

Electronic Supplementary Information

Sequential Sonogashira/intramolecular aminopalladation/cross-coupling of *ortho*-ethynyl-anilines catalyzed by a single Palladium source: rapid access to 2,3-diarylindoles

Jiwei Wang,^{a,b} Gendi Wang,^b Xiang Cheng,^b Ye Liu,^{*a} and Jun Zhang^{*b}

^aKey Laboratory of Green Chemistry and Chemical Processes, School of Chemistry & Molecular Engineering, East China Normal University, 3663 North Zhongshan Road, Shanghai 200062 (China)

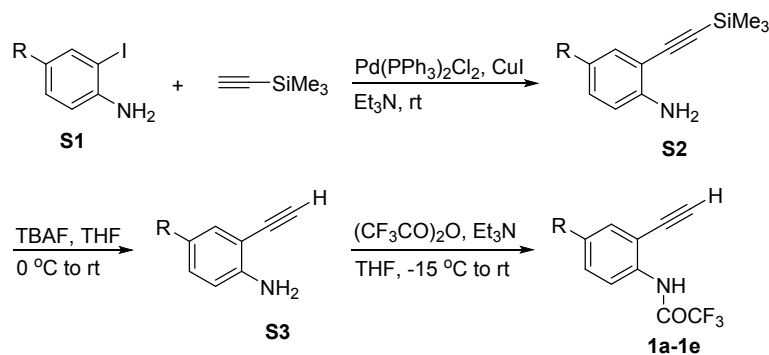
^bKey Laboratory for Advanced Materials and Joint International Research Laboratory of Precision Chemistry and Molecular Engineering, Feringa Nobel Prize Scientist Joint Research Center, School of Chemistry and Molecular Engineering, East China University of Science and Technology, 130 Meilong Road, Shanghai 200237 (China)

General Information:

Unless otherwise stated, all reactions and manipulations were performed using standard Schlenk techniques. All solvents were purified by distillation using standard methods. Commercially available reagents were used without further purification. NMR spectra were recorded by using a Bruker 400 MHz spectrometer. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard (^1H NMR CDCl_3 : 7.26 ppm; ^{13}C NMR CDCl_3 : 77.0 ppm). Mass spectra were recorded on the HP-5989 instrument by EI/ESI methods.

Preparation and characterization

General procedure A for the synthesis of *o*-ethynyltrifluoroacetanilides **1a-1e**:

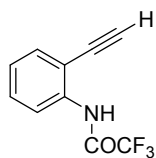


The mixture of **S1** (10 mmol), CuI (95 mg, 0.5 mmol), $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$ (210 mg, 0.3 mmol) under a nitrogen atmosphere was added anhydrous Et_3N (10 mL) and trimethylsilyl acetylene (1.47 g, 15 mmol) in order and the solution was stirred at room temperature. The reaction was monitored by TLC and after completion, then the crude product was purified by silica gel column chromatography (v/v, PE/EtOAc = 200:1) to afford pure **S2** as oil.

The solution of **S2** (5.0 mmol) in THF (20 mL) was added tetrabutylammonium fluoride (1.96 g, 7.5 mmol) at $0\text{ }^\circ\text{C}$, then the mixture was stirred at room temperature for 5 min. The reaction was monitored by TLC and after completion, the reaction mixture was extracted with EtOAc (10 mL \times 3) and washed with brine (10 mL). The combined organic layer was dried over MgSO_4 , and then concentrated in vacuum to afford crude **S3** as oil.

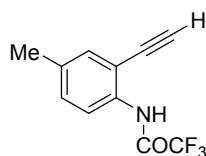
The solution of **S3** (5.0 mmol) in THF (20 mL) was added Et_3N (759 mg, 1.04 mL, 7.5 mmol) at $-15\text{ }^\circ\text{C}$, followed by dropwise addition of trifluoroacetic anhydride (1.26 g, 6.0 mmol). After stirring for 1 h at $-15\text{ }^\circ\text{C}$ and then overnight at room temperature, the mixture was extracted with EtOAc (10 mL \times 3). The combined organic layer was dried over MgSO_4 , then the crude product was purified by silica gel column chromatography (PE) to afford pure **1a-1e** as solid.

***N*-(2-ethynylphenyl)-2,2,2-trifluoroacetamide (1a)**



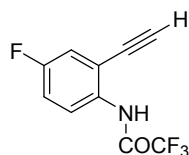
Following the general procedure A, **1a** was purified by silica gel chromatography (v/v, PE/EtOAc = 300:1) as a purple solid (2.0 g, 94 %). ¹H NMR (400 MHz, CDCl₃) δ = 8.75 (brs, 1H), 8.36 (d, *J* = 8.4 Hz, 1H), 7.53 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.46-7.41 (m, 1H), 7.19 (td, *J* = 7.6, 1.2 Hz, 1H), 3.61 (s, 1H). Our data was in full agreement with previous reported in the literature.¹

***N*-(2-ethynyl-4-methylphenyl)-2,2,2-trifluoroacetamide (1b)**



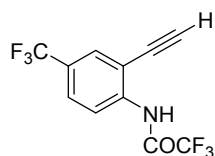
Following the general procedure A, **1b** was purified by silica gel chromatography (v/v, PE/EtOAc = 300:1) as a brown solid (1.63 g, 68 %). ¹H NMR (400 MHz, CDCl₃) δ = 8.67 (brs, 1H), 8.22 (d, *J* = 8.4 Hz, 1H), 7.33 (d, *J* = 1.2 Hz, 1H), 7.24 (d, *J* = 8.4 Hz, 1H), 3.56 (s, 1H), 2.33 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ = 154.3 (q, *J* = 37.1 Hz), 135.3, 134.3, 132.5, 131.0, 119.5, 117.1, 114.2, 112.0, 85.2 (d, *J* = 2.8 Hz), 78.0, 20.6 (d, *J* = 1.6 Hz). ¹⁹F NMR (376 MHz, CDCl₃) δ = -75.9. HRMS (ESI): *m/z* [M-H]⁻ calcd. for C₁₁H₇F₃NO⁻: 226.0480; Found: 226.0480.

***N*-(2-ethynyl-4-fluorophenyl)-2,2,2-trifluoroacetamide (1c)**



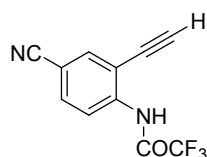
Following the general procedure A, **1c** was purified by silica gel chromatography (v/v, PE/EtOAc = 300:1) as a pale pink solid (1.6 g, 70 %). ¹H NMR (400 MHz, CDCl₃) δ = 8.65 (brs, 1H), 8.34 (dd, *J* = 9.2, 4.8 Hz, 1H), 7.23 (dd, *J* = 8.4, 2.8 Hz, 1H), 7.15 (ddd, *J* = 9.6, 7.6, 3.2 Hz, 1H), 3.65 (s, 1H). ¹³C NMR (100 MHz, CDCl₃) δ = 160.4, 157.9, 154.5 (q, *J* = 37.5 Hz), 133.2 (d, *J* = 2.9 Hz), 121.6 (d, *J* = 8.4 Hz), 118.9 (d, *J* = 24.6 Hz), 117.6 (d, *J* = 22.3 Hz), 117.0, 114.1, 113.9 (d, *J* = 9.5 Hz), 86.6 (d, *J* = 3.2 Hz). ¹⁹F NMR (376 MHz, CDCl₃) δ = -75.9, -115.0. HRMS (ESI): *m/z* [M-H]⁻ calcd. for C₁₀H₄F₄NO⁻: 230.0229; Found: 230.0224.

***N*-(2-ethynyl-4-(trifluoromethyl)phenyl)-2,2,2-trifluoroacetamide (1d)**



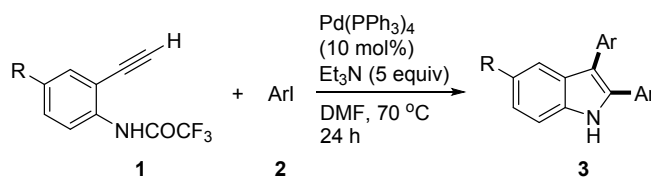
Following the general procedure A, **1d** was purified by silica gel chromatography (PE) as a brown solid (2.2 g, 78 %). ^1H NMR (400 MHz, CDCl_3) δ = 8.84 (brs, 1H), 8.53 (d, J = 8.8 Hz, 1H), 7.79 (s, 1H), 7.69 (dd, J = 8.8, 1.6 Hz, 1H), 3.71 (s, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ = 154.9 (q, J = 37.9 Hz), 139.5, 129.4 (q, J = 3.8 Hz), 127.8, 127.4, 127.3 (q, J = 3.7 Hz), 124.5, 121.8, 119.7, 116.8, 113.9, 112.6, 87.3 (d, J = 3.6 Hz), 76.5. ^{19}F NMR (376 MHz, CDCl_3) δ = -62.7 (d, J = 2.6 Hz), -75.9 (d, J = 3.4 Hz). HRMS (ESI): m/z $[\text{M}-\text{H}]^-$ calcd. for $\text{C}_{11}\text{H}_4\text{F}_6\text{NO}^-$: 280.0197; Found: 280.0178.

***N*-(4-cyano-2-ethynylphenyl)-2,2,2-trifluoroacetamide (1e)**



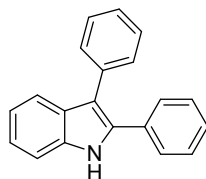
Following the general procedure A, **1e** was purified by silica gel chromatography (v/v, PE/EtOAc = 100:1) as a white solid (0.85 g, 60 %). ^1H NMR (400 MHz, CDCl_3) δ = 8.86 (brs, 1H), 8.55 (d, J = 8.8 Hz, 1H), 7.82 (d, J = 2 Hz, 1H), 7.72 (dd, J = 8.8, 1.6 Hz, 1H), 3.75 (s, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ = 154.8 (q, J = 38.1 Hz), 140.1, 135.8, 134.0, 119.9, 117.2, 113.1, 109.3, 88.1 (d, J = 3.8 Hz), 75.7, 29.6. ^{19}F NMR (376 MHz, CDCl_3) δ = -75.8. HRMS (ESI): m/z $[\text{M}-\text{H}]^-$ calcd. for $\text{C}_{11}\text{H}_4\text{F}_3\text{N}_2\text{O}^-$: 237.0276; Found 237.0275.

General procedure B for the synthesis of 2,3-diaryl indoles 3a-3u:



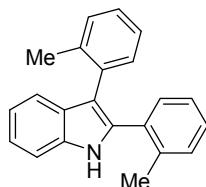
A nitrogen-filled round-bottom flask was charged with **1** (0.47 mmol), $\text{Pd}(\text{PPh}_3)_4$ (54 mg, 0.047 mmol) and anhydrous DMF (3 mL), and then Et_3N (238 mg, 0.33 mL, 2.35 mmol) and aryl iodides **2** (2.35 mmol) were added in order. After the solution was stirred at 70 °C for 24 h, the reaction was quenched with water (3 mL) and the aqueous layer was extracted with DCM (10 mL \times 3). The combined organic layer was dried over MgSO_4 , the volatile was removed under vacuum, and then the resulting residue was purified by silica gel column chromatography (PE/EtOAc) to afford pure product **3a-3u**.

2,3-diphenyl-1H-indole (3a)



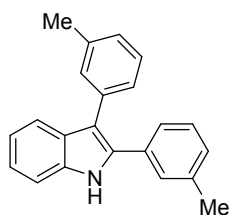
Following the general procedure B, **3a** was purified by silica gel chromatography (v/v, PE/EtOAc = 300:1) as a pale yellow solid (115 mg, 91 %). ¹H NMR (400 MHz, CDCl₃) δ = 8.24 (brs, 1H), 7.71 (d, J = 8.0 Hz, 1H), 7.48-7.37 (m, 7H), 7.37-7.30 (m, 4H), 7.29-7.24 (m, 1H), 7.20-7.15 (m, 1H). Our data was in full agreement with previous reported in the literature.²

2,3-di-*o*-tolyl-1H-indole (3b)



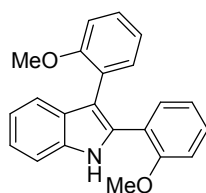
Following the general procedure B, **3b** was purified by silica gel chromatography (v/v, PE/EtOAc = 300:1) as a pale yellow solid (94 mg, 67 %). ¹H NMR (400 MHz, CDCl₃) δ = 8.15 (brs, 1H), 7.48-7.44 (m, 2H), 7.29 (d, J = 8.0 Hz, 2H), 7.25-7.13 (m, 8H), 2.14 (s, 3H), 2.08 (s, 3H). Our data was in full agreement with previous reported in the literature.²

2,3-di-*m*-tolyl-1H-indole (3c)



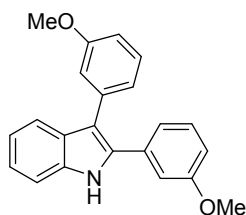
Following the general procedure B, **3c** was purified by silica gel chromatography (v/v, PE/EtOAc = 300:1) as a pale yellow solid (118 mg, 85 %). ¹H NMR (400 MHz, CDCl₃) δ = 8.24 (brs, 1H), 7.72 (d, J = 8.0 Hz, 1H), 7.50-7.38 (m, 2H), 7.35-7.26 (m, 3H), 7.25-7.21 (m, 6H), 2.39 (s, 3H), 2.35 (s, 3H). Our data was in full agreement with previous reported in the literature.³

2,3-bis(2-methoxyphenyl)-1H-indole (3d)



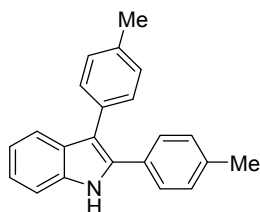
Following the general procedure B, **3d** was purified by silica gel chromatography (v/v, PE/EtOAc = 300:1) as a pale yellow solid (54 mg, 35 %). ^1H NMR (400 MHz, CDCl_3) δ = 9.19 (s, 1H), 7.50 (d, J = 8.0 Hz, 1H), 7.43 (d, J = 8.4 Hz, 1H), 7.37-7.29 (m, 2H), 7.25-7.19 (m, 3H), 7.12-7.07 (m, 1H), 7.02-6.95 (m, 3H), 6.78 (td, J = 7.6, 0.8 Hz, 1H), 3.90 (s, 3H), 3.57 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ = 157.3, 156.2, 135.3, 132.4, 132.0, 130.8, 128.5, 128.2, 127.9, 124.8, 122.0, 121.7, 120.7, 120.6, 119.9, 119.5, 111.6, 111.4, 111.2, 110.7, 55.7 (d, J = 4.5 Hz), 55.1 (d, J = 3.2 Hz). HRMS (ESI): m/z $[\text{M}+\text{H}]^+$ calcd. for $\text{C}_{22}\text{H}_{20}\text{NO}_2^+$: 330.1494; Found 330.1488.

2,3-bis(3-methoxyphenyl)-1H-indole (**3e**)



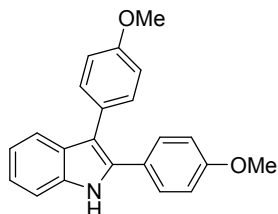
Following the general procedure B, **3e** was purified by silica gel chromatography (v/v, PE/EtOAc = 300:1) as a pale yellow solid (106 mg, 69 %). ^1H NMR (400 MHz, CDCl_3) δ = 8.27 (brs, 1H), 7.70 (d, J = 8.0 Hz, 1H), 7.44 (d, J = 8.0 Hz, 1H), 7.32-7.27 (m, 1H), 7.26-7.23 (m, 2H), 7.18-7.13 (m, 1H), 7.06-7.00 (m, 3H), 6.99-6.95 (m, 1H), 6.87-6.82 (m, 2H), 3.76 (s, 3H), 3.68 (s, 3H). Our data was in full agreement with previous reported in the literature.³

2,3-di-*p*-tolyl-1H-indole (**3f**)



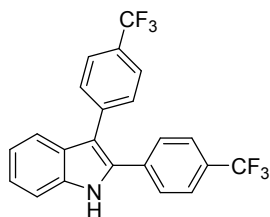
Following the general procedure B, **3f** was purified by silica gel chromatography (v/v, PE/EtOAc = 300:1) as a pale yellow solid (106 mg, 59 %). ^1H NMR (400 MHz, CDCl_3) δ = 8.19 (s, 1H), 7.67 (d, J = 7.6 Hz, 1H), 7.47-7.39 (m, 2H), 7.37-7.30 (m, 4H), 7.22-7.12 (m, 5H), 2.40 (s, 3H), 2.36 (s, 3H). Our data was in full agreement with previous reported in the literature.³

2,3-bis(4-methoxyphenyl)-1H-indole (3g)



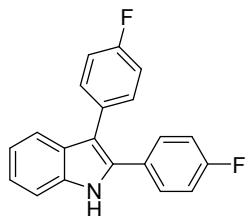
Following the general procedure B, **3g** was purified by silica gel chromatography (v/v, PE/EtOAc = 300:1) as a pale yellow solid (76 mg, 50 %). ^1H NMR (400 MHz, CDCl_3) δ = 8.18 (brs, 1H), 7.65 (d, J = 8.0 Hz, 1H), 7.42-7.34 (m, 5H), 7.23 (t, J = 7.4 Hz, 1H), 7.15 (t, J = 7.4 Hz, 1H), 6.95 (d, J = 8.0 Hz, 2H), 6.87 (d, J = 8.8 Hz, 2H), 3.86 (s, 3H), 3.82 (s, 3H). Our data was in full agreement with previous reported in the literature.³

2,3-bis(4-(trifluoromethyl)phenyl)-1H-indole (3h)



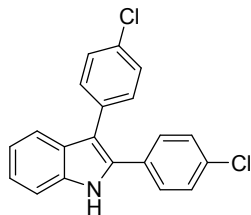
Following the general procedure B and the reaction was reacted for 48 h, **3g** was purified by silica gel chromatography (v/v, PE/EtOAc = 200:1) as a pale yellow solid (165 mg, 87%). ^1H NMR (400 MHz, CDCl_3) δ = 8.40 (brs, 1H), 7.69-7.60 (m, 5H), 7.55-7.47 (m, 5H), 7.34-7.29 (m, 1H), 7.23-7.19 (m, 1H). Our data was in full agreement with previous reported in the literature.⁴

2,3-bis(4-fluorophenyl)-1H-indole (3i)



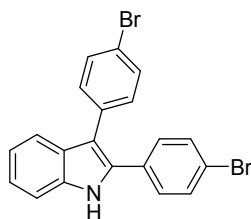
Following the general procedure B, **3i** was purified by silica gel chromatography (v/v, PE/EtOAc = 300:1) as a pale yellow solid (106 mg, 74 %). ^1H NMR (400 MHz, CDCl_3) δ = 8.20 (brs, 1H), 7.63 (d, J = 8.0 Hz, 1H), 7.44 (d, J = 8.0 Hz, 1H), 7.40-7.34 (m, 4H), 7.29-7.24 (m, 1H), 7.19-7.15 (m, 1H), 7.12-7.01 (m, 4H). Our data was in full agreement with previous reported in the literature.³

2,3-bis(4-chlorophenyl)-1H-indole (3j)



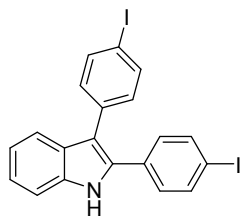
Following the general procedure B, **3j** was purified by silica gel chromatography (v/v, PE/EtOAc = 300:1) as a white solid (93 mg, 59 %). ¹H NMR (400 MHz, CDCl₃) δ = 8.24 (brs, 1H), 7.63 (d, J = 8.0 Hz, 1H), 7.44 (d, J = 8.4 Hz, 1H), 7.35 (dd, J = 9.4, 1.4 Hz, 8H), 7.29-7.25 (m, 1H), 7.17 (t, J = 7.4 Hz, 1H). Our data was in full agreement with previous reported in the literature.³

2,3-bis(4-bromophenyl)-1H-indole (3k)



Following the general procedure B, **3k** was purified by silica gel chromatography (v/v, PE/EtOAc = 300:1) as a white solid (116 mg, 58 %). ¹H NMR (400 MHz, CDCl₃) δ = 8.25 (brs, 1H), 7.63 (d, J = 8.0 Hz, 1H), 7.49 (dd, J = 13.6, 8.4 Hz, 4H), 7.44 (d, J = 8.0 Hz, 1H), 7.30-7.26 (m, 5H), 7.20-7.15 (m, 1H). Our data was in full agreement with previous reported in the literature.⁵

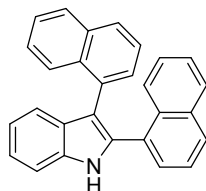
2,3-bis(4-iodophenyl)-1H-indole (3l)



Following the general procedure B, **3l** was purified by silica gel chromatography (v/v, PE/EtOAc = 300:1) as a pale yellow solid (102 mg, 42 %). ¹H NMR (400 MHz, CDCl₃) δ = 8.26 (brs, 1H), 7.73-7.65 (m, 4H), 7.63 (d, J = 8.0 Hz, 1H), 7.43 (d, J = 8.0 Hz, 1H), 7.29-7.24 (m, 1H), 7.20-7.12 (m, 5H). ¹³C NMR (100 MHz, CDCl₃) δ = 137.8, 137.7, 135.9, 134.3, 133.1, 131.8, 131.7, 129.7, 128.1, 123.2, 120.7, 119.4, 114.2, 111.1, 93.6, 91.8, 65.8. HRMS (ESI):

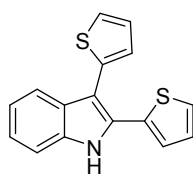
m/z [M+H]⁺ calcd. for C₂₀H₁₄I₂N⁺: 521.9216; Found: 521.9202.

2,3-di(naphthalen-1-yl)-1H-indole (3m)



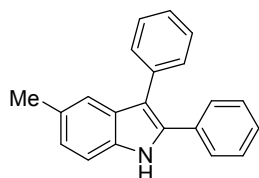
Following the general procedure B, **3m** was purified by silica gel chromatography (v/v, PE/EtOAc = 300:1) as a pale yellow solid (55 mg, 32%). ¹H NMR (400 MHz, CDCl₃) δ = 8.44 (brs, 1H), 8.06 (d, *J* = 8.4 Hz, 1H), 8.00 (d, *J* = 8.4 Hz, 1H), 7.84 (dd, *J* = 8.0, 5.6 Hz, 2H), 7.76 (d, *J* = 8.4 Hz, 1H), 7.72 (dd, *J* = 7.2, 1.6 Hz, 1H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.47-7.41 (m, 2H), 7.39-7.28 (m, 7H), 7.27-7.24 (m, 1H), 7.15 (t, *J* = 7.6 Hz, 1H). Our data was in full agreement with previous reported in the literature.²

2,3-di(thiophen-2-yl)-1H-indole (3n)



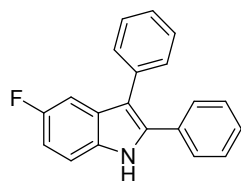
Following the general procedure B, **3n** was purified by silica gel chromatography (v/v, PE/EtOAc = 200:1) as a pale yellow solid (85 mg, 65%). ¹H NMR (400 MHz, CDCl₃) δ = 8.27 (brs, 1H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.42-7.38 (m, 2H), 7.31 (dd, *J* = 5.2, 1.2 Hz, 1H), 7.29-7.24 (m, 1H), 7.23-7.19 (m, 2H), 7.19-7.15 (m, 2H), 7.05 (dd, *J* = 4.8, 3.6 Hz, 1H). Our data was in full agreement with previous reported in the literature.⁶

5-methyl-2,3-diphenyl-1H-indole (3o)



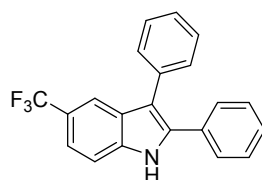
Following the general procedure B, **3o** was purified by silica gel chromatography (v/v, PE/EtOAc = 200:1) as a pale yellow solid (105 mg, 84%). ¹H NMR (400 MHz, CDCl₃) δ = 8.14 (brs, 1H), 7.48-7.38 (m, 7H), 7.35-7.28 (m, 5H), 7.09 (d, *J* = 8.0 Hz, 1H), 2.46 (s, 3H). Our data was in full agreement with previous reported in the literature.³

5-fluoro-2,3-diphenyl-1H-indole (3p)



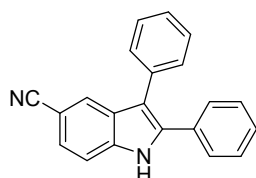
Following the general procedure B, **3p** was purified by silica gel chromatography (v/v, PE/EtOAc = 200:1) as a pale yellow solid (90 mg, 72%). ¹H NMR (400 MHz, CDCl₃) δ = 8.21 (brs, 1H), 7.44-7.38 (m, 6H), 7.37-7.30 (m, 6H), 7.00 (td, J = 9.2, 2.4 Hz, 1H). Our data was in full agreement with previous reported in the literature.³

2,3-diphenyl-5-(trifluoromethyl)-1H-indole (3q)



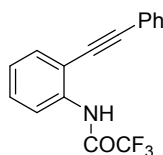
Following the general procedure B, **3q** was purified by silica gel chromatography (v/v, PE/EtOAc = 400:1) as a pale yellow solid (60 mg, 50%). ¹H NMR (400 MHz, CDCl₃) δ = 8.46 (brs, 1H), 7.94 (s, 1H), 7.53-7.46 (m, 2H), 7.45-7.40 (m, 6H), 7.38-7.32 (m, 4H). Our data was in full agreement with previous reported in the literature.⁷

2,3-diphenyl-1H-indole-5-carbonitrile (3r)



Following the general procedure B, **3r** was purified by silica gel chromatography (v/v, PE/EtOAc = 100:1) as a pale yellow solid (40 mg, 32%). ¹H NMR (400 MHz, CDCl₃) δ = 8.47 (brs, 1H), 7.94 (s, 1H), 7.53-7.46 (m, 2H), 7.45-7.40 (m, 6H), 7.38-7.31 (m, 4H). Our data was in full agreement with previous reported in the literature.³

The synthesis of internal alkyne 4a



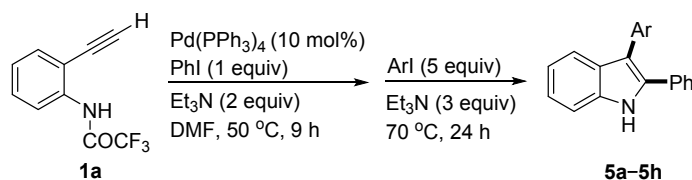
A nitrogen-filled round-bottom flask was charged with **1a** (0.47 mmol), Pd(PPh₃)₄ (54 mg,

0.047 mmol) and anhydrous DMF (3 mL), and then Et₃N (238 mg, 0.33 mL, 2.35 mmol) and PhI (479 mg, 0.26 mL, 2.35 mmol) were added in order. After the solution was stirred at 70 °C for 0.5 h, the reaction was quenched with water (3 mL) and the aqueous layer was extracted with DCM (10 mL × 3). The combined organic layer was dried over MgSO₄, the volatile was removed under vacuum, and then the resulting residue was purified by silica gel column chromatography (PE/EtOAc) to afford pure product **4a** as pale yellow solid (117 mg, 86%). ¹H NMR (400 MHz, CDCl₃) δ = 8.90 (brs, 1H), 8.38 (d, *J* = 8.0 Hz, 1H), 7.59-7.52 (m, 3H), 7.45-7.40 (m, 4H), 7.23 (t, *J* = 7.6 Hz, 1H). Our data are in full agreement with previous reported in the literature.⁸

The cyclization of **4a** with PhI under the catalysis of Pd(PPh₃)₄

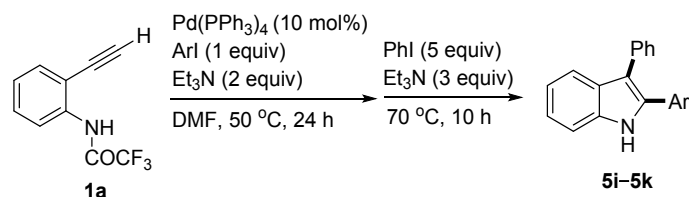
A nitrogen-filled round-bottom flask was charged with **4a** (136 mg, 0.47 mmol), Pd(PPh₃)₄ (54 mg, 0.047 mmol) and anhydrous DMF (3 mL), and then Et₃N (238 mg, 0.33 mL, 2.35 mmol) and PhI (479 mg, 0.26 mL, 2.35 mmol) were added in order. After the solution was stirred at 70 °C for 24 h, the reaction was quenched with water (3 mL) and the aqueous layer was extracted with DCM (10 mL × 3). The combined organic layer was dried over MgSO₄, the volatile was removed under vacuum, and then the resulting residue was purified by silica gel column chromatography (PE/EtOAc) to afford pure product **3a** as pale yellow solid (109 mg, 86%).

General procedure C for the synthesis of 2,3-diaryl indoles **5a-5i**:



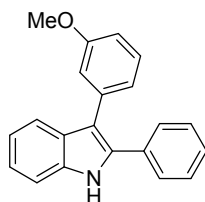
A nitrogen-filled round-bottom flask was charged with **1a** (100 mg, 0.47 mmol), Pd(PPh₃)₄ (54 mg, 0.047 mmol) and anhydrous DMF (3 mL), and then Et₃N (95 mg, 0.13 mL, 0.94 mmol) and PhI (96 mg, 52 μL, 0.47 mmol) were added in order. After the solution was stirred at 50 °C for 9 h, another portion of Et₃N (143 mg, 0.2 mL, 1.41 mmol) and second aryl iodide (2.35 mmol) were added to the reaction mixture. After the solution was stirred at 70 °C for another 24 h, the reaction was quenched with water, and the aqueous layer was extracted with DCM. The combined organic layer was dried over MgSO₄, the volatile was removed under vacuum, and then the crude product was purified by silica gel column chromatography (PE/EtOAc) to afford pure products **5a-5h**.

General procedure D for the synthesis of 2,3-diaryl indoles 5i-5k:



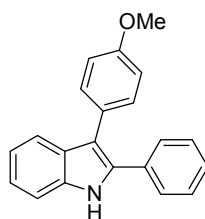
A nitrogen-filled round-bottom flask was charged with **1a** (100 mg, 0.47 mmol), Pd(PPh₃)₄ (54 mg, 0.047 mmol) and anhydrous DMF (3 mL), and then Et₃N (95 mg, 0.13 mL, 0.94 mmol) and aryl iodide (0.94 mmol) were added in order. After the solution was stirred at 50 °C for 24 h, another portion of Et₃N (143 mg, 0.2 mL, 1.41 mmol) and PhI (479 mg, 0.26 mL, 0.47 mmol) were added to the reaction mixture. After the solution was stirred at 70 °C for another 10 h, the reaction was quenched with water, and the aqueous layer was extracted with DCM. The combined organic layer was dried over MgSO₄, the volatile was removed under vacuum, and then the crude product was purified by silica gel column chromatography (PE/EtOAc) to afford pure products **5i-5k**.

3-(3-methoxyphenyl)-2-phenyl-1H-indole (**5a**)



Following the general procedure C, **5a** was purified by silica gel chromatography (v/v, PE/EtOAc = 200:1) as a pale yellow solid (120 mg, 86%). ¹H NMR (400 MHz, CDCl₃) δ = 8.26 (brs, 1H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.47-7.42 (m, 3H), 7.37-7.24 (m, 5H), 7.19-7.15 (m, 1H), 7.05-7.01 (m, 2H), 6.86 (ddd, *J* = 8.0, 3.2, 0.8 Hz, 1H), 3.75 (s, 3H). Our data was in full agreement with previous reported in the literature.⁹

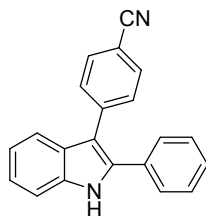
3-(4-methoxyphenyl)-2-phenyl-1H-indole (**5b**)



Following the general procedure C, **5b** was purified by silica gel chromatography (v/v, PE/EtOAc = 400:1) as a pale yellow solid (70 mg, 50%). ¹H NMR (400 MHz, CDCl₃) δ = 8.31 (brs, 1H), 7.48 (d, *J* = 7.6 Hz, 1H), 7.44-7.39 (m, 3H), 7.36-7.28 (m, 4H), 7.27-7.20 (m, 2H),

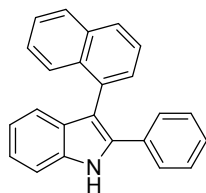
7.14-7.10 (m, 1H), 7.02-6.96 (m, 2H), 3.55 (s, 3H). Our data was in full agreement with previous reported in the literature.⁹

4-(2-phenyl-1H-indol-3-yl)benzonitrile (**5c**)



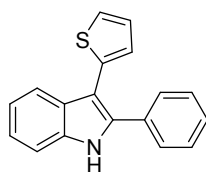
Following the general procedure C, **5c** was purified by silica gel chromatography (v/v, PE/EtOAc = 200:1) as a pale yellow solid (114 mg, 83%). ¹H NMR (400 MHz, CDCl₃) δ = 8.36 (brs, 1H), 7.68 (d, J = 8.0 Hz, 1H), 7.64 (d, J = 8.4 Hz, 2H), 7.54 (d, J = 8.4 Hz, 2H), 7.47 (d, J = 8.0 Hz, 1H), 7.41-35 (m, 5H), 7.31-7.27 (m, 1H), 7.23-7.18 (m, 1H). Our data was in full agreement with previous reported in the literature.⁹

3-(naphthalen-1-yl)-2-phenyl-1H-indole (**5d**)



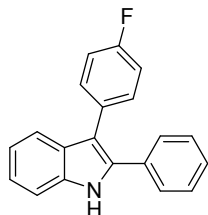
Following the general procedure C, **5d** was purified by silica gel chromatography (v/v, PE/EtOAc = 200:1) as a pale yellow solid (108 mg, 73%). ¹H NMR (400 MHz, CDCl₃) δ = 8.44 (brs, 1H), 7.92 (dd, J = 16.4, 8.0 Hz, 2H), 7.80 (d, J = 8.4 Hz, 1H), 7.52-7.44 (m, 4H), 7.34-7.28 (m, 3H), 7.27-7.26 (m, 1H), 7.23-7.17 (m, 4H), 7.09- 7.05 (m, 1H). Our data was in full agreement with previous reported in the literature.¹⁰

2-phenyl-3-(thiophen-2-yl)-1H-indole (**5e**)



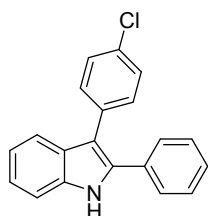
Following the general procedure C, **5e** was purified by silica gel chromatography (v/v, PE/EtOAc = 200:1) as a pale yellow solid (100 mg, 78%). ¹H NMR (400 MHz, CDCl₃) δ = 8.28 (brs, 1H), 7.80 (d, J = 8.0 Hz, 1H), 7.52 (dd, J = 8.4, 1.6 Hz, 2H), 7.44-7.36 (m, 4H), 7.31-7.28 (m, 1H), 7.27-7.24 (m, 1H), 7.22-7.18 (m, 1H), 7.10-7.05 (m, 2H). Our data was in full agreement with previous reported in the literature.¹⁰

3-(4-fluorophenyl)-2-phenyl-1H-indole (5f)



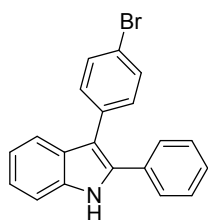
Following the general procedure C, the crude product was purified by silica gel chromatography (v/v, PE/EtOAc = 300:1) to afford a mixture of **5f** and **3a** in the ratio of 5 : 2 (118 mg, 89%). Our data was in full agreement with previous reported in the literature.¹⁰

3-(4-chlorophenyl)-2-phenyl-1H-indole (5g)



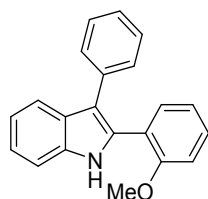
Following the general procedure C, the crude product was purified by silica gel chromatography (v/v, PE/EtOAc = 300:1) to afford a mixture of **5g** and **3a** in the ratio of 3 : 1 (122 mg, 88%). Our data was in full agreement with previous reported in the literature.¹⁰

3-(4-bromophenyl)-2-phenyl-1H-indole (5h)



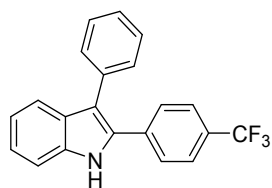
Following the general procedure C, the crude product was purified by silica gel chromatography (v/v, PE/EtOAc = 300:1) to afford a mixture of **5h** and **3a** in the ratio of 3 : 1 (125 mg, 81%). Our data was in full agreement with previous reported in the literature.⁵

2-(2-methoxyphenyl)-3-phenyl-1H-indole (5i)



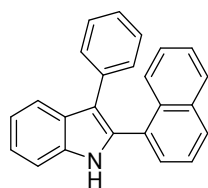
Following the general procedure D, **5i** was purified by silica gel chromatography (v/v, PE/EtOAc = 100:1) as a pale yellow solid (55 mg, 40%). ¹H NMR (400 MHz, CDCl₃) δ = 9.02 (brs, 1H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.45 (dd, *J* = 7.2, 5.6 Hz, 3H), 7.38 (t, *J* = 7.6 Hz, 2H), 7.31-7.22 (m, 4H), 7.14 (t, *J* = 8.0 Hz, 1H), 7.01 (d, *J* = 8.0 Hz, 1H), 6.82 (t, *J* = 7.6 Hz, 1H), 3.87 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ = 156.7, 135.8, 135.4, 132.0, 131.1, 130.1, 129.0, 128.4, 127.8, 125.9, 122.4, 120.9, 120.8, 119.9, 119.4, 115.7, 111.6, 110.7, 55.7, 55.6, 26.9. HRMS (ESI): *m/z* [M+H]⁺ calcd. for C₂₁H₁₈NO⁺: 300.1388; found: 300.1383.

3-phenyl-2-(4-(trifluoromethyl)phenyl)-1H-indole (**5j**)



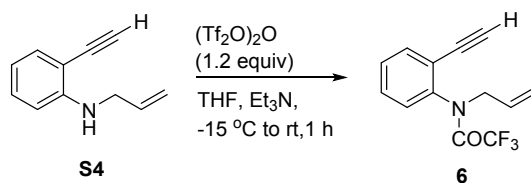
Following the general procedure D, **5j** was purified by silica gel chromatography (v/v, PE/EtOAc = 100:1) as a pale yellow solid (64 mg, 41%). ¹H NMR (400 MHz, CDCl₃) δ = 8.29 (s, 1H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.55 (dd, *J* = 18.4, 8.8 Hz, 4H), 7.46 (d, *J* = 8.0 Hz, 1H), 7.44-7.39 (m, 4H), 7.36-7.32 (m, 1H), 7.31-7.27 (m, 1H), 7.20-7.16 (m, 1H). ¹³C NMR (100 MHz, CDCl₃) δ = 136.1, 134.4, 132.2, 130.1, 129.4, 129.1, 128.7, 128.7, 128.1, 126.7, 125.5 (q, *J* = 11.2 Hz), 125.4, 123.4, 122.7, 120.7, 220.0, 116.6, 111.1, 29.7. ¹⁹F NMR (376 MHz, CDCl₃) δ = -62.5. HRMS (ESI): *m/z* [M+H]⁺ calcd. for 338.1157; found: 338.1105.

2-(naphthalen-1-yl)-3-phenyl-1H-indole (**5k**)



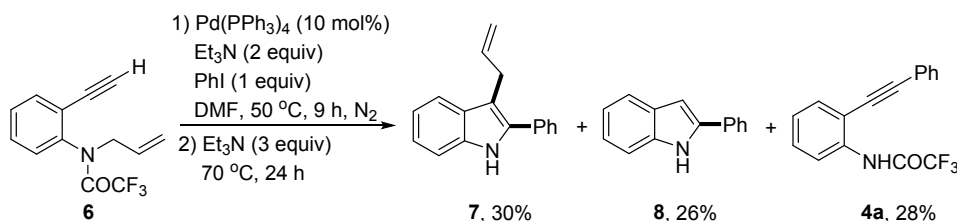
Following the general procedure D, **5k** was purified by silica gel chromatography (v/v, PE/EtOAc = 100:1) as a pale yellow solid (57 mg, 38%). ¹H NMR (400 MHz, CDCl₃) δ = 8.28 (s, 1H), 7.93-7.87 (m, 4H), 7.51-7.43 (m, 4H), 7.40-7.29 (m, 4H), 7.25-7.18 (m, 3H), 7.15-7.11 (m, 1H). ¹³C NMR (100 MHz, CDCl₃) δ = 135.8, 134.9, 133.6, 133.2, 132.2, 130.5, 129.2, 128.8, 128.2, 128.2, 127.5, 126.5, 126.0, 125.9, 125.7, 125.3, 122.5, 120.4, 119.7, 116.6, 110.9. HRMS (ESI): *m/z* [M+H]⁺ calcd. for C₂₄H₁₈N⁺: 320.1439; found: 320.1438.

The synthesis of *N*-allyl-*N*-(2-ethynylphenyl)-2,2,2-trifluoroacetamide **6**:



In a round-bottom flask, Et₃N (1 mL) was added to a solution of **S4** (0.5 g, 3.18 mmol) in THF (10 mL) at -15°C, followed by dropwise addition of trifluoroacetic anhydride (0.54 mL, 1.2 equiv). The reaction mixture was stirred at room temperature for 1h. Then the solution was quenched with water (10 mL) and the aqueous layer was extracted with EtOAc (10 mL × 3). The combined organic layer was dried over MgSO₄, and then the filtrate was concentrated to afford pure **6** as brown oil (773 mg, 96%). ¹H NMR (400 MHz, CDCl₃) δ = 7.60-7.57 (m, 1H), 7.40-7.36 (m, 2H), 7.18-7.15 (m, 1H), 5.90-5.80 (m, 1H), 5.19-5.09 (m, 2H), 4.87 (dd, *J* = 14.4, 5.6 Hz, 1H), 3.86 (dd, *J* = 14.4, 7.6 Hz, 1H), 3.31 (s, 1H). ¹³C NMR (100 MHz, CDCl₃) δ = 156.6 (q, *J* = 36.3 Hz), 140.3, 134.4, 132.8, 131.4 (dd, *J* = 8.0, 5.0 Hz), 130.6, 129.8, 129.0, 128.3, 122.1, 121.6 (t, *J* = 5.8 Hz), 120.0 (dd, *J* = 10.0, 5.7 Hz), 118.5 (t, *J* = 5.8 Hz), 117.5, 114.7, 84.5, 82.0, 53.3. ¹⁹F NMR (376 MHz, CDCl₃) δ = -68.5. HRMS (EI): *m/z* M⁺ calcd. for C₁₃H₁₀F₃NO⁺: 253.0709; Found: 253.0692.

The domino Sonogashira coupling/cyclization to *N*-allyl *o*-ethynylaniline **6**:



A nitrogen-filled round-bottom flask was charged with **6** (100 mg, 0.40 mmol), Pd(PPh₃)₄ (54 mg, 0.04 mmol) and anhydrous DMF (3 mL), and then Et₃N (0.11 mL, 0.80 mmol), PhI (0.044 mL, 0.40 mmol) were added in order. After the solution was stirred at 50 °C for 9 h, another portion of Et₃N (0.165 mL, 1.20 mmol) was added to the reaction mixture. After the solution was stirred at 70 °C for another 24 h, the reaction was quenched with water, and the aqueous layer was extracted with DCM. The combined organic layer was dried over MgSO₄, the volatile was removed under vacuum, and then the crude product was purified by column chromatography using silica gel (v/v, PE/EtOAc = 300:1) to afford pure product **7** as a pale yellow solid (28 mg, 30%), along with the minor product **8** as a pale yellow solid (20 mg, 26%) and **4b** (32 mg, 28%). Product **7**: ¹H NMR (400 MHz, CDCl₃) δ = 8.07 (brs, 1H), 7.62 (d, *J* = 8.0 Hz, 1H), 7.59-7.56 (m, 2H), 7.48 (t, *J* = 7.2 Hz, 2H), 7.41-7.36 (m, 2H), 7.25-7.20 (m, 1H), 7.17-7.13 (m, 1H), 6.20-6.10 (m, 1H), 5.13 (dd, *J* = 6.8, 2.0 Hz, 1H), 5.09 (t, *J* = 2.0 Hz, 1H), 3.65 (dt, *J* = 6.0, 1.6 Hz, 2H). Product **8**: ¹H NMR (400 MHz, CDCl₃) δ = 8.35 (s, 1H), 7.68

(dd, $J = 8.4, 1.2$ Hz, 2H), 7.65 (d, $J = 8.4$ Hz, 1H), 7.46 (t, $J = 7.6$ Hz, 2H), 7.41 (dd, $J = 8.2, 0.6$ Hz, 1H), 7.34 (t, $J = 7.6$ Hz, 1H), 7.23-7.18 (m, 1H), 7.16-7.11 (m, 1H), 6.84 (dd, $J = 2.0, 0.4$ Hz, 1H). Our data of 7^{11} , 8^{12} and $4a^8$ were in full agreement with previous reported in the literatures.

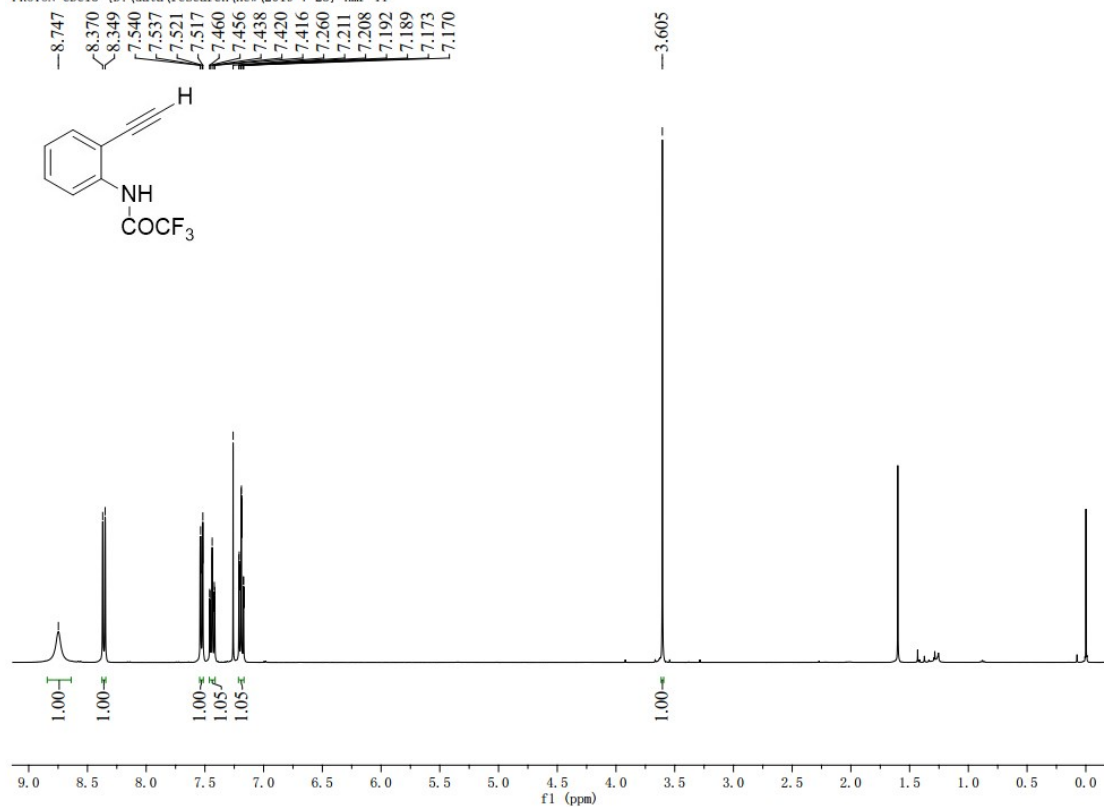
Reference:

1. P. Cironi, J. Tulla-Puche, G. Barany, F. Albericio and M. Álvarez, *Org. Lett.*, 2004, **6**, 1405-1408.
2. Z. Zhou, G. X. Liu, Y. Chen and X. Y. Lu, *Adv. Synth. Catal.*, 2015, **357**, 2944-2950.
3. D. B. Zhao, Z. Z. Shi and F. Glorius, *Angew. Chem. Int. Ed.*, 2013, **52**, 12426-12429.
4. M. Thangaraj, S. S. Bhojgude, S. Jain, R. G. Gonnade and A. T. Biju, *J. Org. Chem.*, 2016, **81**, 8604-8611.
5. G. Y. Zhang, H. Yu, G. P. Qin and H. M. Huang, *Chem. Commun.*, 2014, **50**, 4331-4334.
6. A. Lerchen, S. Vásquez-Céspedes and F. Glorius, *Angew. Chem. Int. Ed.*, 2016, **55**, 3208-3211.
7. K. Muralirajan and C.-H. Cheng, *Adv. Synth. Catal.*, 2014, **356**, 1571-1576.
8. N. K. Swamy, A. Yazici and S. G. Pyne, *J. Org. Chem.* **2010**, *75*, 3412-3419.
9. S. Cacchi, G. Fabrizia, D. Lambab, F. Marinellie and L. M. Parisi, *Synthesis*, 2003, 728-734.
10. L. J. Gu, C. Jin, W. Wang, Y. H. He, G. Y. Yang and G. P. Li, *Chem. Commun.*, 2017, **53**, 4203-4206.
11. H. Lauwick, Y. Sun, H. Akdas-Kilig, S. Dérien and M. Achard, *Chem. Eur. J.*, 2018, **24**, 7964-7969
12. P. Rubio-Marqués, M. A. Rivero-Crespo, A. Leyva-Pérez and A. Corma, *J. Am. Chem. Soc.*, 2015, **137**, 11832-11837.

NMR Spectra

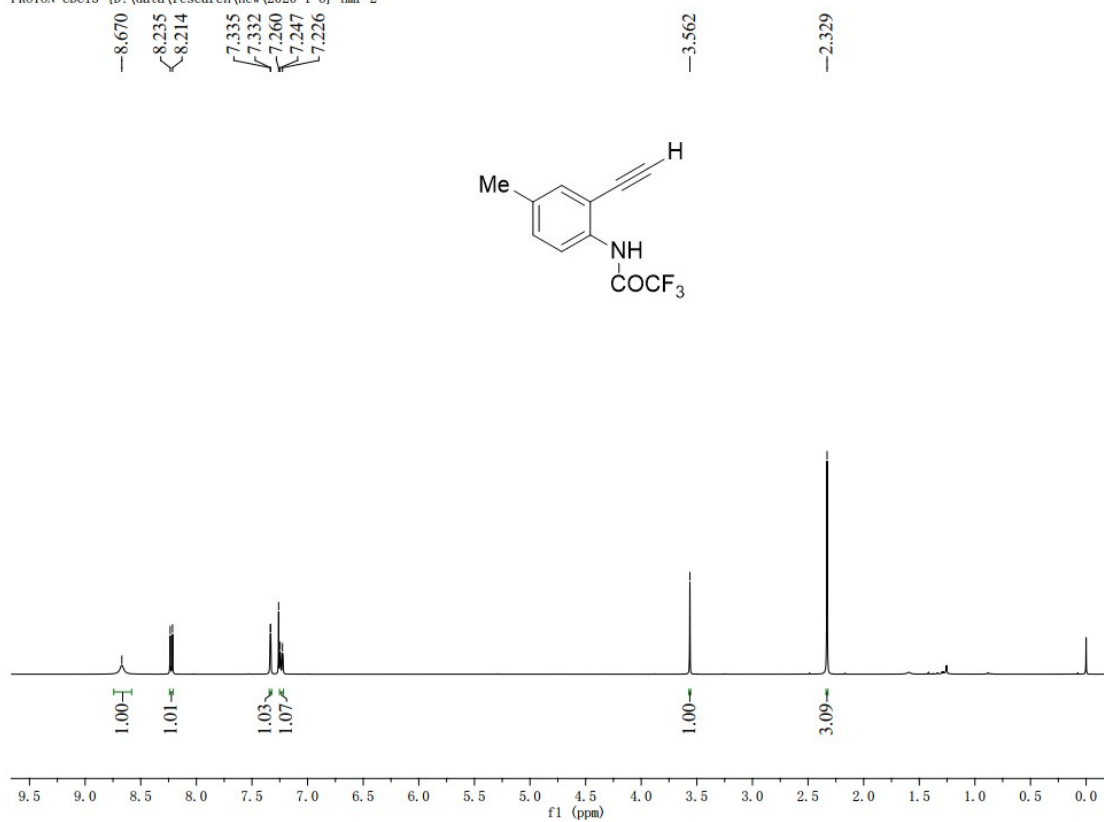
Compound 1a

PROTON CDCl3 {D:\data\research\new\2019-7-23} nmr 44



Compound 1b

PROTON CDCl3 {D:\data\research\new\2020-1-6} nmr 2



C13CPD CDC13 {D:\data\research\new\2020-1-13} nmr 43

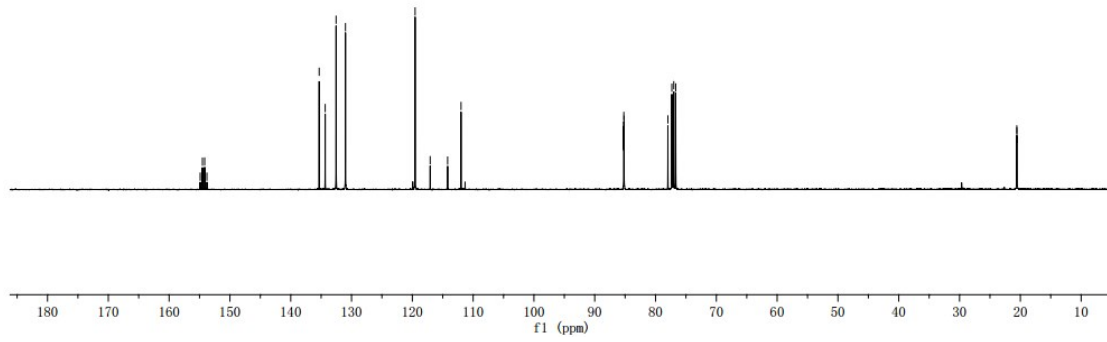
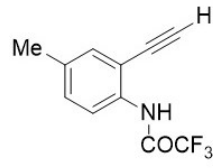
154.894
154.523
154.151
153.780

135.321
134.332
132.537
130.995

119.540
117.062
114.193
111.989

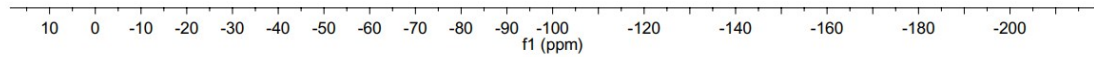
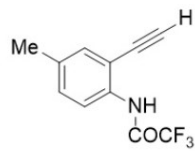
85.213
85.185
77.967
77.318
77.000
76.682

20.587
20.571



ju-wgd-005
F19CPD CDC13 {D:\data\research\new\2020-11-4} nmr 41

75.890

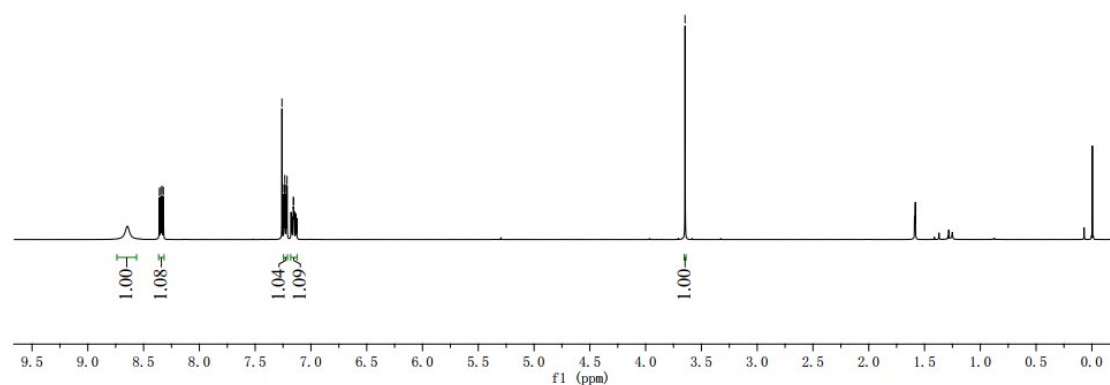
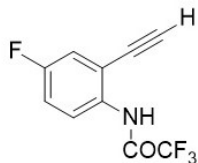


Compound 1c

PROTON CDC13 {D:\data\research\new\20190-5-10} nmr 11

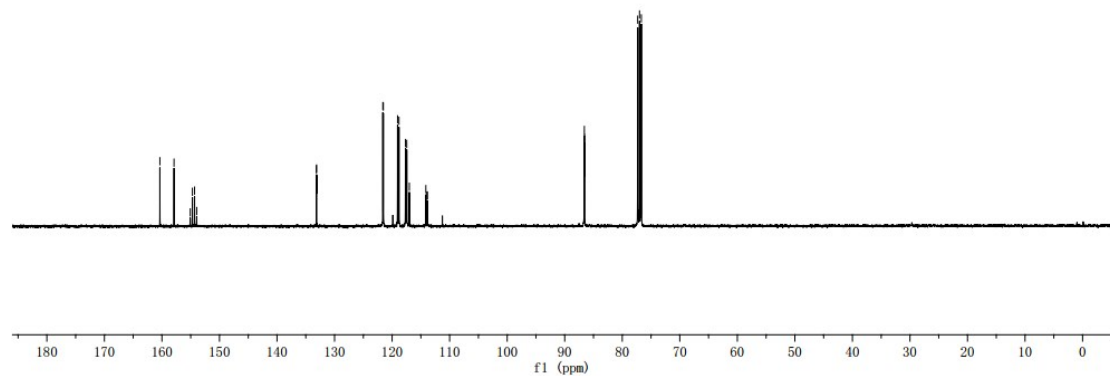
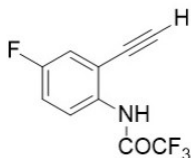
8.358
8.346
8.335
8.323
7.260
7.242
7.235
7.221
7.214
7.158
7.155

3.646

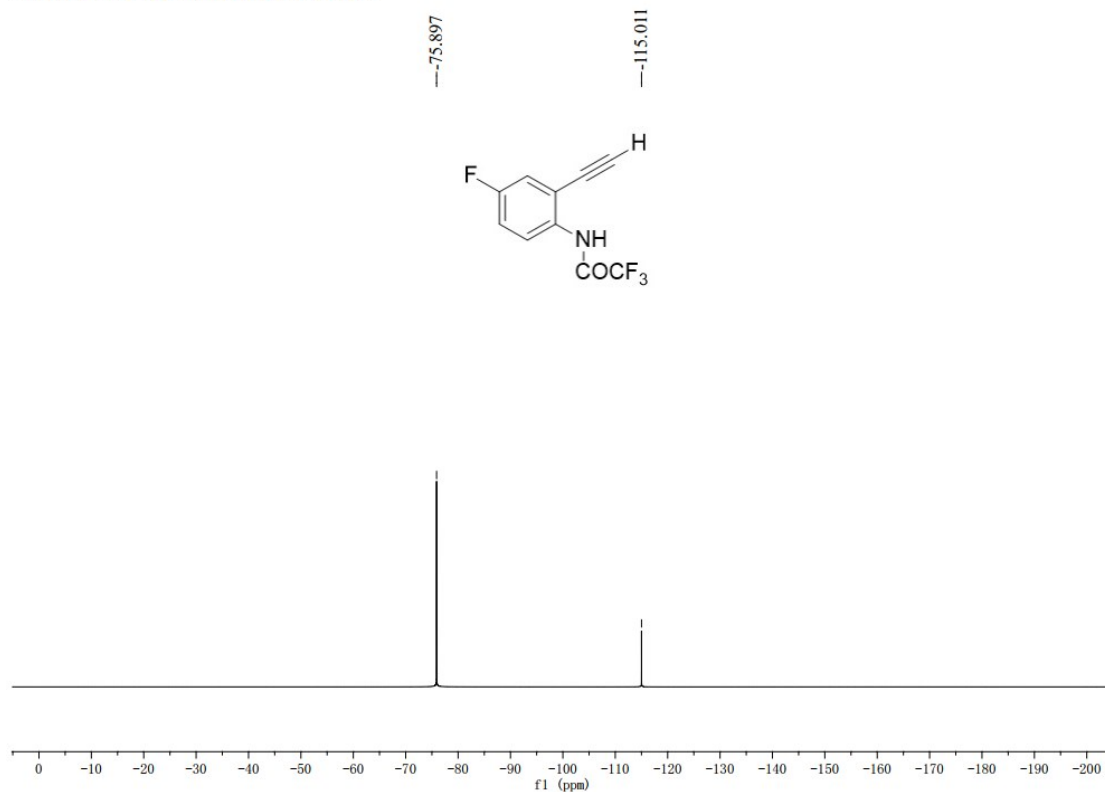


C13CPD CDC13 {D:\data\research\new\2020-1-13} nmr 44

160.357
157.901
155.079
154.704
154.329
153.955
133.160
133.131
121.609
121.525
119.052
118.806
117.674
117.451
117.003
114.135
113.957
113.862
86.587
86.555
77.318
77.000
76.682

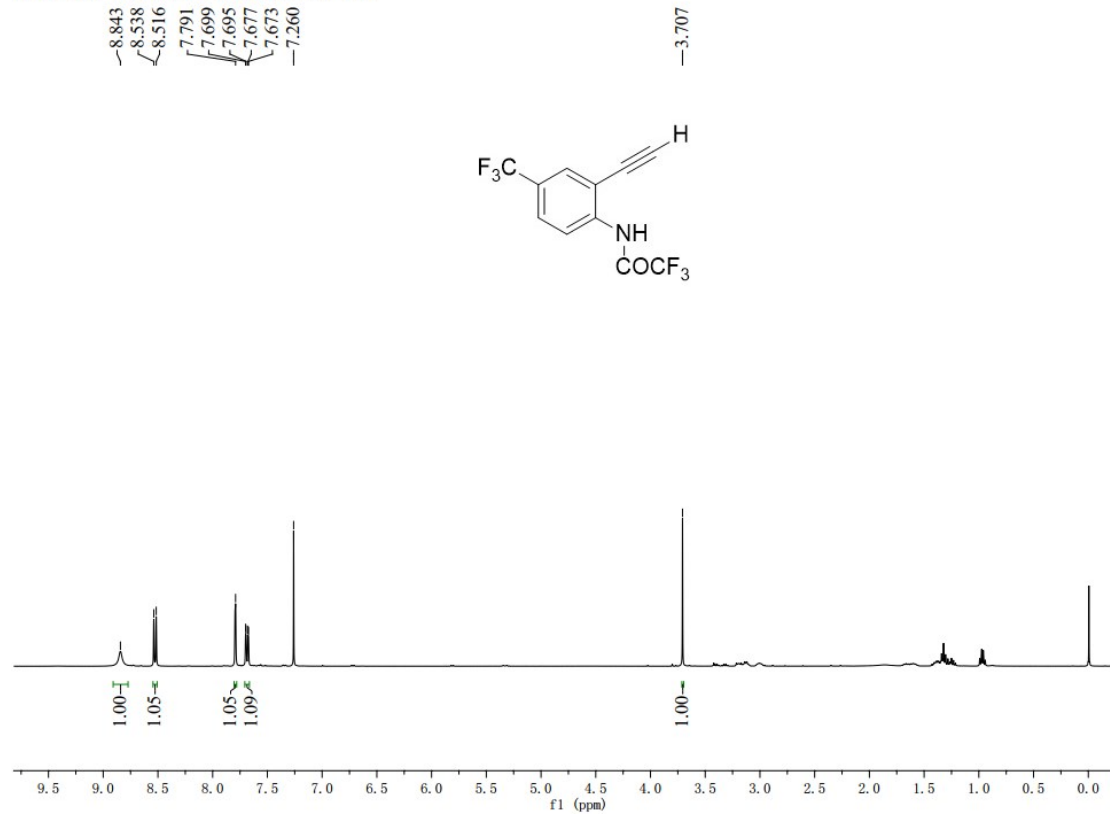


F19CPD CDC13 {D:\data\research\new\2019-5-13} nmr 9



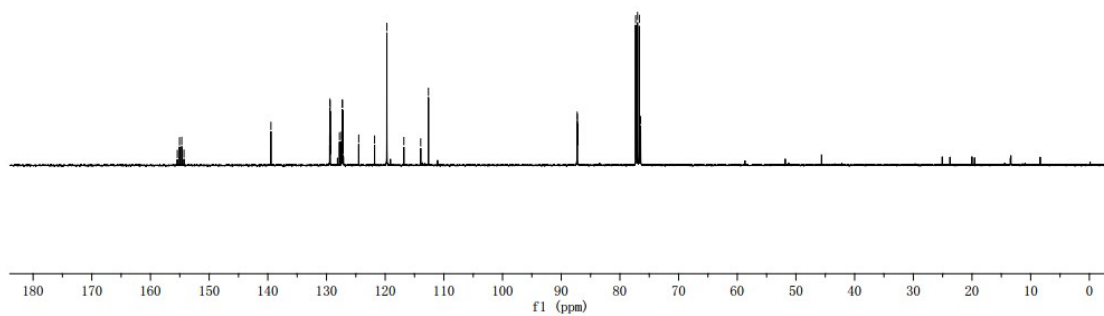
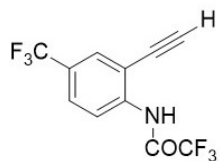
Compound 1d

PROTON CDC13 {D:\data\research\new\2020-1-6} nmr 1



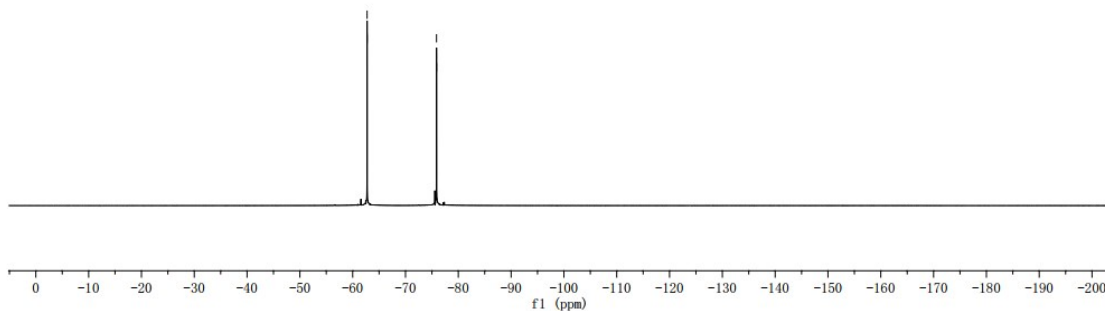
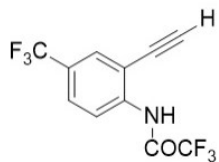
C13CPD CDC13 {D:\data\research\new\2020-1-13} nmr 42

155.427
155.048
154.669
154.289
139.469
129.454
129.416
129.377
127.789
127.455
127.351
127.314
127.278
127.241
124.511
121.807
119.715
112.624
87.246
87.246
77.318
77.000
76.682
76.473



F19CPD CDC13 {D:\data\research\new\2020-1-14} nmr 17

62.728
62.735
75.874
75.883



Compound 1e

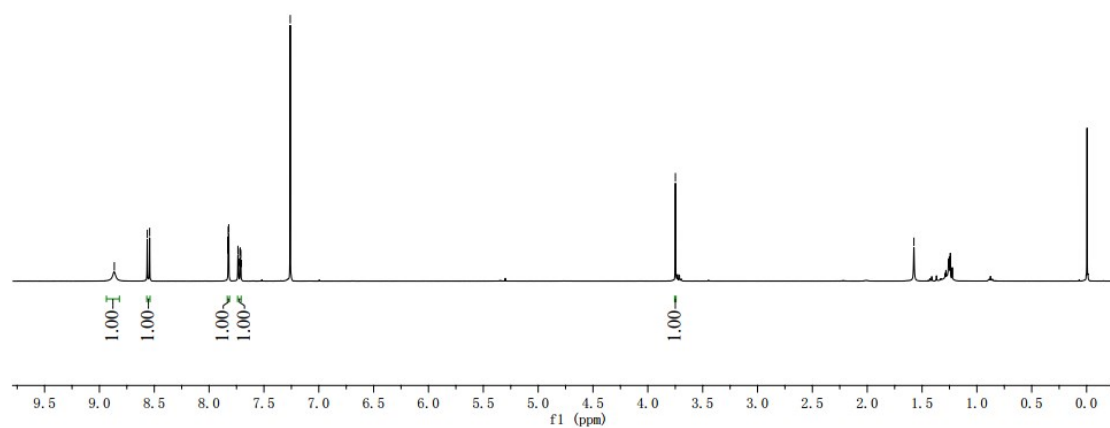
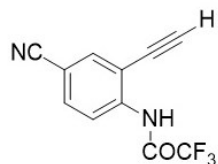
PROTON CDC13 {D:\data\research\new\2019-11-7} nmr 31

8.864
8.564
8.542

7.826
7.821
7.737
7.733
7.715
7.710

3.749

1.574



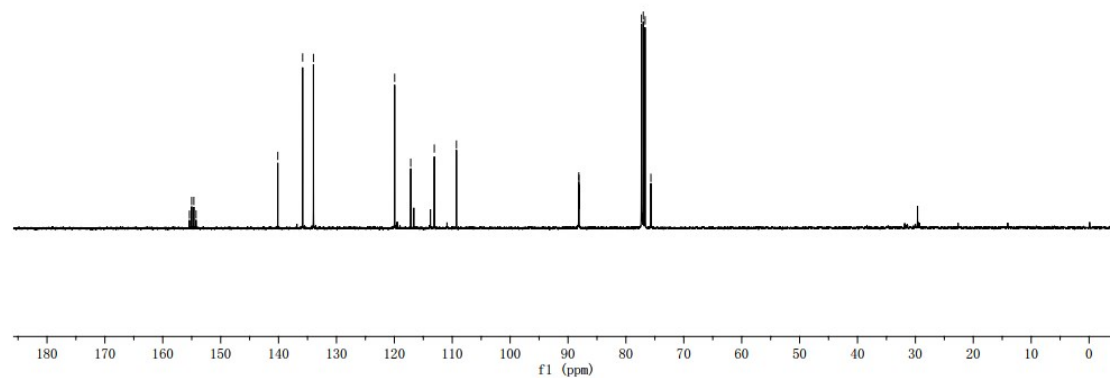
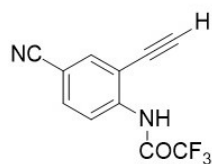
¹³CPD CDC13 {D:\data\research\new\2020-1-13} nmr 45

155.397
155.016
154.634
154.252

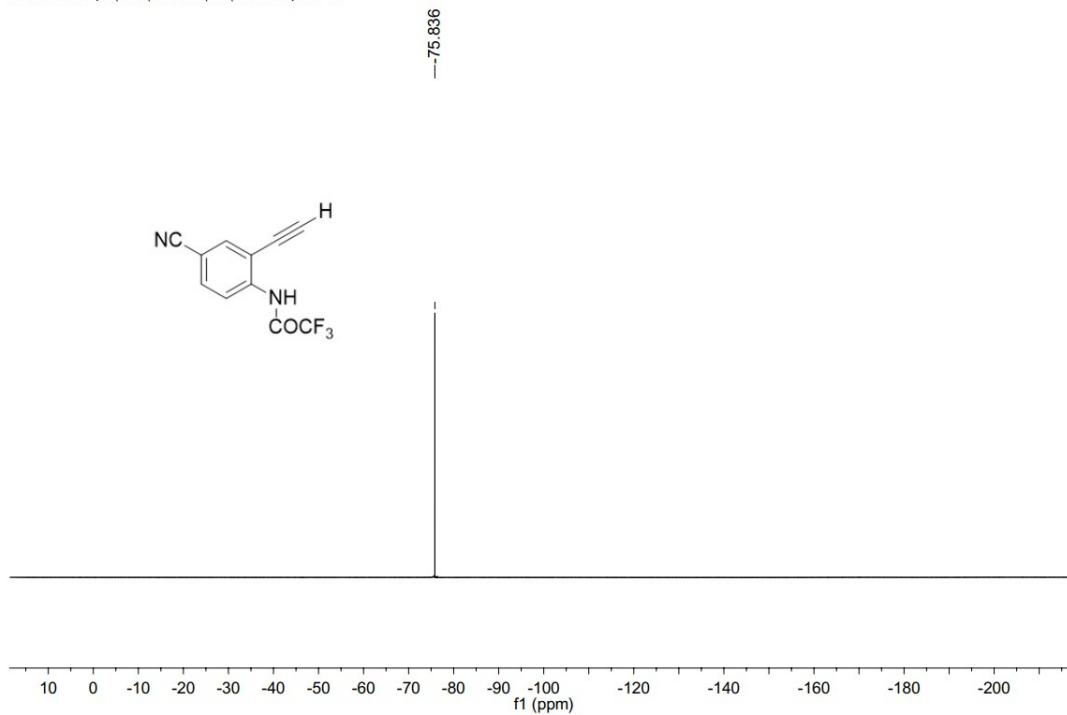
140.132
135.841
133.972

119.945
117.170
113.099
109.272

88.141
88.103
77.318
77.000
76.682
75.685

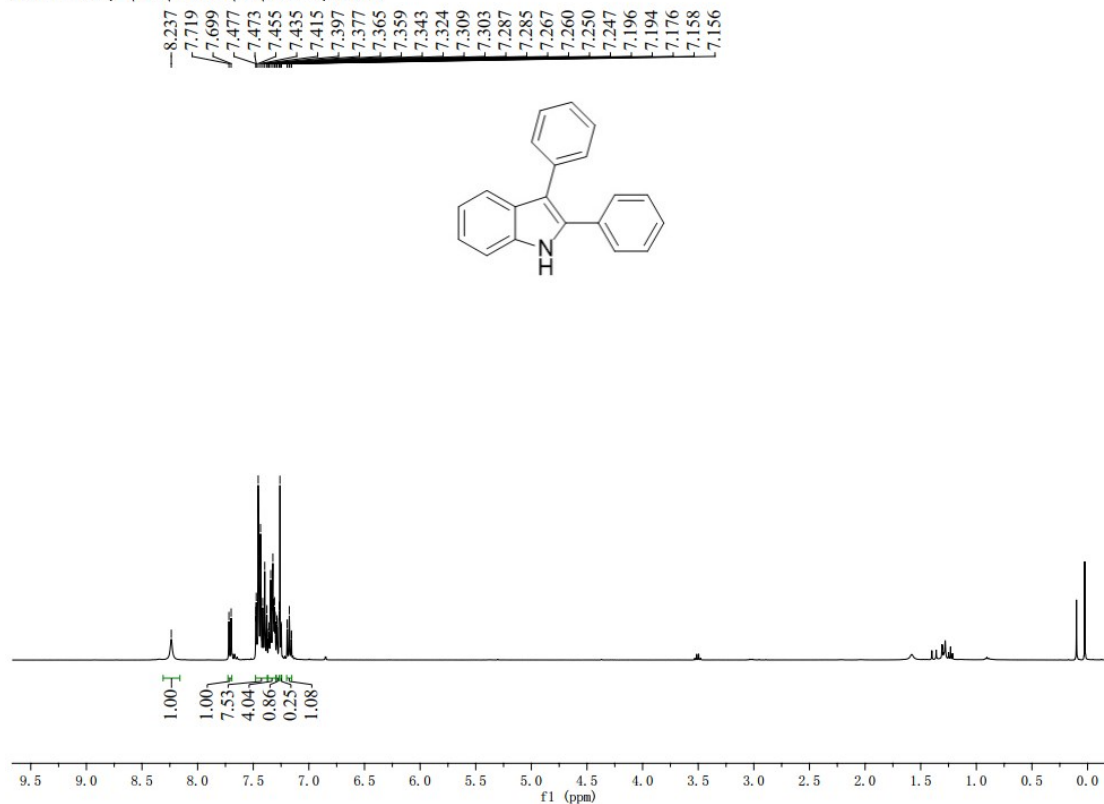


ju-wgd-002
F19CPD CDC13 {D:\data\research\new\2020-11-1} nmr 40



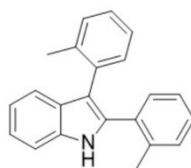
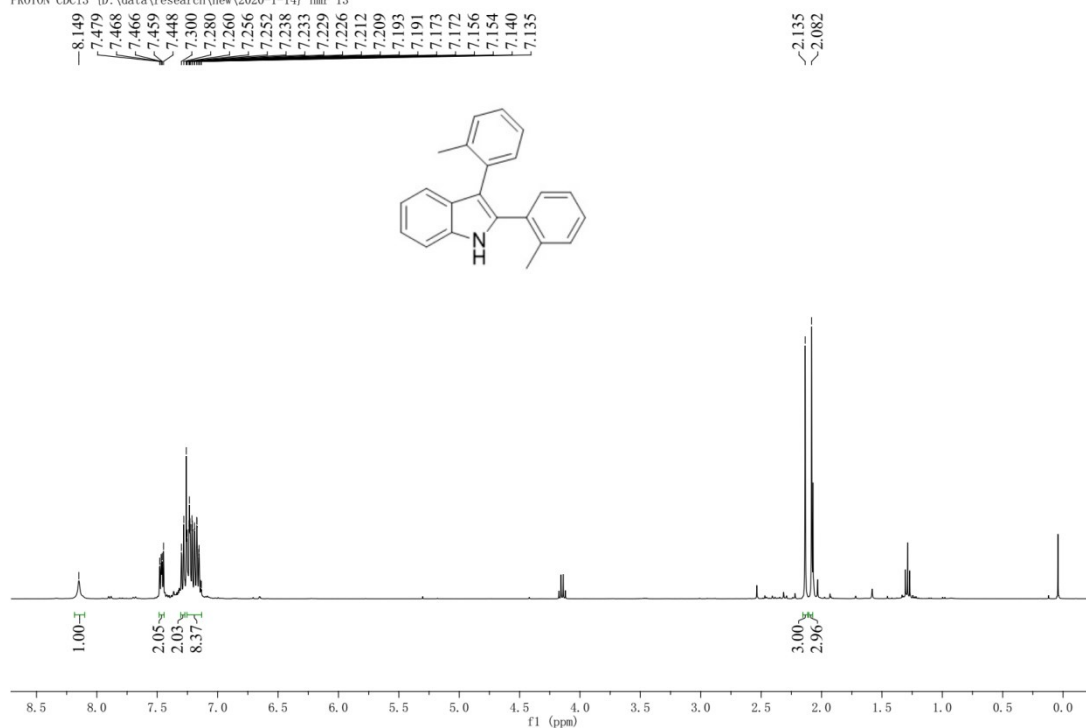
Compound 3a

PROTON CDC13 {D:\data\research\new\2020-1-7} nmr 55



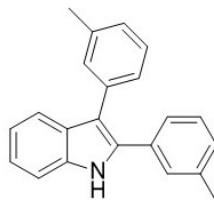
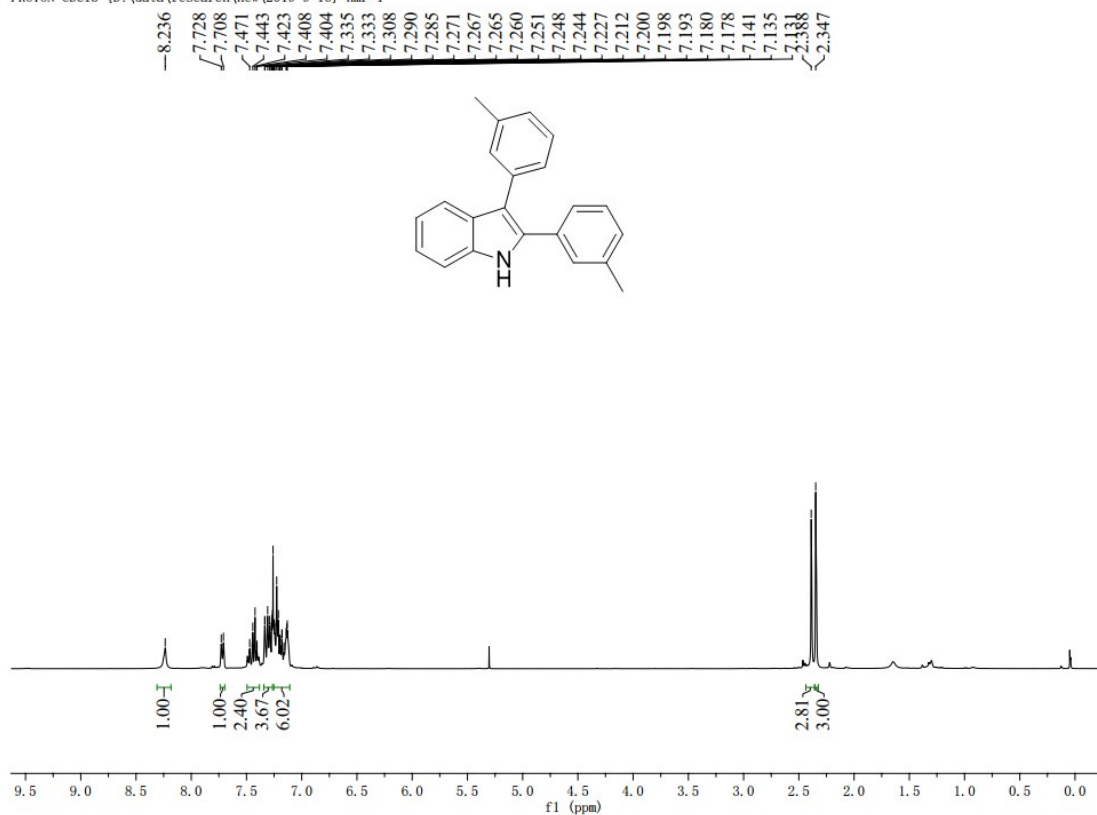
Compound 3b

PROTON CDCl3 [D:\data\research\new\2020-1-14] nmr 13



Compound 3c

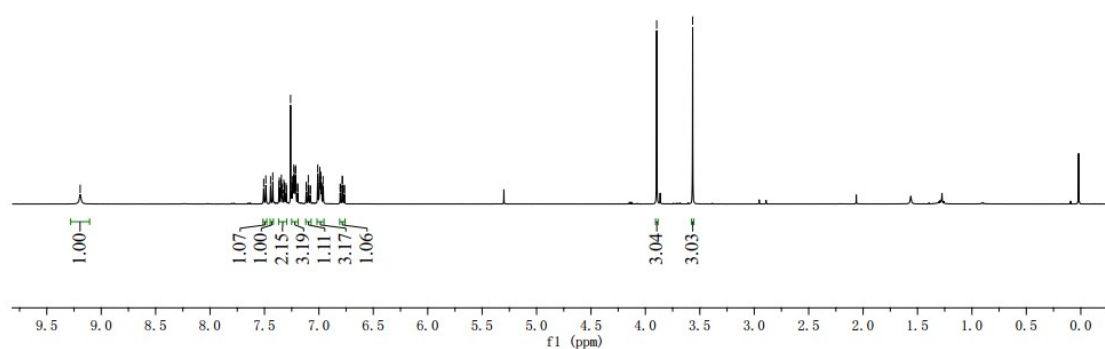
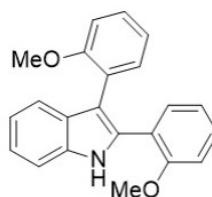
PROTON CDCl3 [D:\data\research\new\2019-9-16] nmr 4



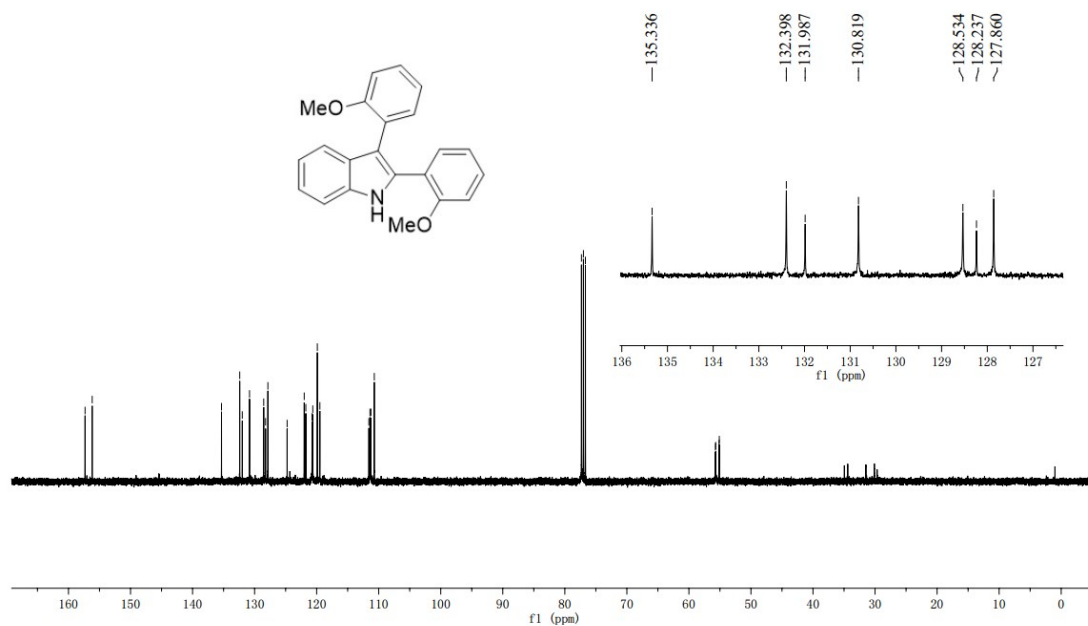
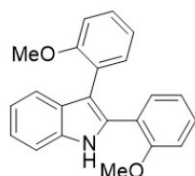
Compound 3d

PROTON CDCl3 {D:\data\research\new\2020-1-9} nmr 47

9.193 7.507 7.487 7.444 7.423 7.367 7.363 7.349 7.344 7.322 7.317 7.260 7.248 7.242 7.231 7.218 7.213 7.117 7.097 7.010 6.994 6.992 6.987 6.982 6.962 6.785 6.886 3.566

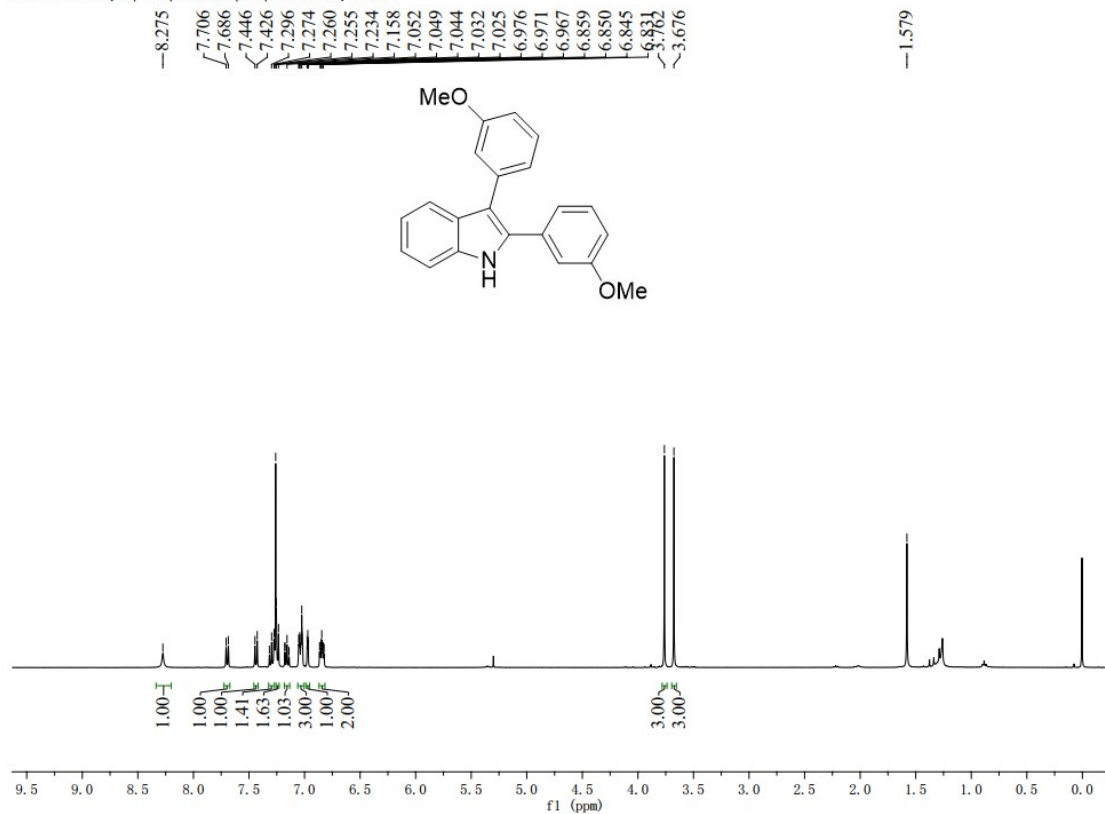


157.325 156.177 135.336 132.398 131.987 130.819 128.534 127.860 122.003 121.747 120.737 120.624 119.891 119.482 117.584 111.408 111.249 110.709 77.318 77.000 76.683 55.725 55.680 55.134 55.102

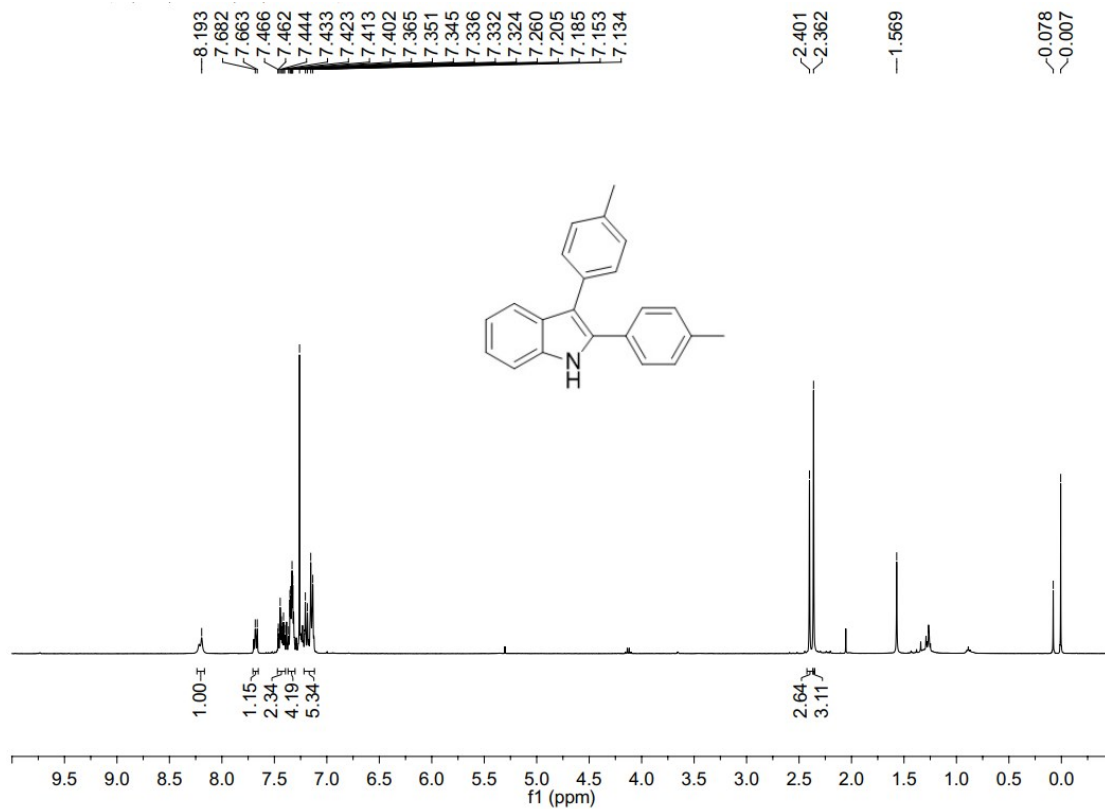


Compound 3e

PROTON CDC13 {D:\data\research\new\2019-10-15} nmr 33



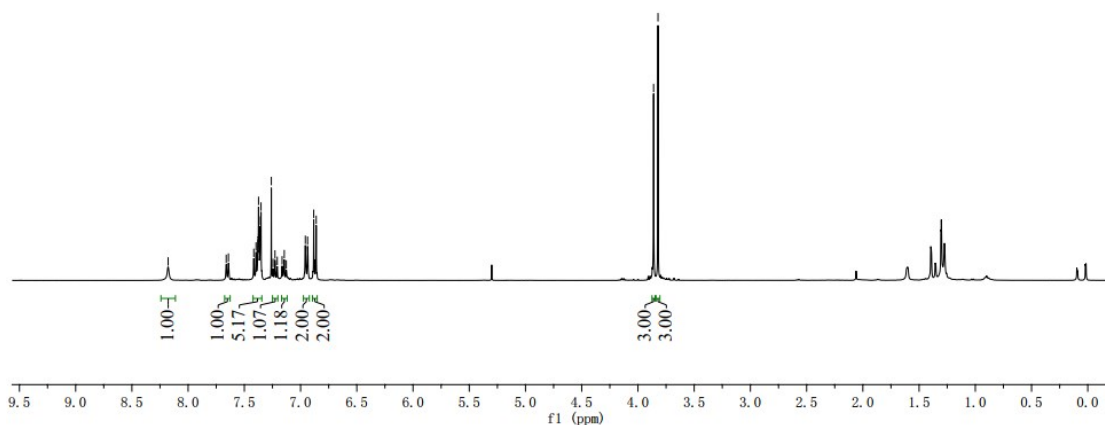
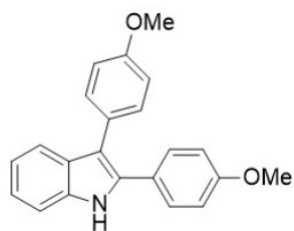
Compound 3f



Compound 3g

PROTON CDCl3 {D:\data\research\new\2019-6-19} nmr 38

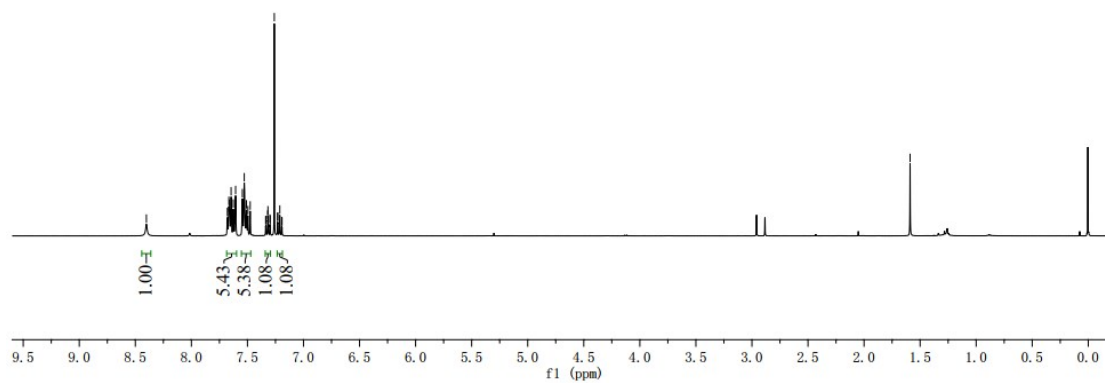
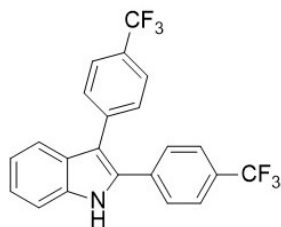
8.178
7.661
7.641
7.416
7.396
7.374
7.357
7.352
7.260
7.245
7.228
7.208
7.164
7.145
7.127
6.958
6.883
6.861
3.861
3.822



Compound 3h

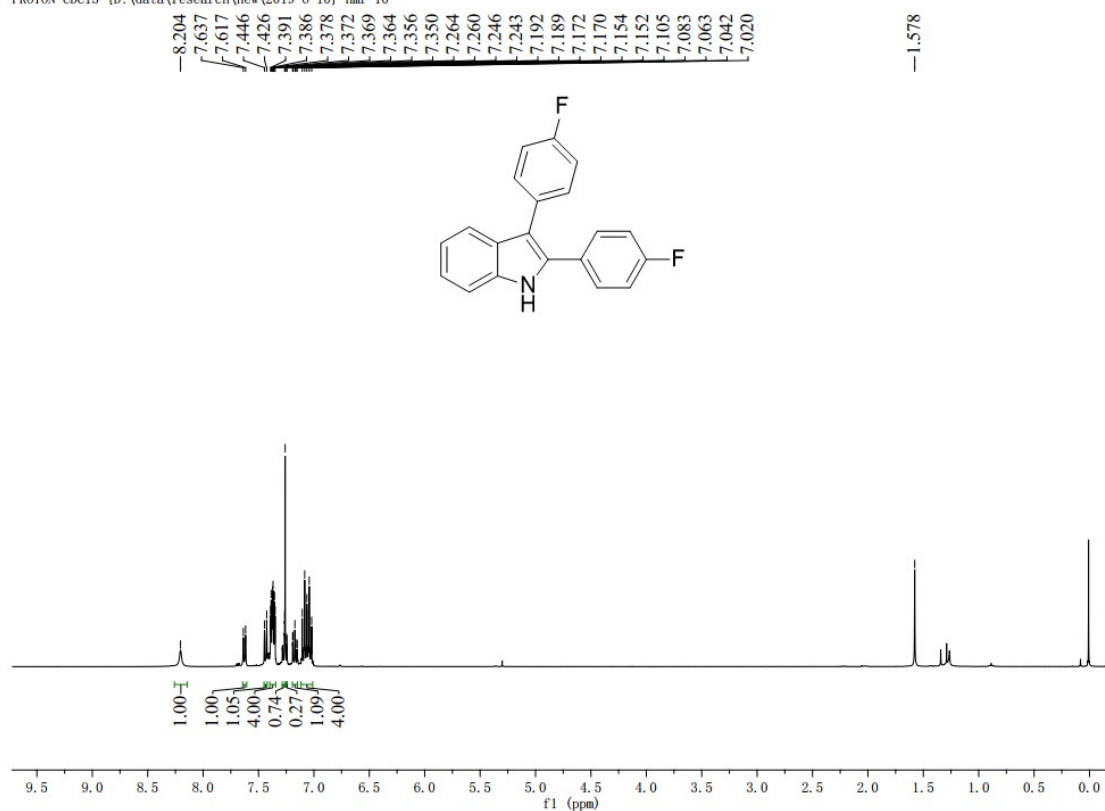
PROTON CDCl3 {D:\data\research\new\2020-1-13} nmr 13

8.401
7.679
7.666
7.660
7.646
7.626
7.606
7.545
7.528
7.509
7.496
7.475
7.337
7.335
7.320
7.317
7.299
7.297
7.260
7.231
7.229
7.211
7.194
7.192
1.589



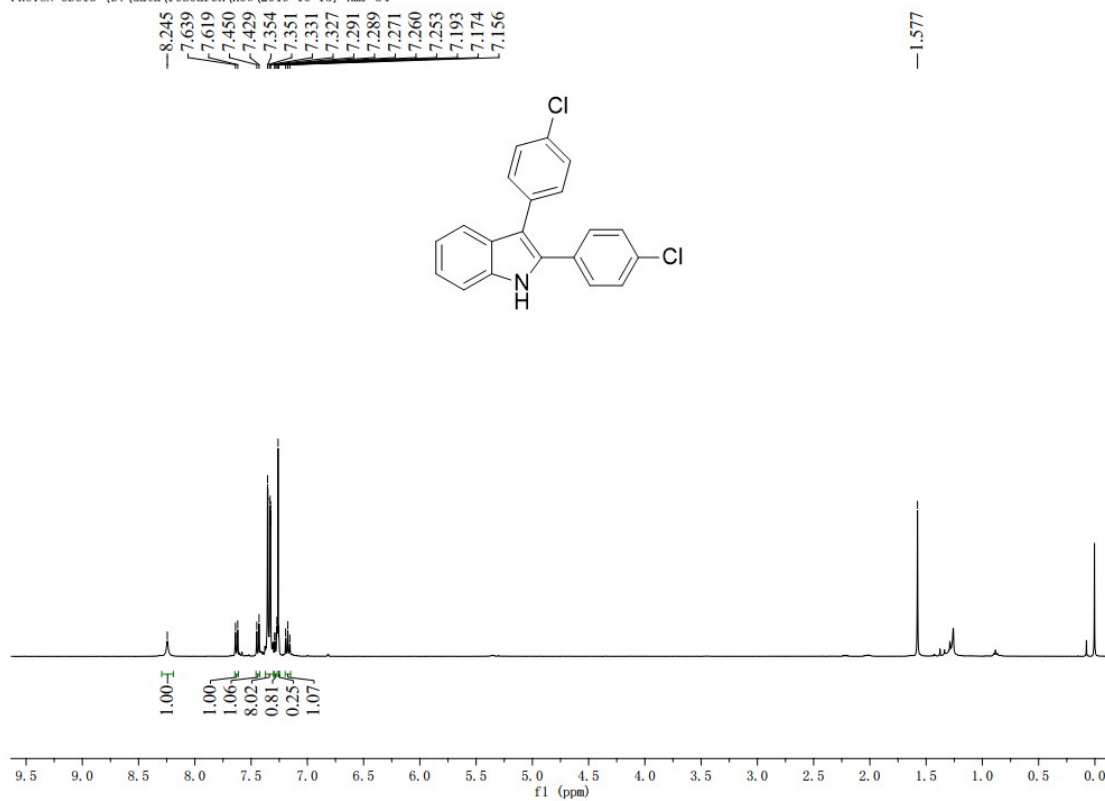
Compound 3i

PROTON CDC13 {D:\data\research\new\2019-6-10} nmr 10



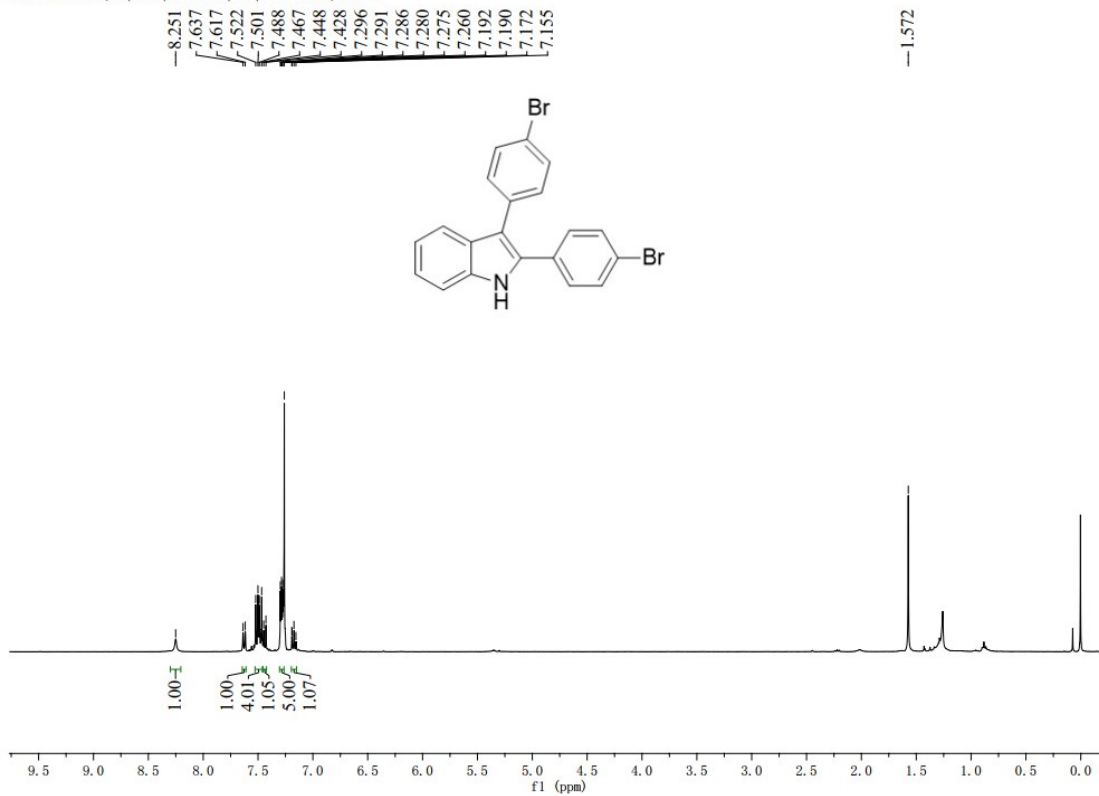
Compound 3j

PROTON CDC13 {D:\data\research\new\2019-10-15} nmr 34



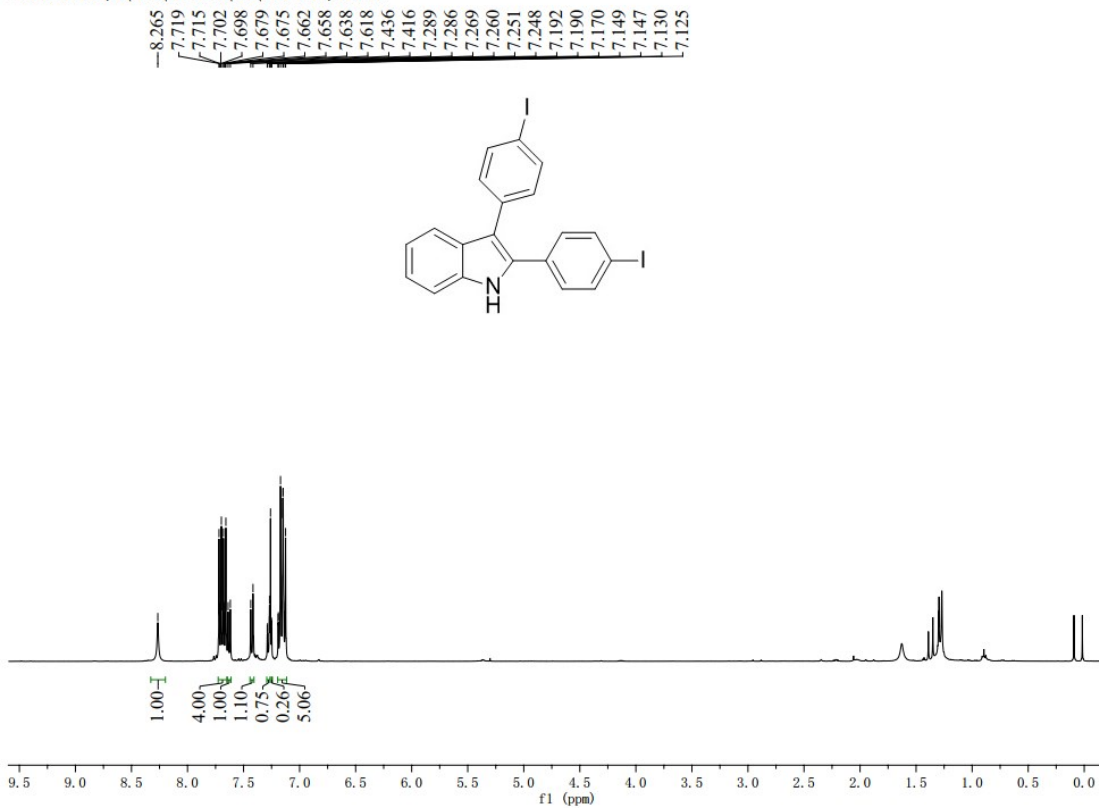
Compound 3k

PROTON CDC13 {D:\data\research\new\2019-10-11} nmr 7



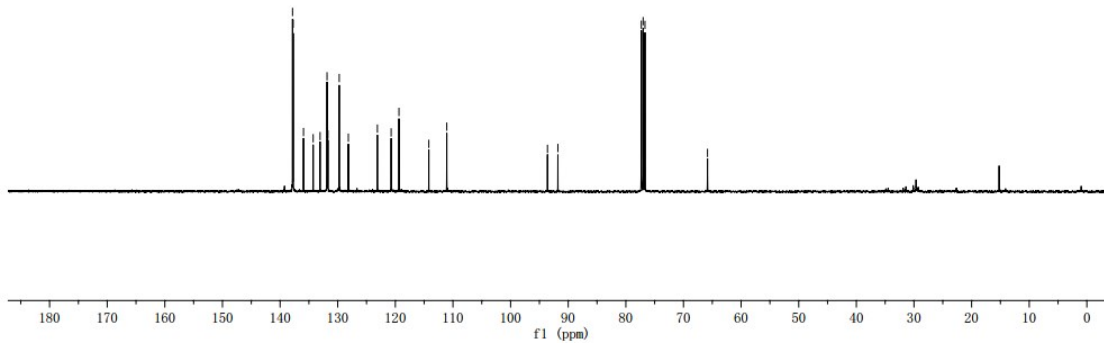
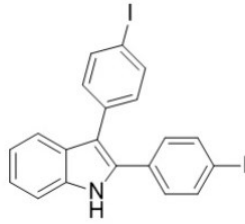
Compound 3l

PROTON CDC13 {D:\data\research\new\2019-6-14} nmr 36



C13CPD CDC13 {D:\data\research\new\2019-6-17} nmr 23

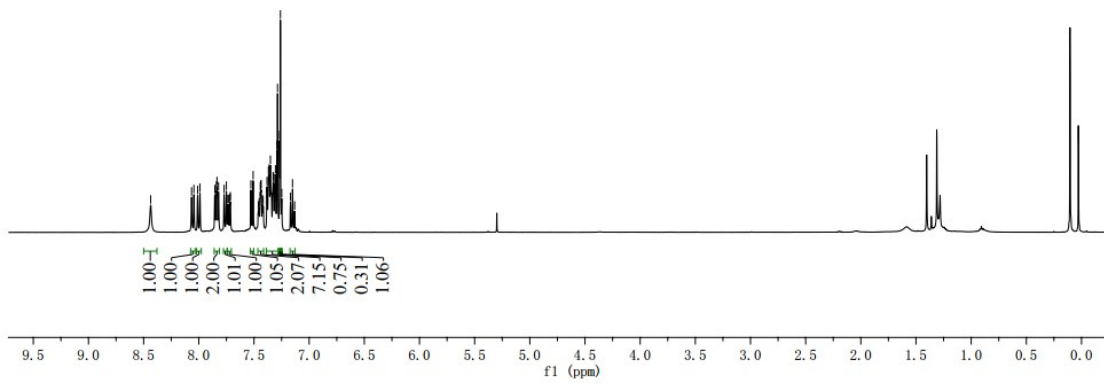
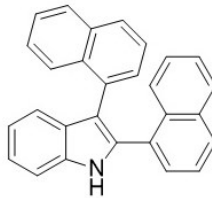
137.838
137.726
135.939
134.259
133.058
131.850
131.690
129.734
128.153
123.114
120.727
119.370
114.192
111.076
93.597
91.790
77.318
77.000
76.682
65.828



Compound 3m

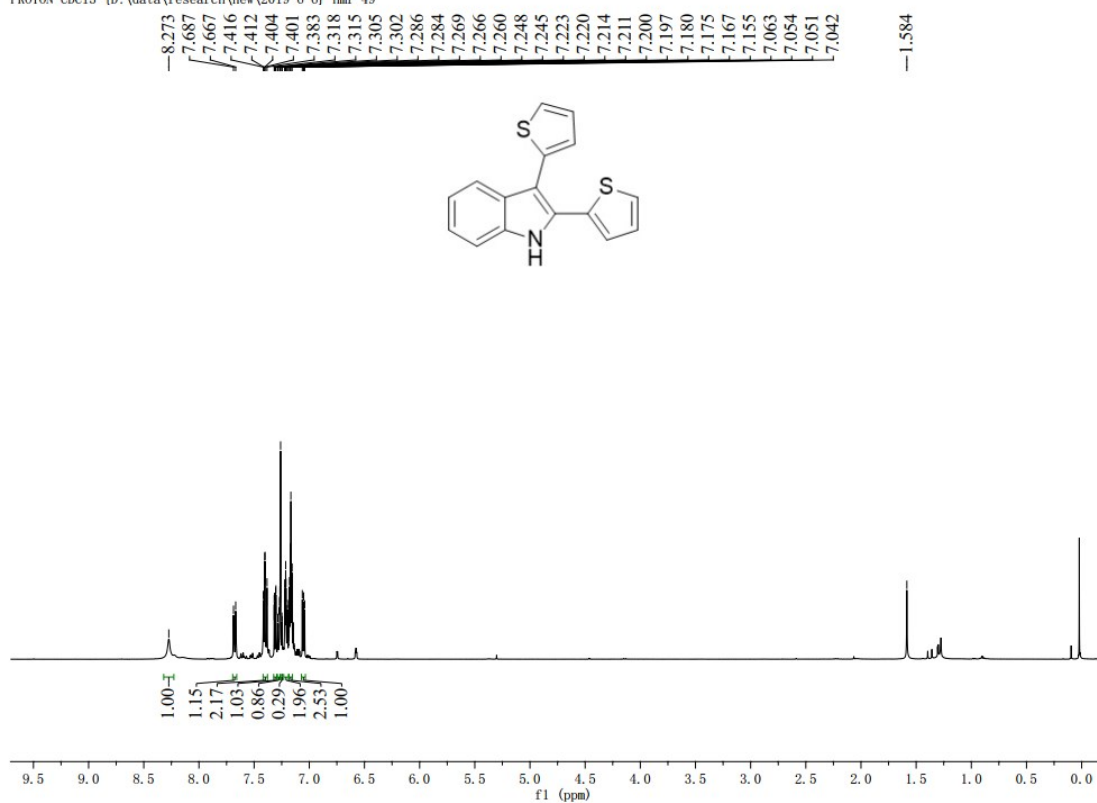
PROTON CDC13 {D:\data\research\new\2020-1-13} nmr 18

8.436
8.066
8.045
8.011
7.990
7.855
7.841
7.835
7.821
7.771
7.750
7.736
7.732
7.718
7.714
7.528
7.508
7.460
7.453
7.442
7.438
7.435
7.424
7.417
7.382
7.369
7.362
7.351
7.326
7.323
7.310
7.306
7.292
7.287
7.268
7.260
7.248
7.169
7.151
7.131



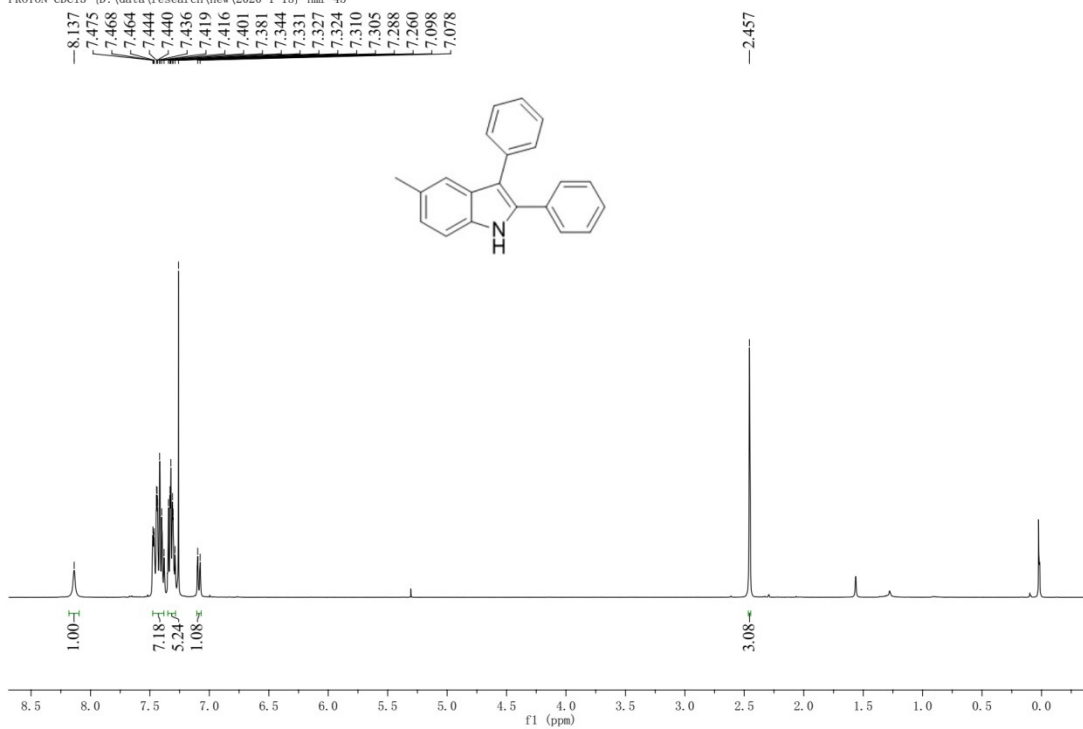
Compound 3n

PROTON CDC13 (D:\data\research\new\2019-6-6) nmr 49



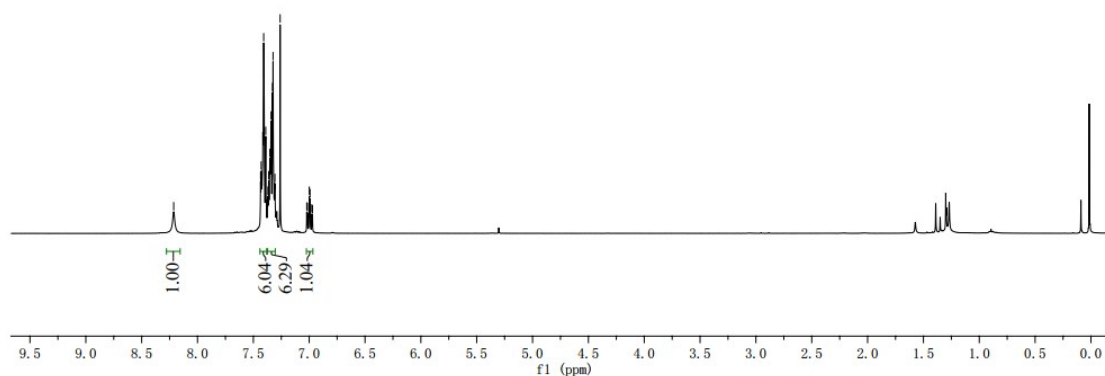
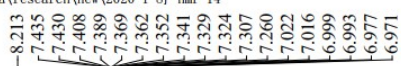
Compound 3o

PROTON CDC13 (D:\data\research\new\2020-1-15) nmr 45



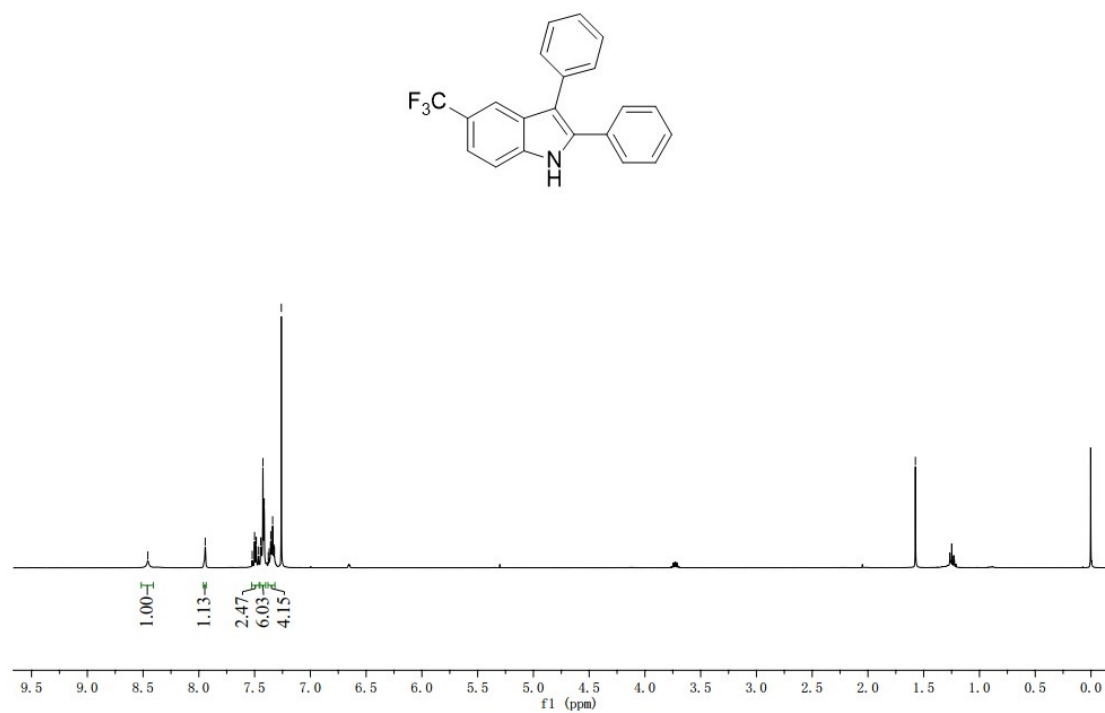
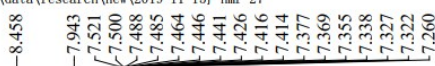
Compound 3p

PROTON CDC13 {D:\data\research\new\2020-1-8} nmr 14



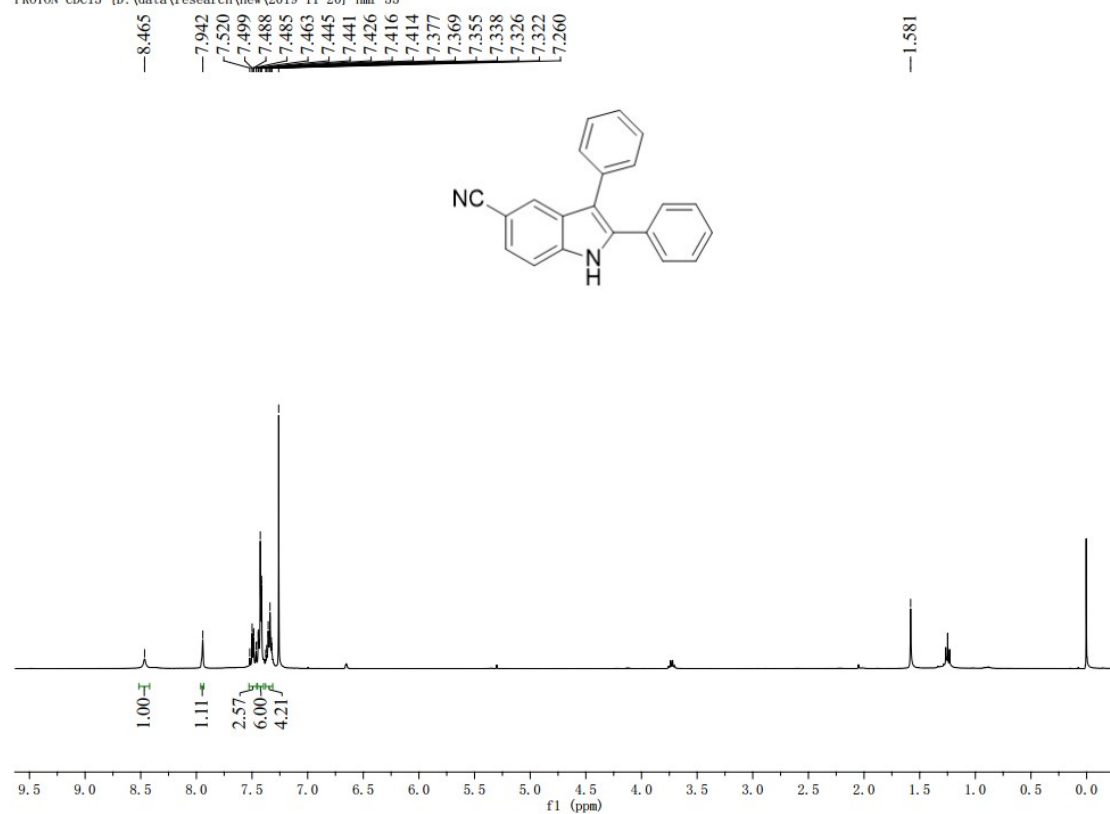
Compound 3q

PROTON CDC13 {D:\data\research\new\2019-11-15} nmr 27



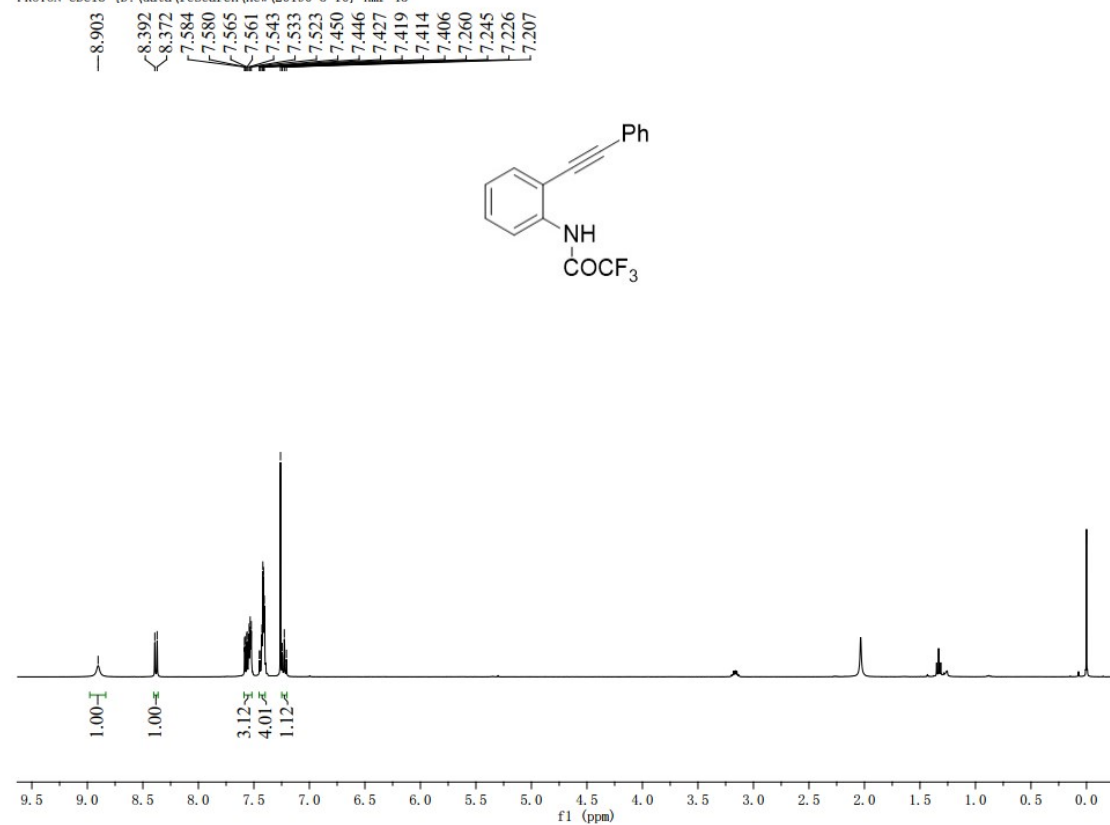
Compound 3r

PROTON CDCl3 {D:\data\research\new\2019-11-20} nmr 55



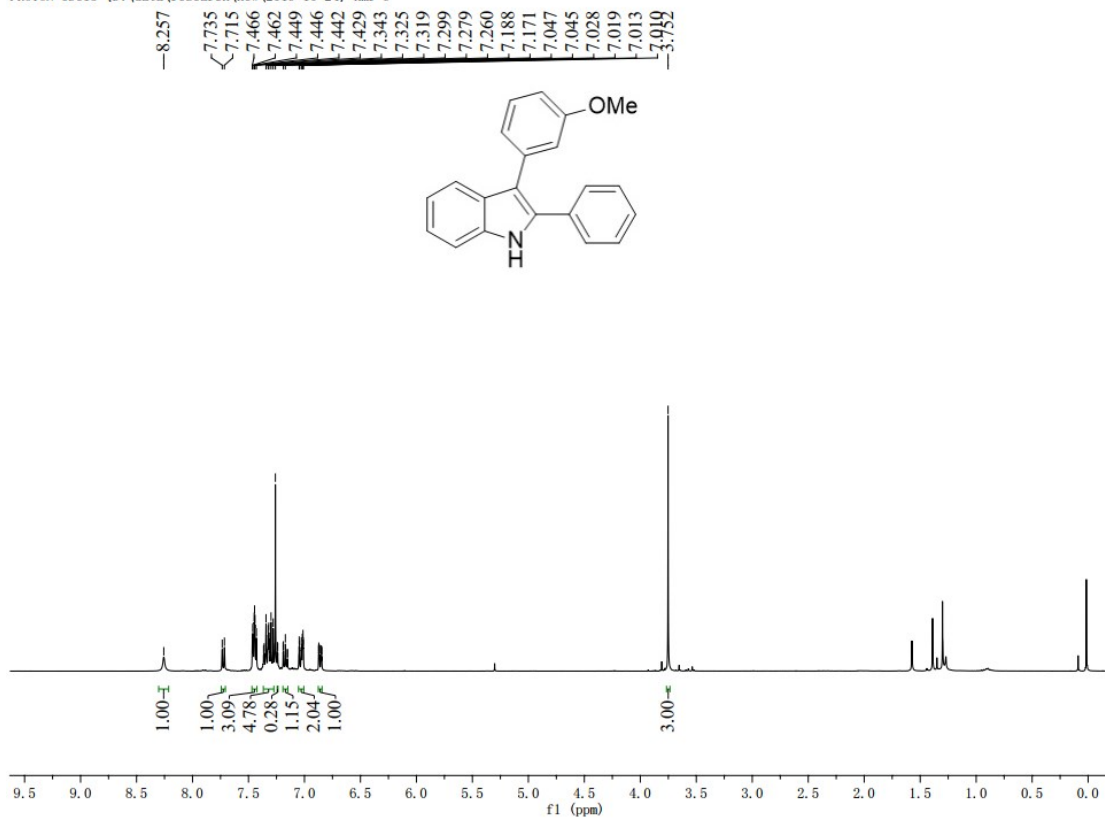
Compound 4a

PROTON CDCl3 {D:\data\research\new\20190-5-10} nmr 45



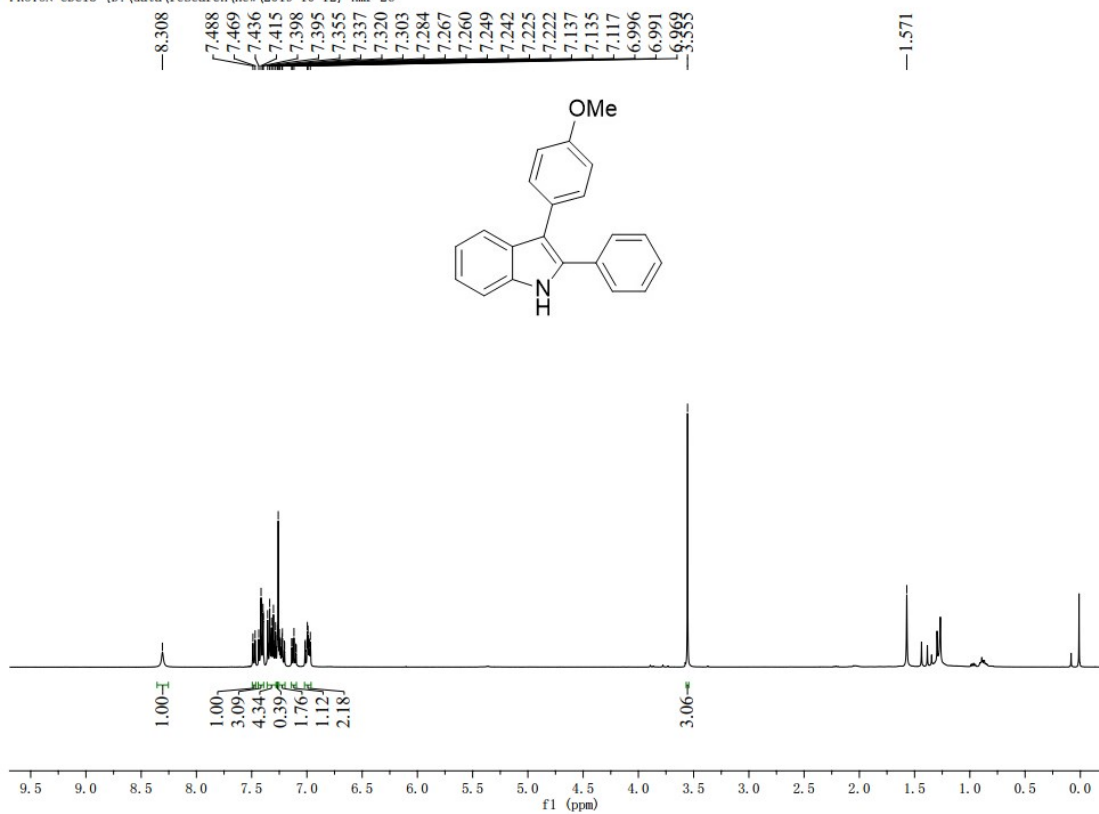
Compound 5a

PROTON CDC13 {D:\data\research\new\2019-10-24} nmr 9



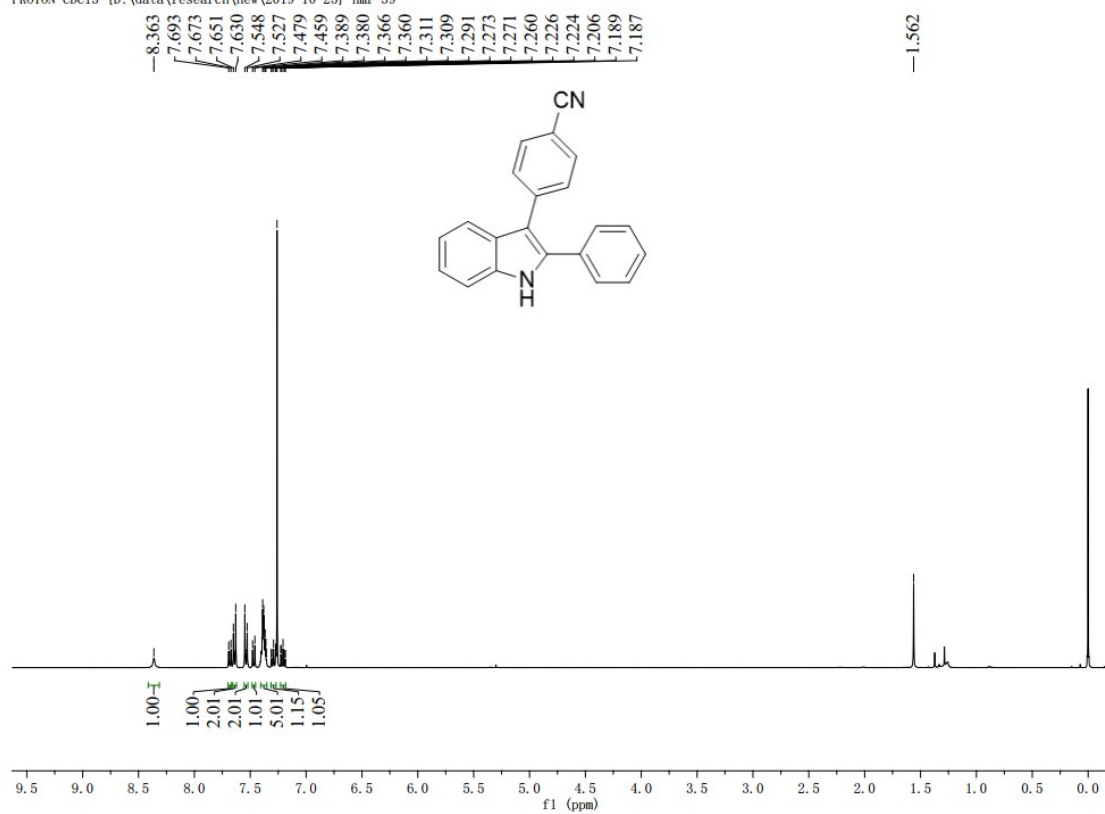
Compound 5b

PROTON CDC13 {D:\data\research\new\2019-10-12} nmr 26



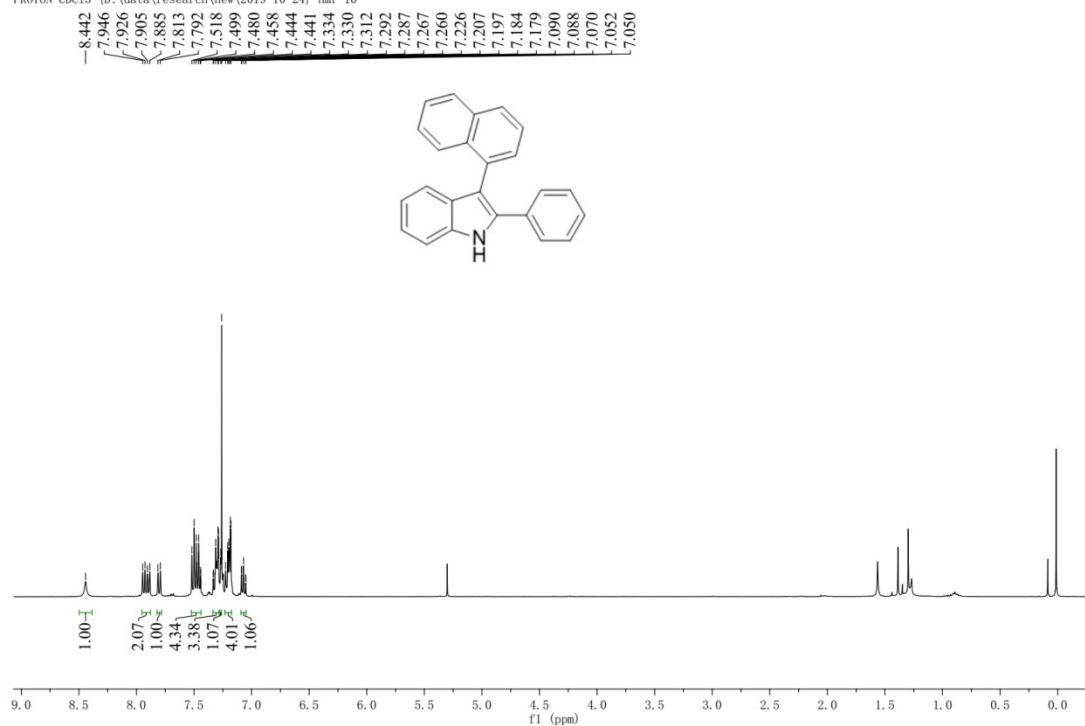
Compound 5c

PROTON CDC13 {D:\data\research\new\2019-10-25} nmr 39



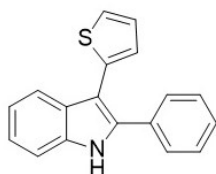
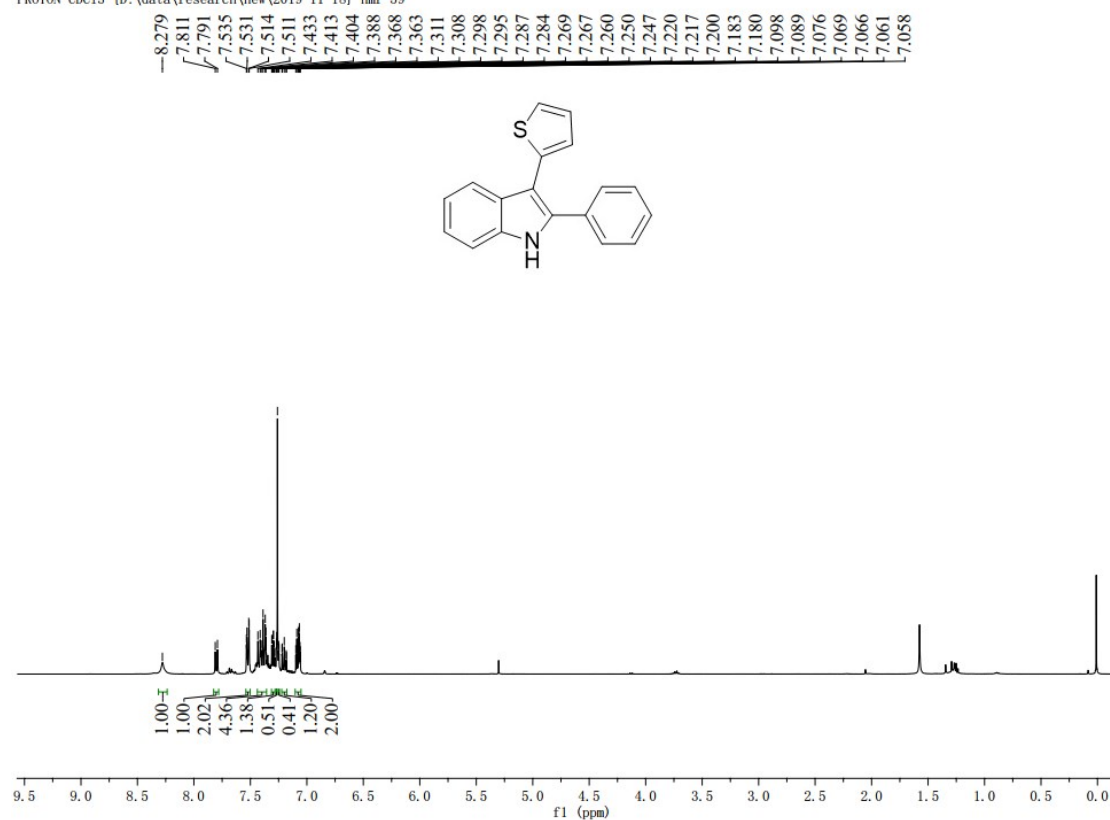
Compound 5d

PROTON CDC13 {D:\data\research\new\2019-10-24} nmr 10

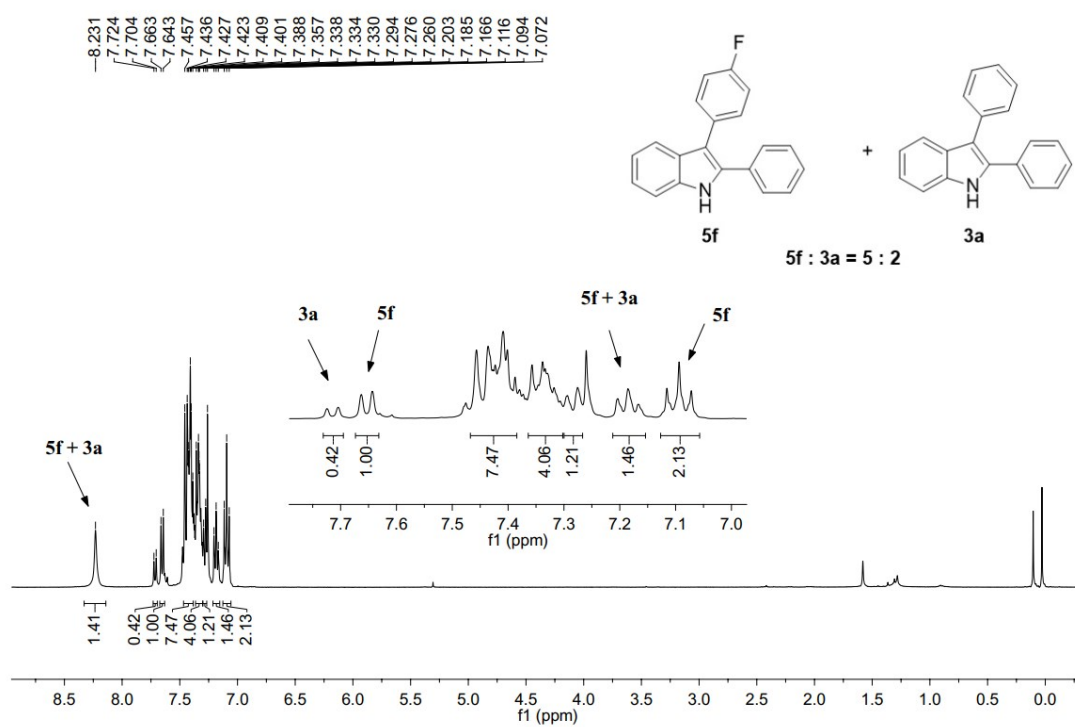


Compound 5e

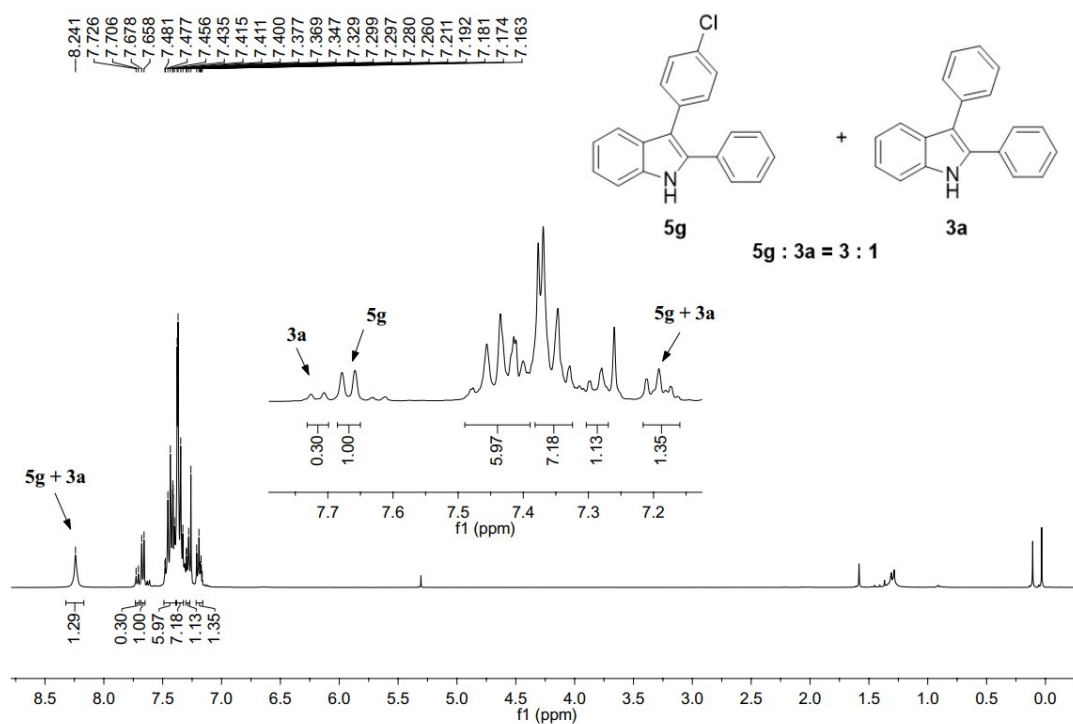
PROTON CDCl3 {D:\data\research\new\2019-11-18} nmr 59



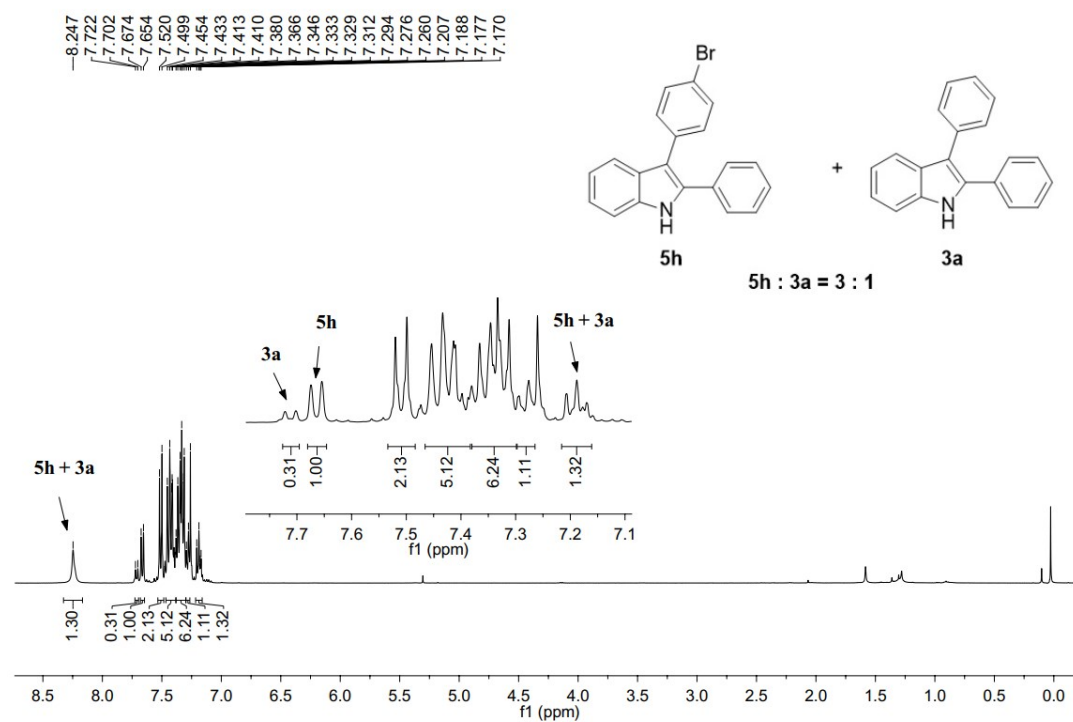
Compound 5f



Compound 5g



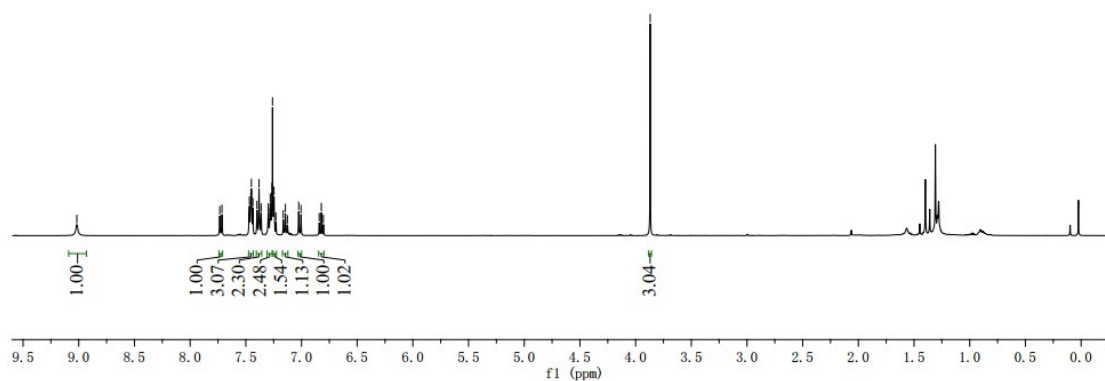
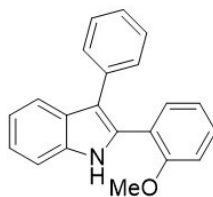
Compound 5h



Compound 5i

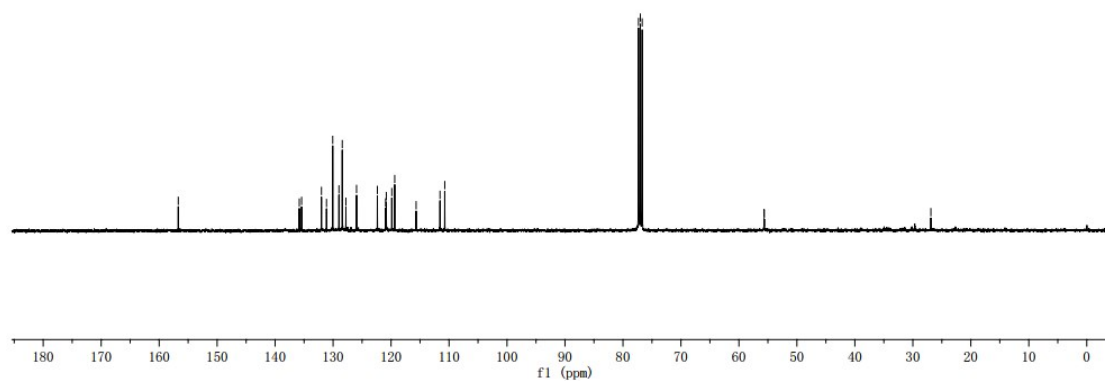
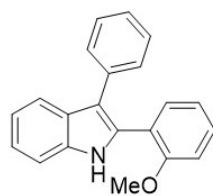
PROTON CDCl3 {D:\data\research\new\2020-5-29} nmr 17

9.017
7.734
7.714
7.468
7.454
7.450
7.437
7.400
7.381
7.362
7.299
7.295
7.280
7.275
7.265
7.260
7.247
7.230
7.164
7.144
7.126
7.025
7.005
6.841
6.822
6.803
-3.869



C13CPD CDCl3 {D:\data\research\new\2020-6-22} nmr 18

156.703
135.827
135.428
132.009
131.135
130.060
128.988
128.417
127.789
125.953
122.361
120.938
120.820
119.873
119.368
115.679
111.559
110.737
77.317
77.000
76.682
55.669
55.629
26.889

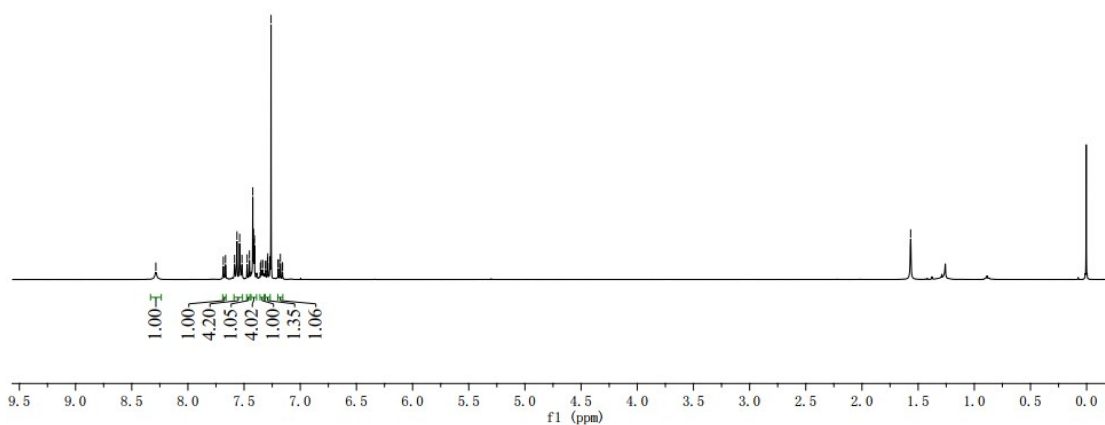
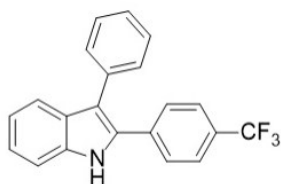


Compound 5j

PROTON CDC13 {D:\data\research\new\2020-6-19} nmr 7

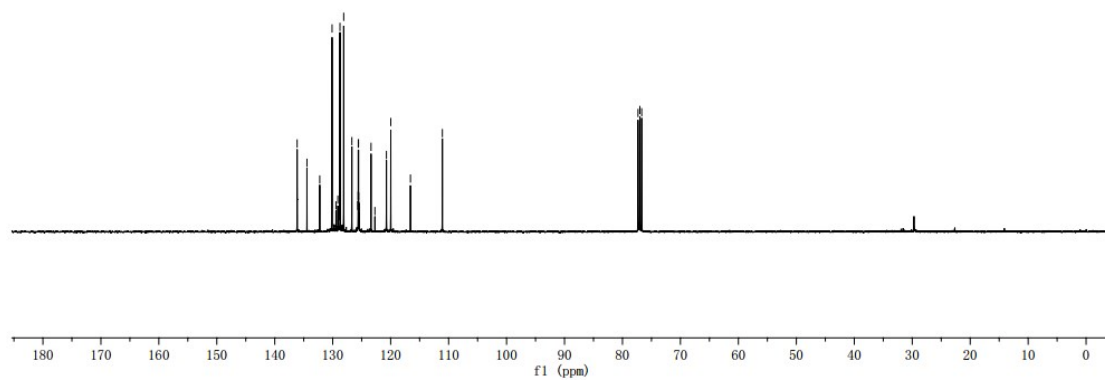
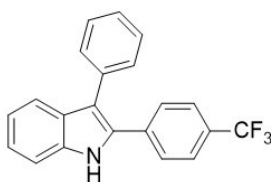
8.285
7.685
7.665
7.585
7.563
7.539
7.519
7.473
7.453
7.423
7.416
7.408
7.355
7.348
7.333
7.310
7.307
7.292
7.289
7.271
7.269
7.260
7.197
7.195
7.177
7.159
7.157

1.567

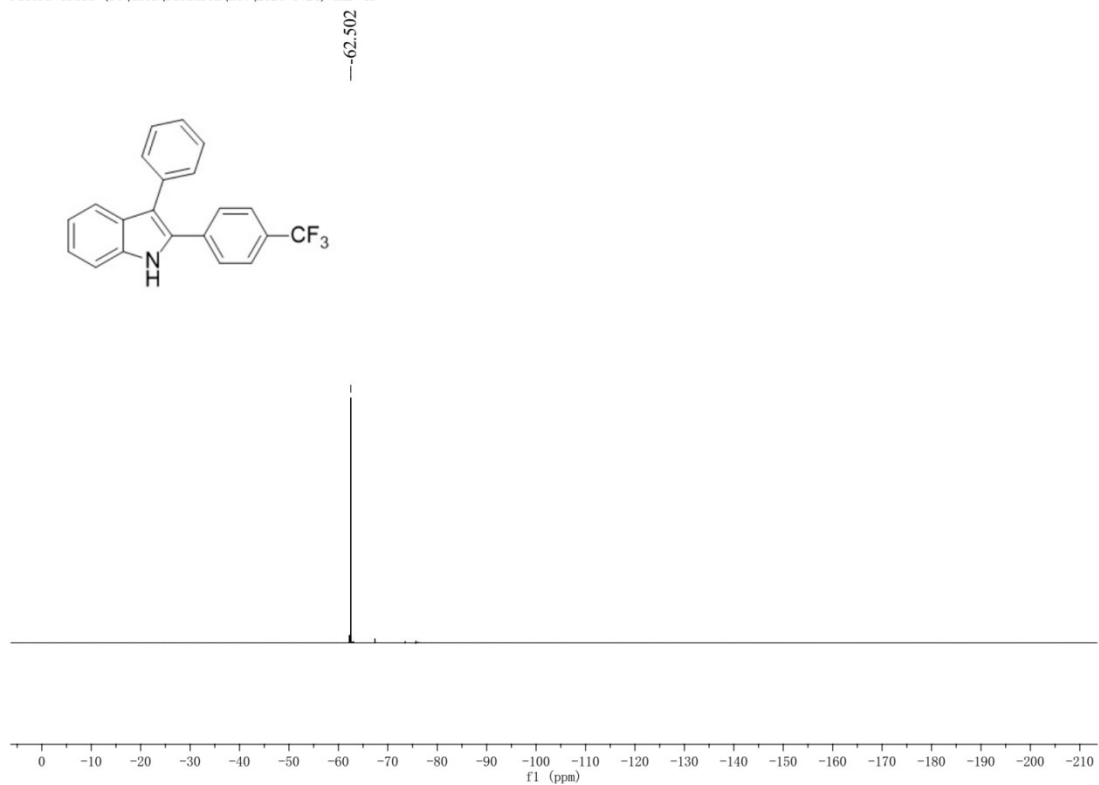


C13CPD CDC13 {D:\data\research\new\2020-6-22} nmr 21

136.139
134.440
132.235
130.108
129.435
129.112
128.746
128.673
128.100
126.694
125.621
125.584
125.546
125.509
125.421
123.385
122.716
120.729
119.977
116.582
111.079
77.318
77.000
76.683

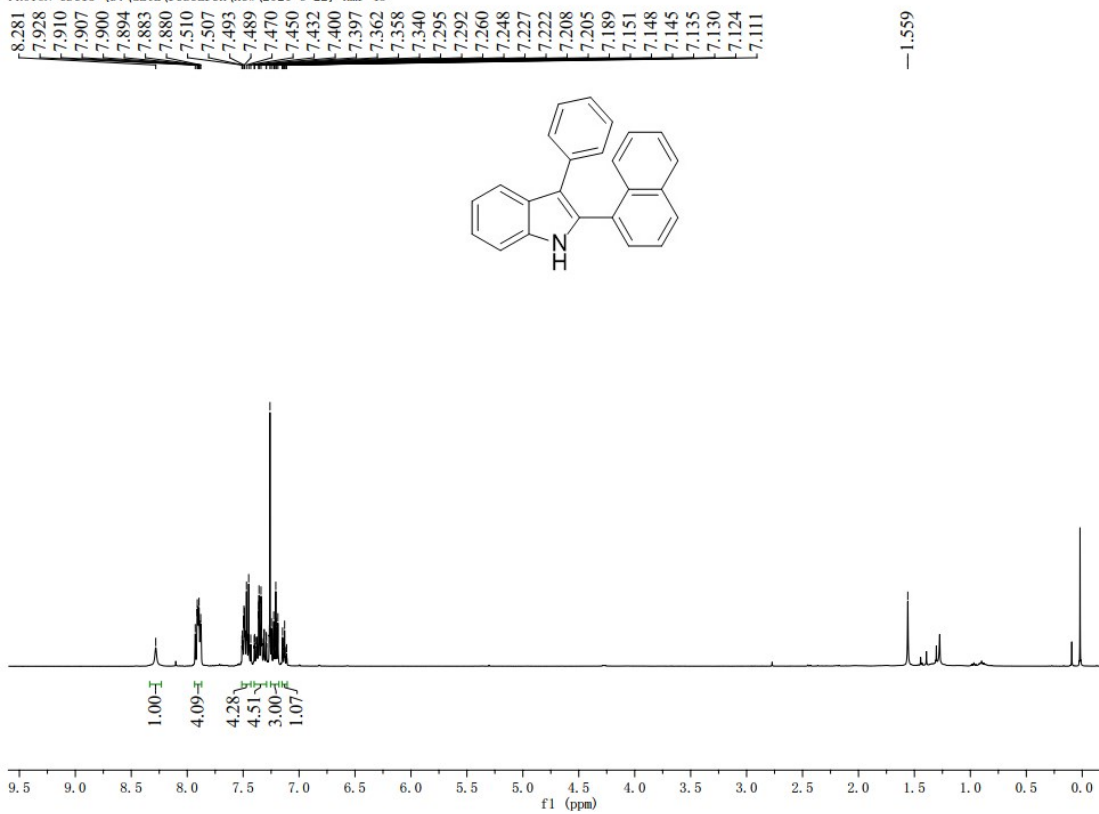


F19CPD CDC13 {D:\data\research\new\2020-6-24} nmr 43



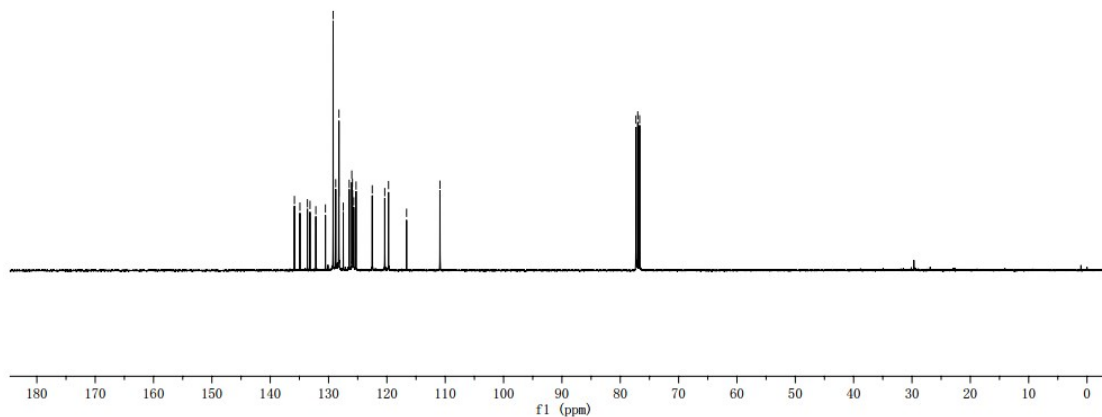
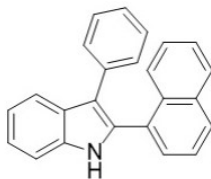
Compound 5k

PROTON CDC13 {D:\data\research\new\2020-6-22} nmr 48



C13CPD CDC13 {D:\data\research\new\2020-6-22} nmr 22

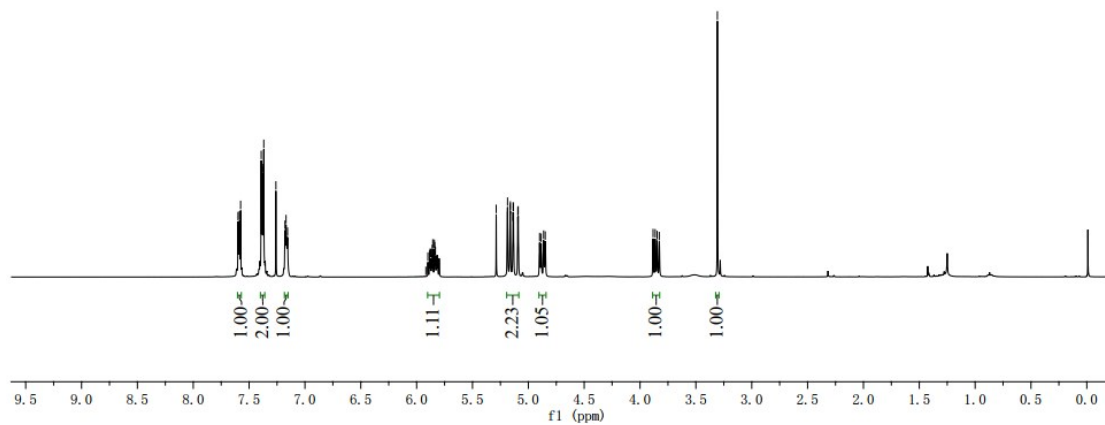
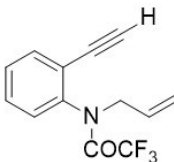
135.852
134.911
133.627
133.181
132.181
130.540
129.216
128.774
128.248
128.218
127.477
126.456
126.017
125.907
125.678
125.289
122.512
120.366
119.724
116.629
110.903
77.318
77.000
76.682



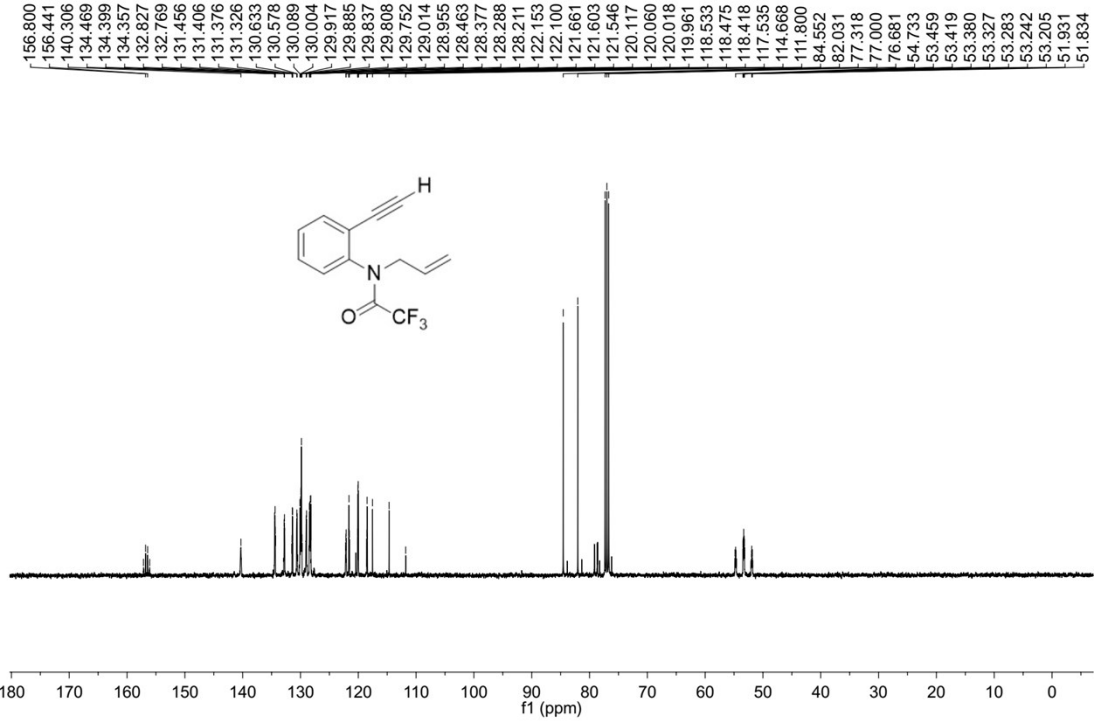
Compound 6

PROTON CDC13 {D:\data\research\new\2019-12-30} nmr 15

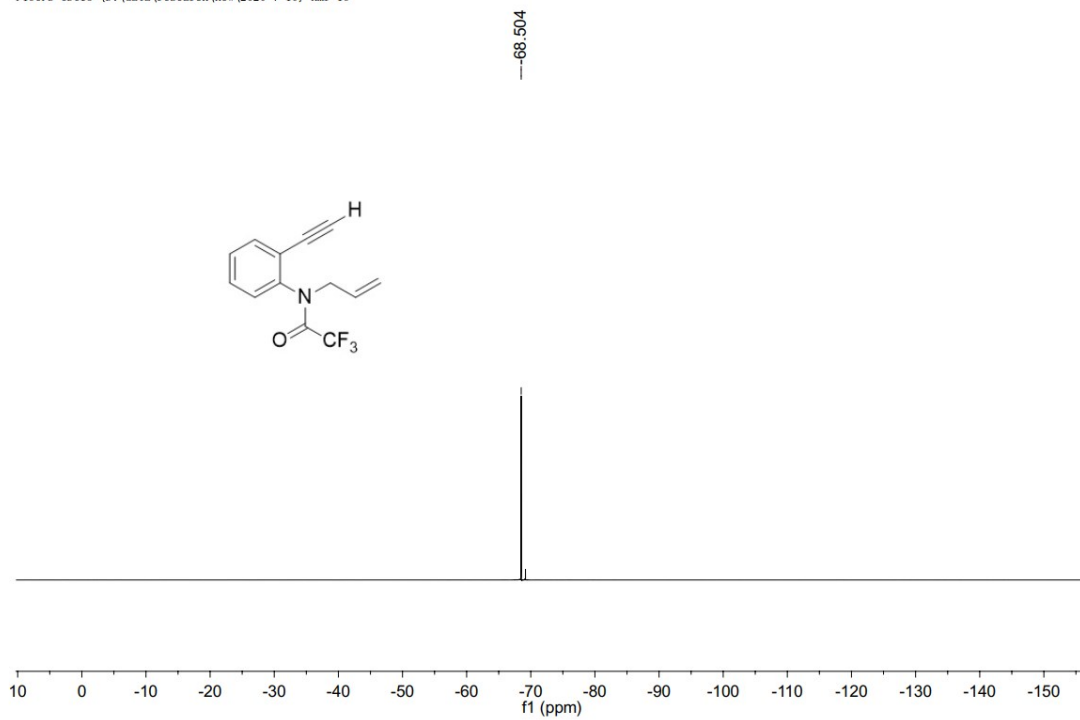
7.599
7.593
7.587
7.576
7.392
7.381
7.379
7.369
7.260
7.179
7.169
7.156
5.860
5.856
5.841
5.838
5.832
5.288
5.186
5.163
5.161
5.136
5.833
3.864
3.847
3.828
3.308



C13GD CDC13 [D:\data\research\new\2020-7-10] nmr 23

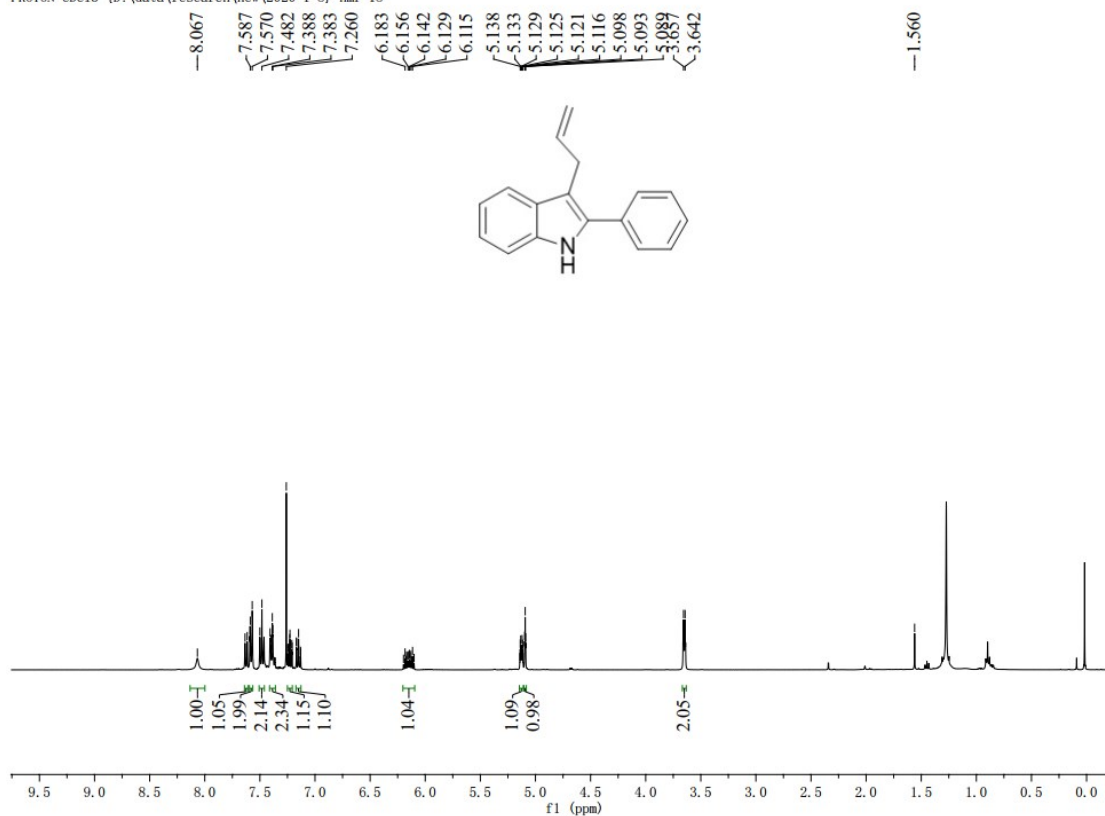


ju-wgd-001
F19CPD CDC13 [D:\data\research\new\2020-7-10] nmr 16



Compound 7

PROTON CDC13 {D:\data\research\new\2020-1-8} nmr 18



Compound 8

PROTON CDC13 {D:\data\research\new\2020-1-13} nmr 16

