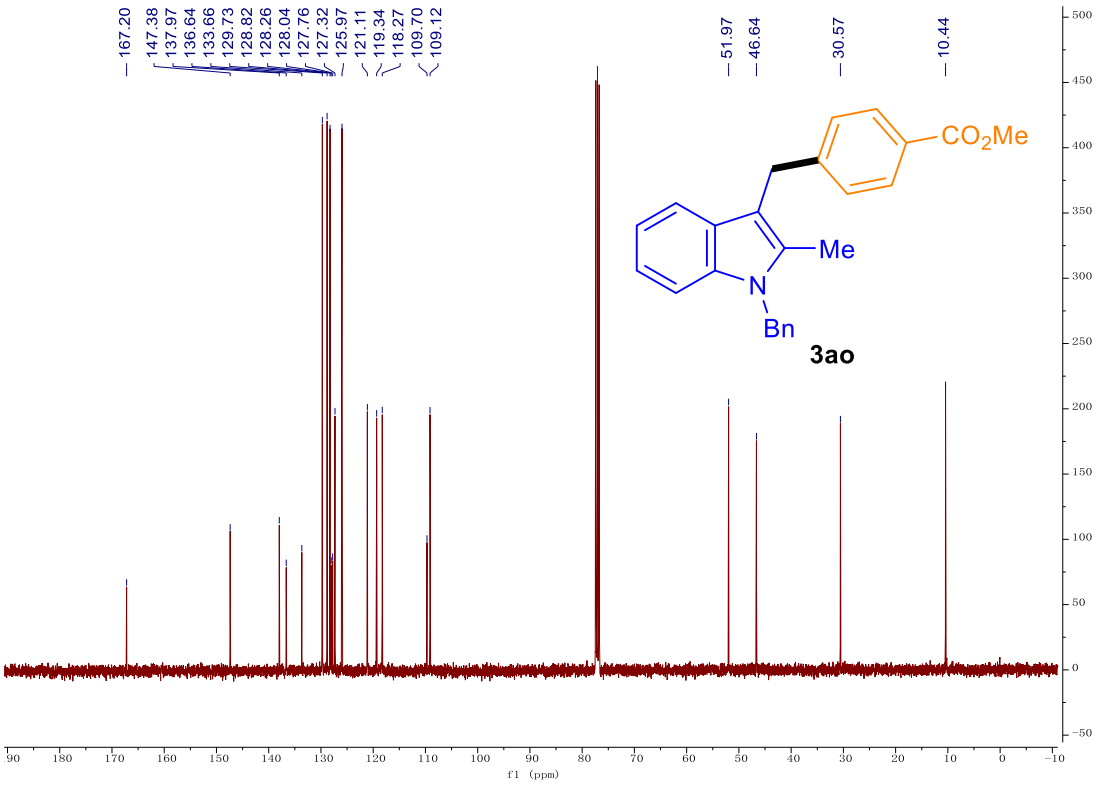


^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3am** ($CDCl_3$, rt).

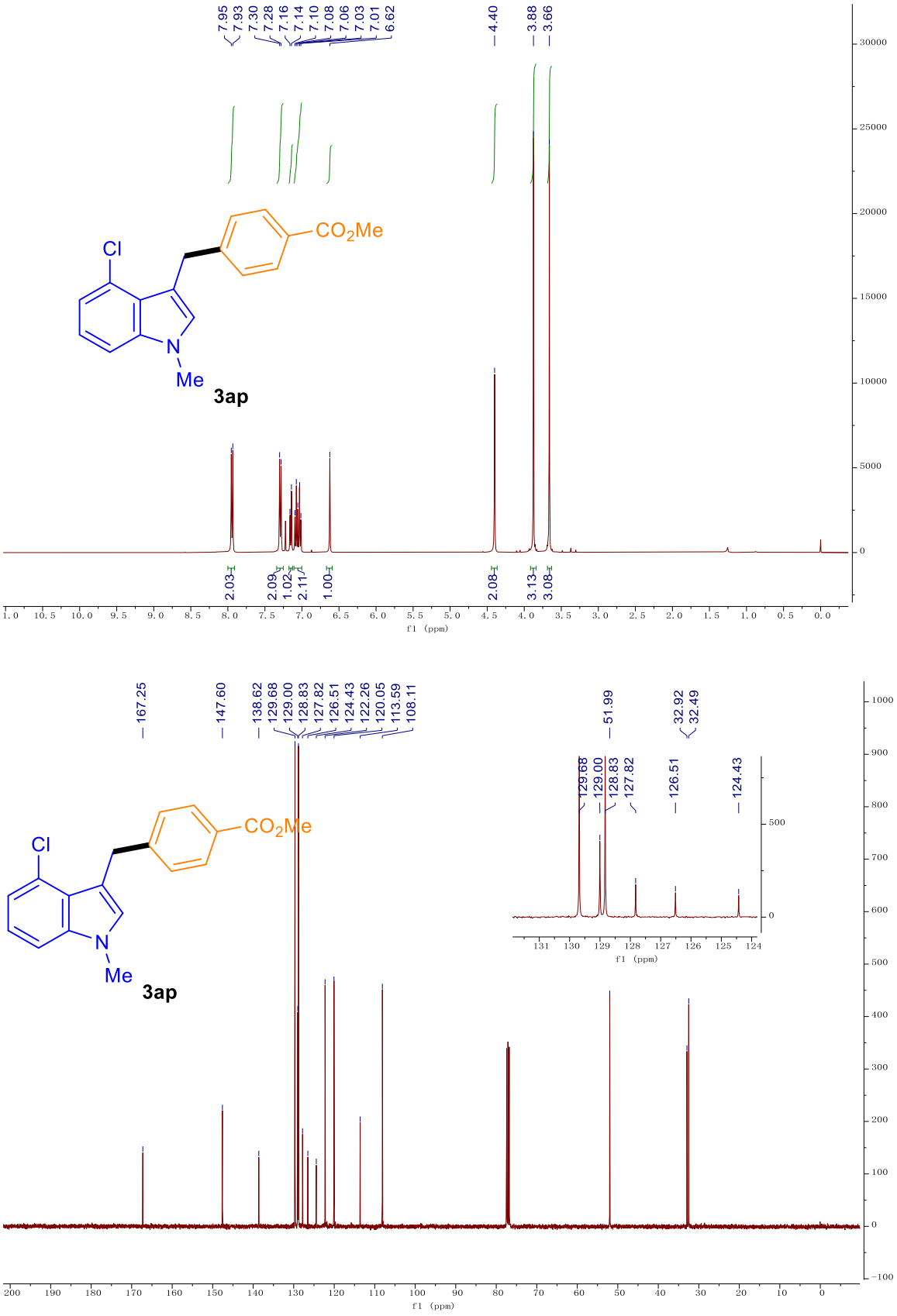


^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3an** ($CDCl_3$, rt).

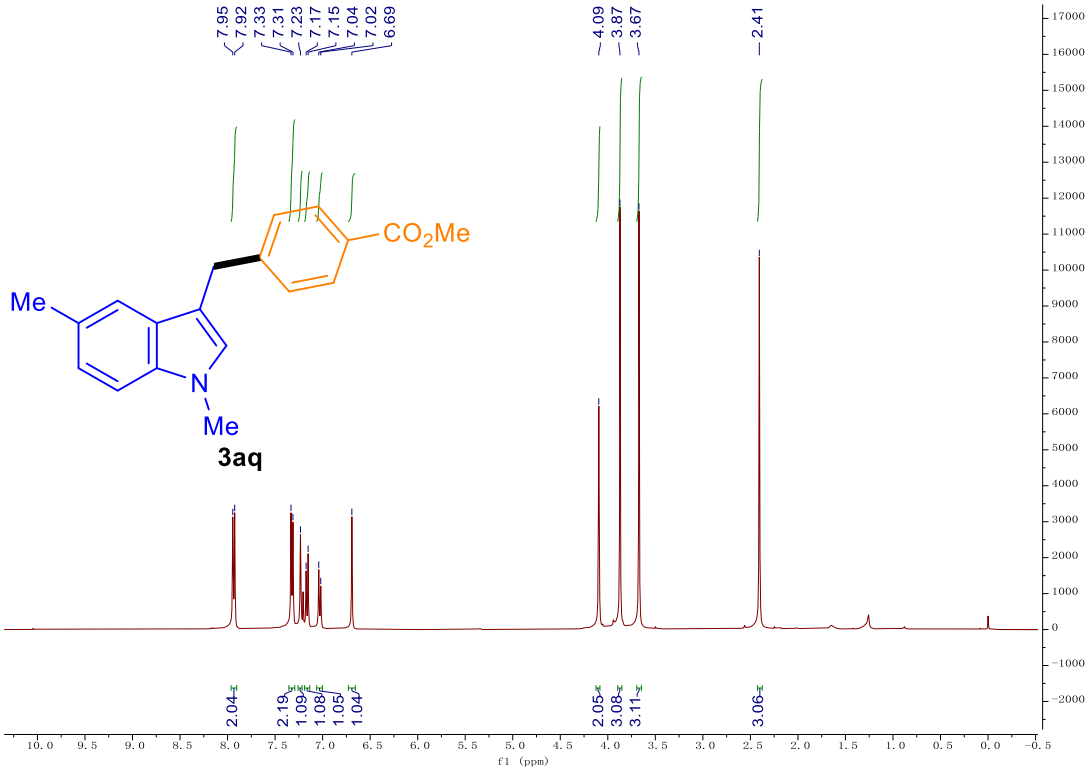


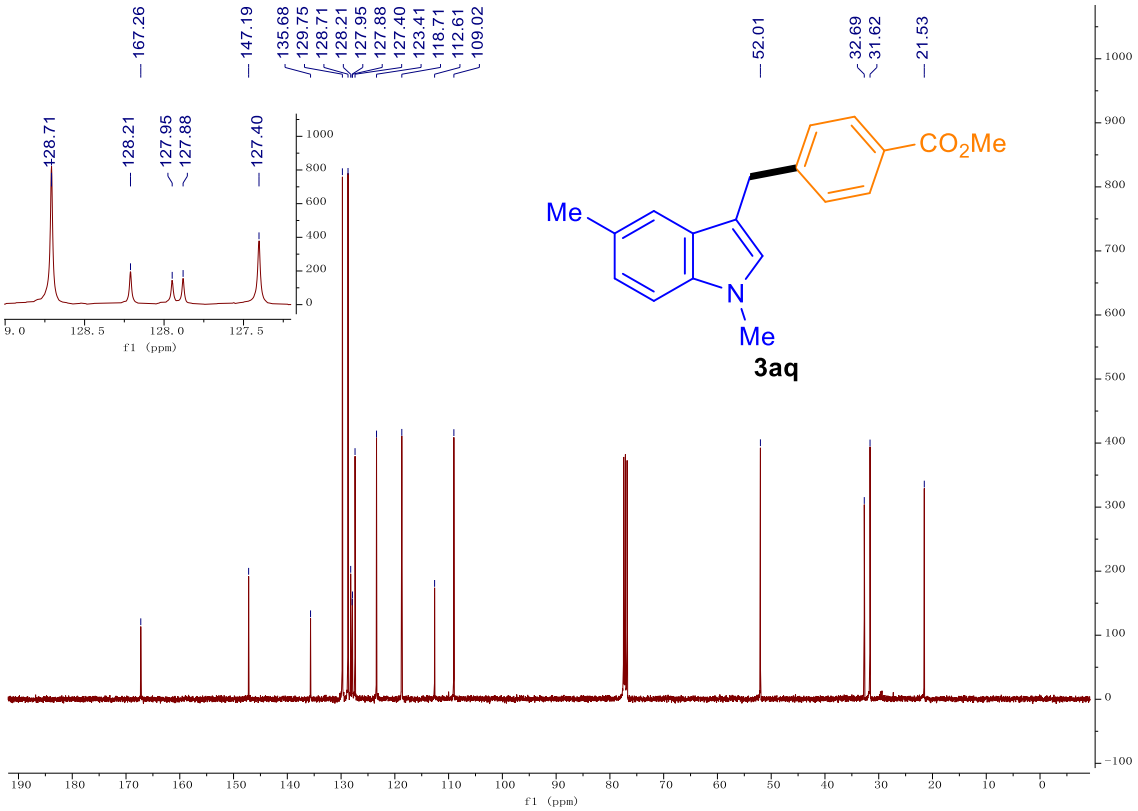


^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3ao** ($CDCl_3$, rt).

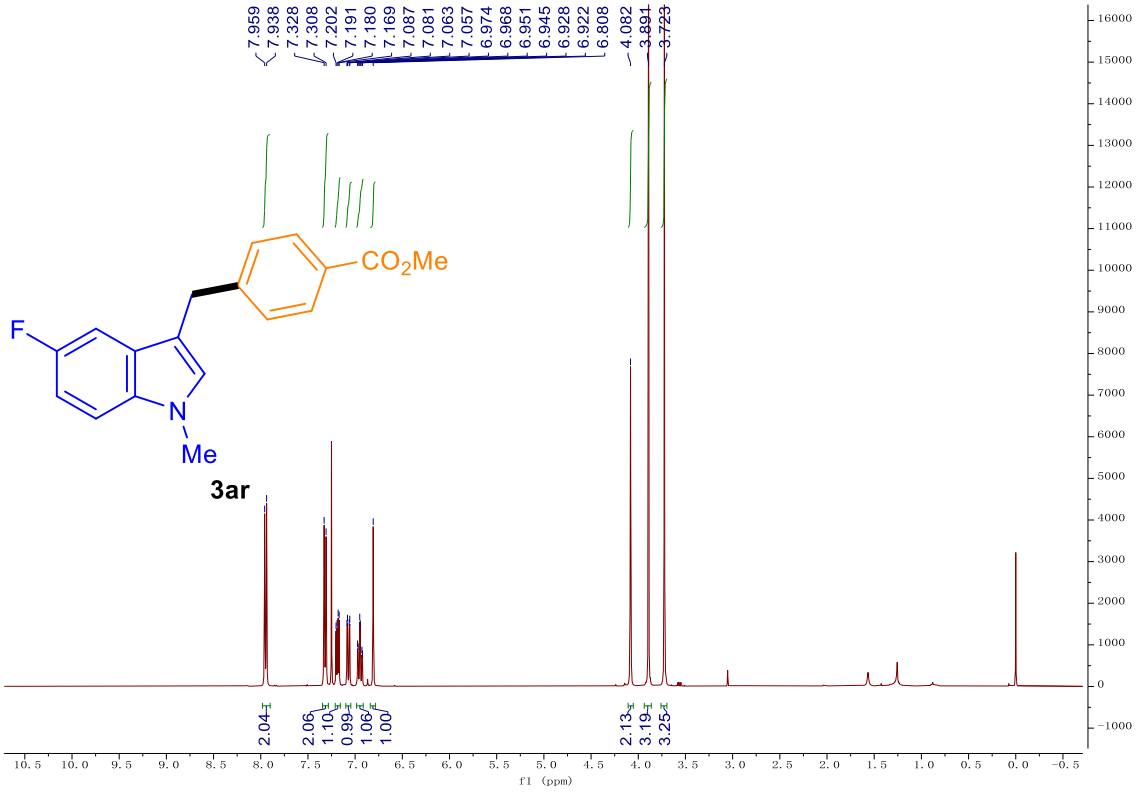


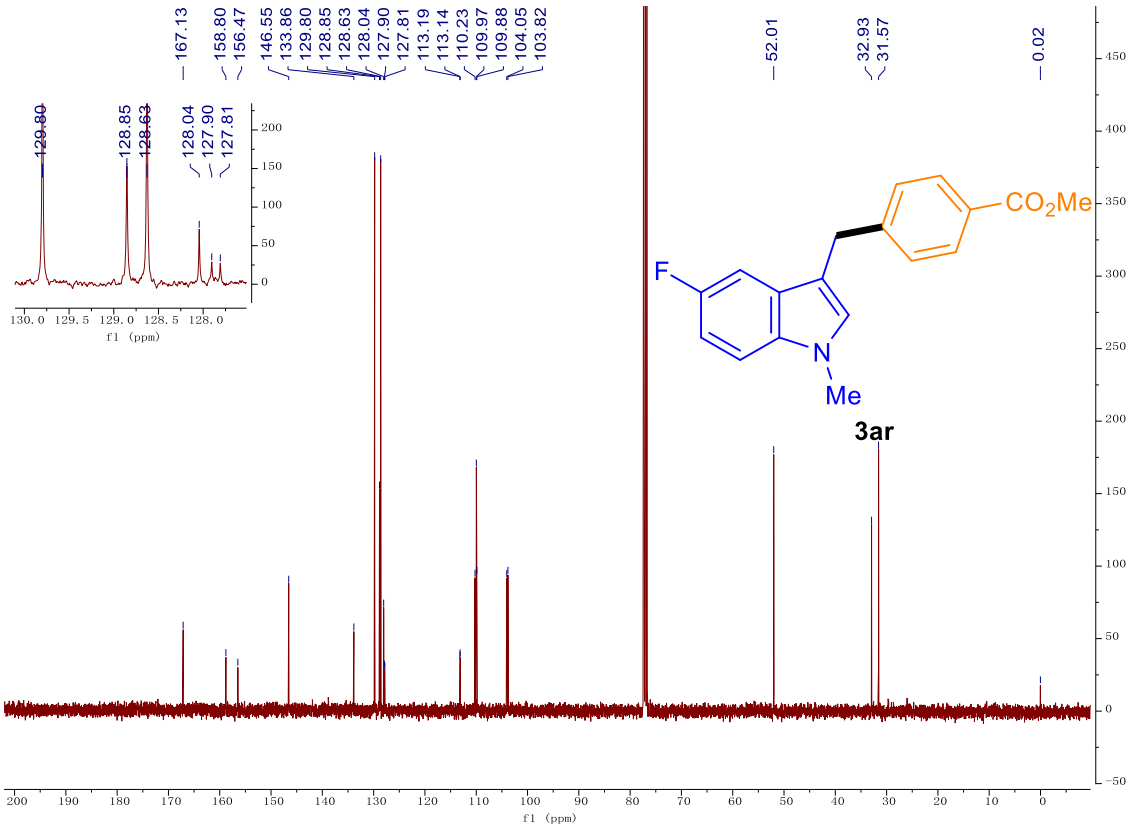
^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3ap** ($CDCl_3$, rt).

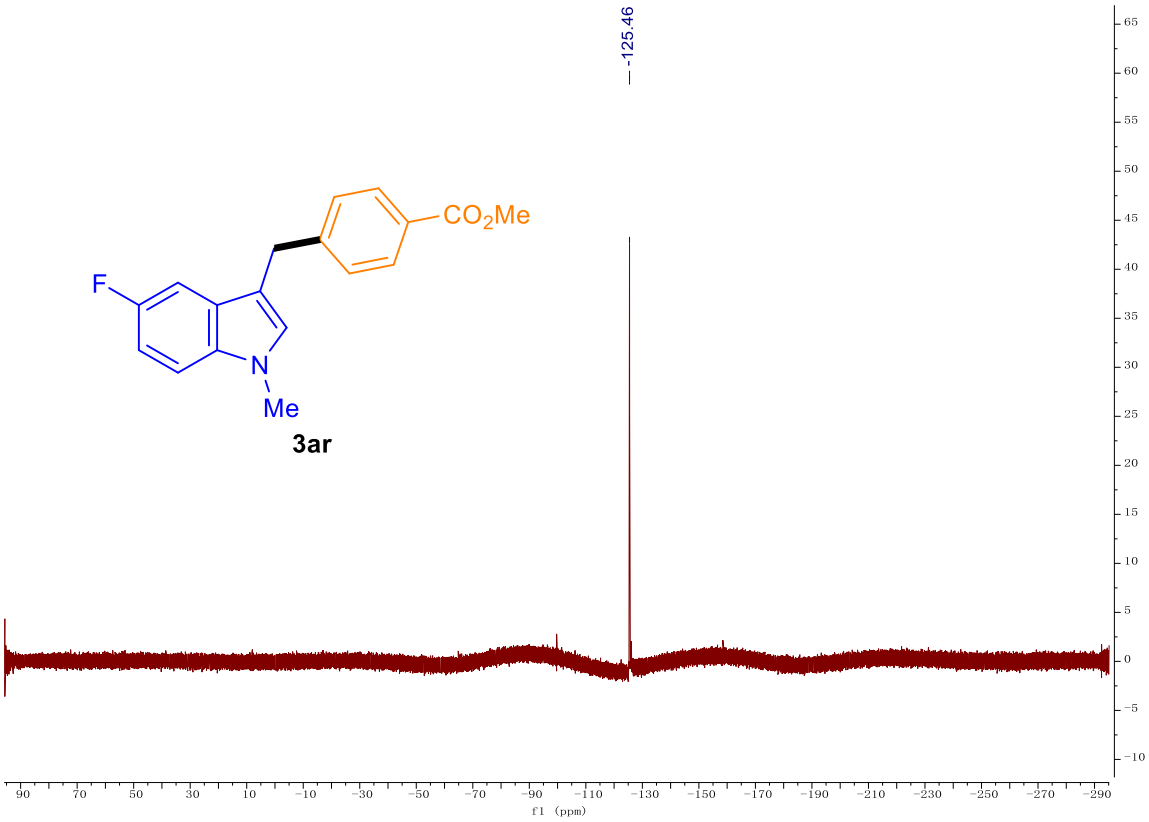




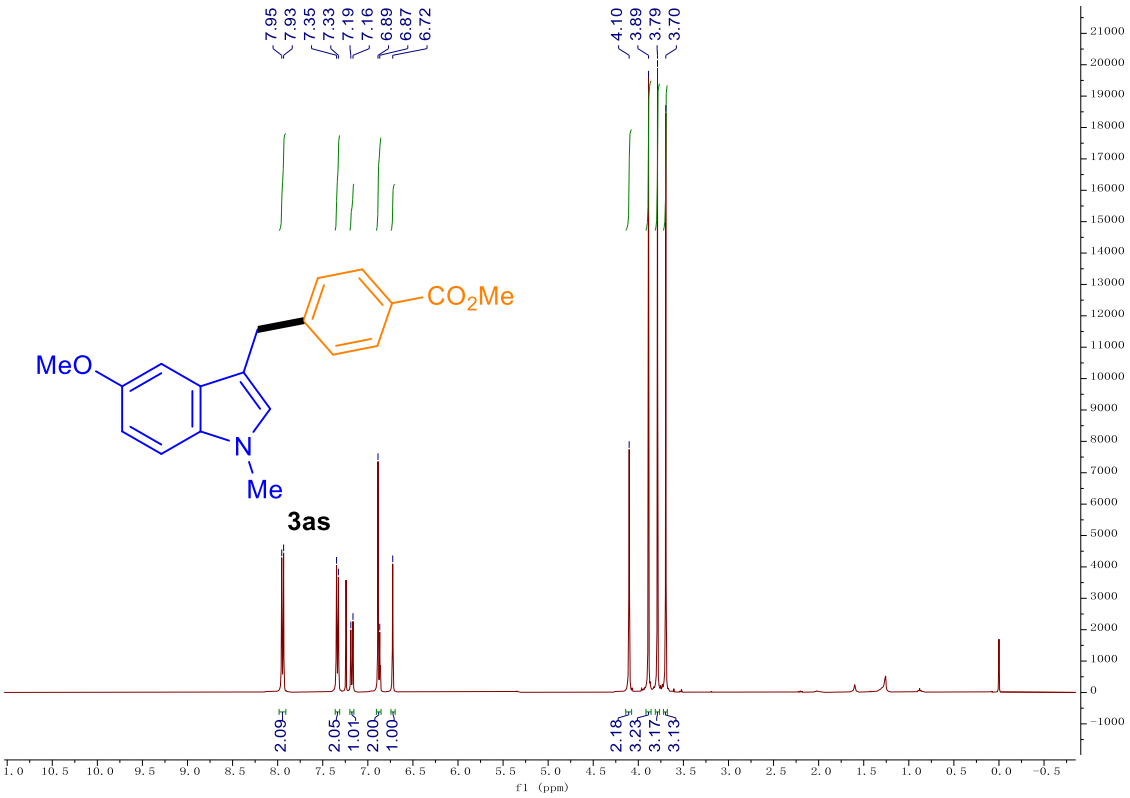
^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3aq** ($CDCl_3$, rt).

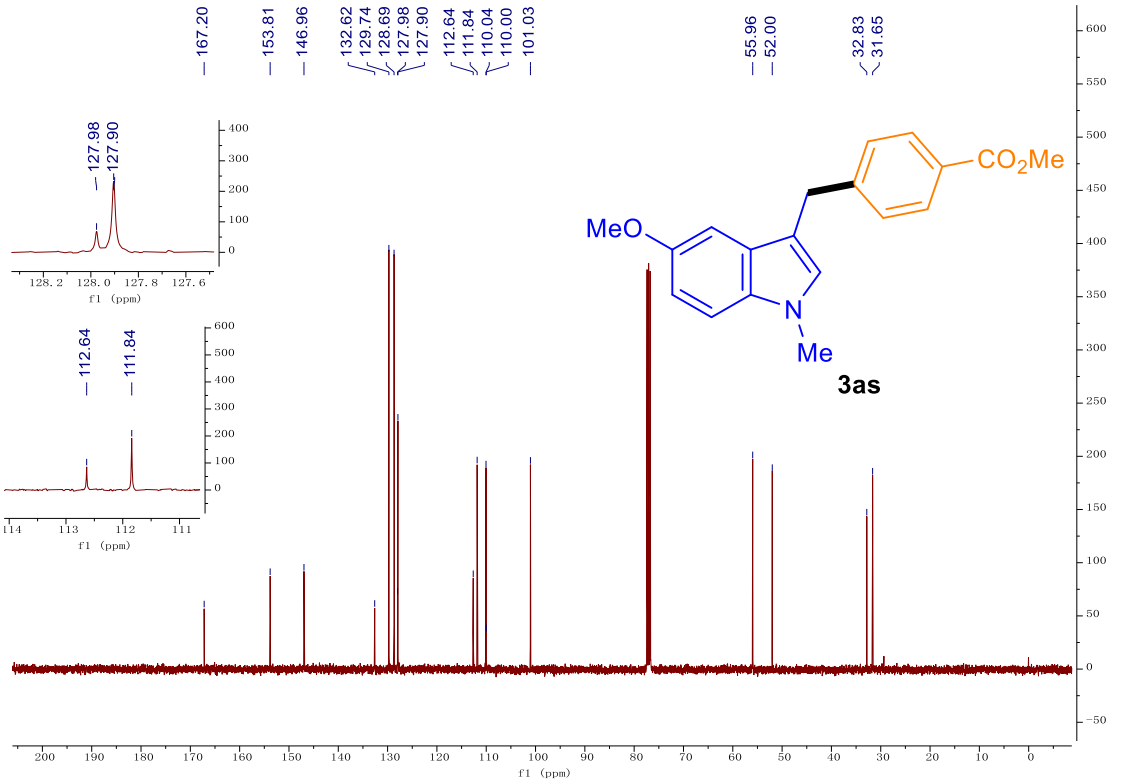

7.959
7.938
7.328
7.308
7.202
7.191
7.180
7.169
7.087
7.081
7.063
7.057
6.974
6.968
6.951
6.945
6.928
6.922
6.808
4.082
3.891
3.723
CO2Me
F
N
Me
3ar
2.04
2.06
1.10
0.99
1.06
1.00
2.13
3.19
3.25
f1 (ppm)


167.13
158.80
156.47
146.55
133.86
129.80
128.85
128.63
128.04
127.90
127.81
113.19
113.14
110.23
109.97
109.88
104.05
103.82
52.01
32.93
31.57
0.02
129.80
128.85
128.63
128.04
127.90
127.81
CO2Me
F
N
Me
3ar
f1 (ppm)

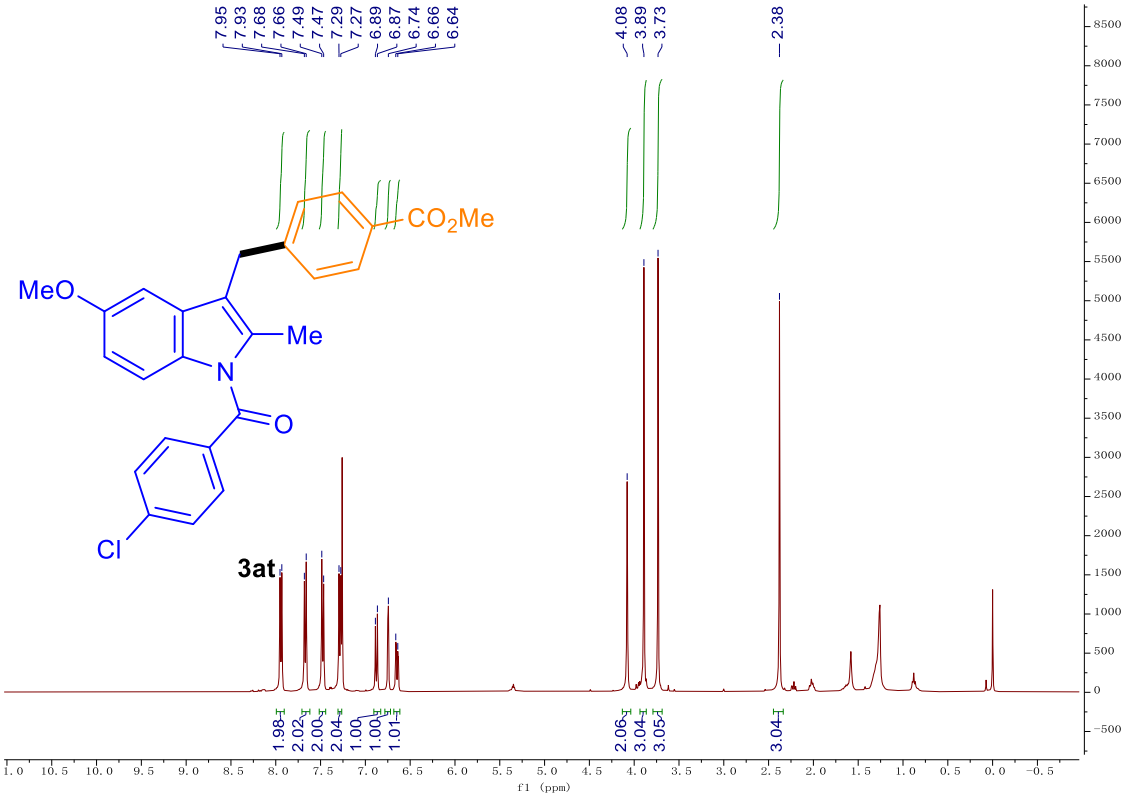


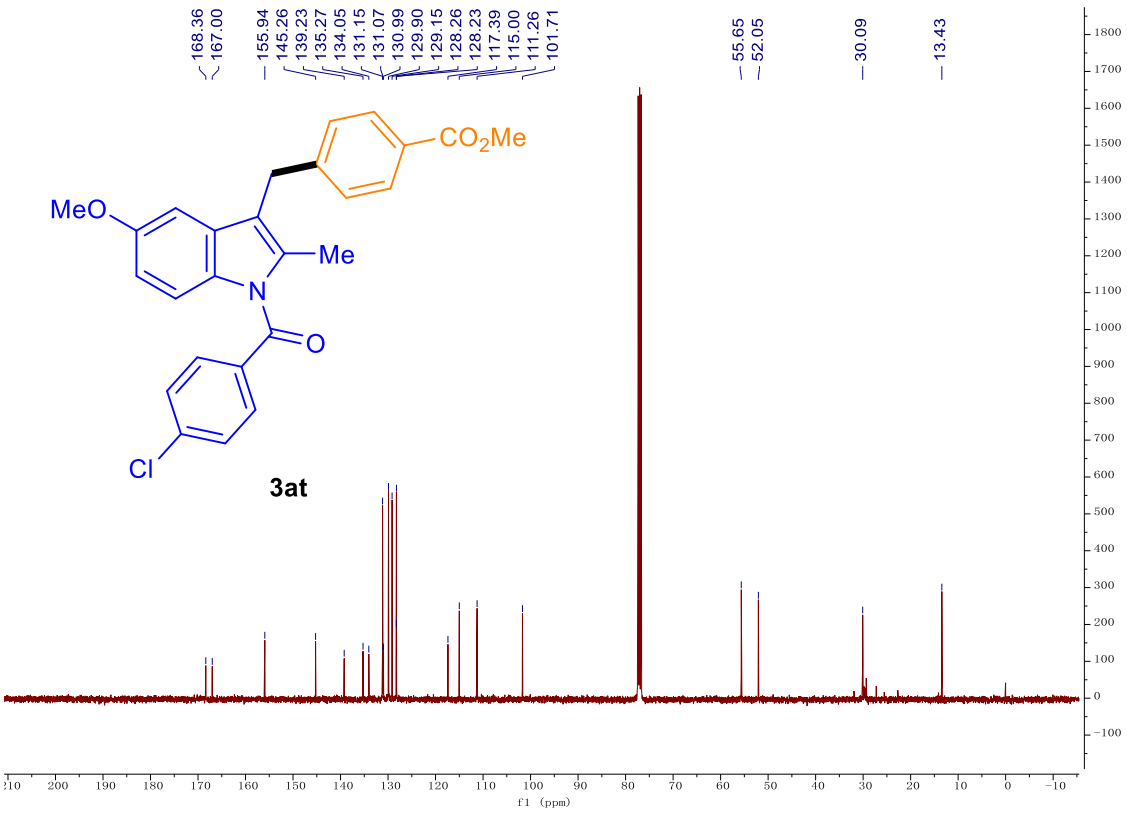
^{1}H NMR (400 MHz), ^{13}C{^{1}H} NMR (100 MHz) and ^{19}F NMR (376 MHz) spectra of **3ar** ($CDCl_3$,





^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3as** ($CDCl_3$, rt).





^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **3at** ($CDCl_3$, rt).