Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Visible light-promoted, photocatalyst-free decarboxylative alkylations of 2*H*-indazoles via electron donor-acceptor-complex activation

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1. General information

Cesium Carbonate (Cs_2CO_3) was purchased from Titan Technology, Shanghai, China. Other reagents were purchased from Bidepharm.com. Unless otherwise stated, all commercially available reagents were directly used without further purification. All solvents were purified by standard methods prior to use. All reactions were monitored by thin layer chromatography (TLC), and column chromatography was carried out on 100-200 mesh of silica gel purchased from Tansoole, Shanghai, China. All nuclear magnetic resonance (NMR) spectra were recorded on a Bruker Avance 600 MHz in $CDCl_3$ at room temperature (20 ± 3 °C), using tetramethylsilane as internal standard. High-resolution mass spectra (HRMS) were conducted on a 3000-mass spectrometer, using Bruker compact Qq TOF MS/MS system with the ESI technique.

Photochemical reaction was carried out under visible light irradiation by a blue LED at 25 ºC. RLH-18 8-position Photo Reaction System manufactured by Beijing Roger Tech Ltd. was used in this system (See Figure A). Eight 10W blue LEDs were equipped in this Photo reactor. The blue LED's energy peak wavelength is 455 nm, peak width at half-height is 22.9 nm, lirradiance@10 W is 172.29 mW/cm^2. The reaction vessel is borosilicate glass test tube and no filters were applied.

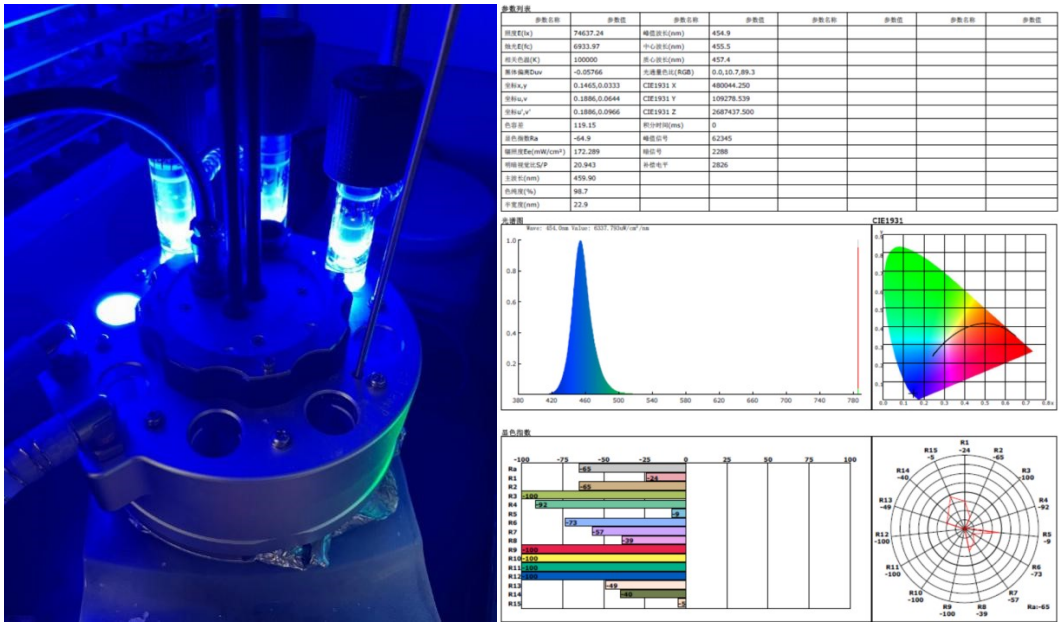
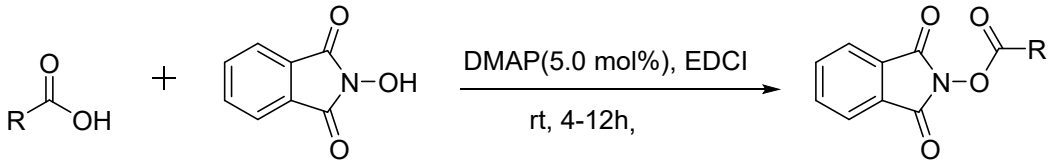


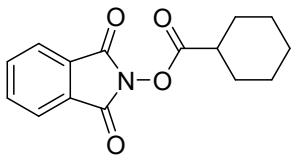
Figure S1. The reaction apparatus and spectrum of blue LED

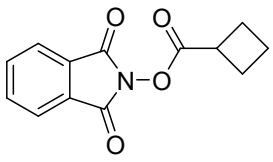
2. Experimental procedures

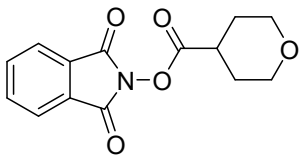
2.1 General Procedure for Redox-Active Esters Synthesis



To the round bottom flask were added carboxylic acid (5.0 mmol), *N*-hydroxyphthalimide (815.7 mg, 5.0 mmol), DMAP (30.5 mg, 0.25 mmol, 5.0 mol%) and DCM (25 mL), and then the mixture was stirred at room temperature. Then the EDCI (1.05 g, 5.5 mmol) was added and stirred for 4-12 hours. Upon completion monitored by the TLC, the mixture was filtered through a pad of Celite, washed with dichloromethane. The solution was washed with saturated sodium carbonate solution, and the organic layer was dried over anhydrous Na_2SO_4. The solution was then concentrated under reduced pressure and purified by silica gel column chromatography. Spectroscopic data for **2a**,[1] **2o**,[2] **2p**,[1] **2q**,[1] **2r**,[3] **2s**,[1] **2t**,[3] **2u**,[4] and **2v**[1] were in agreement with the literature.


2a


2o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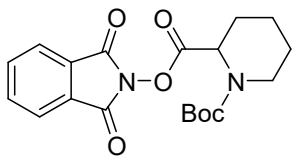
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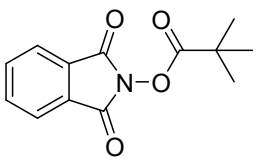
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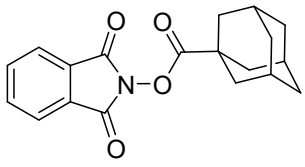
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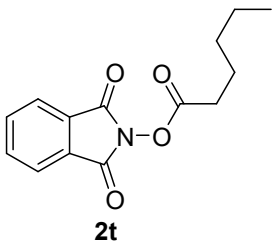
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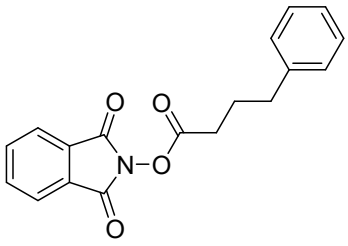
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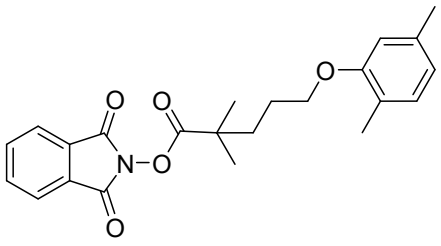
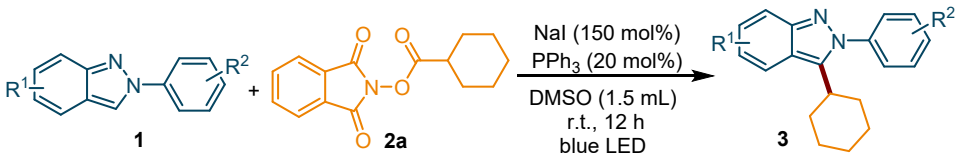
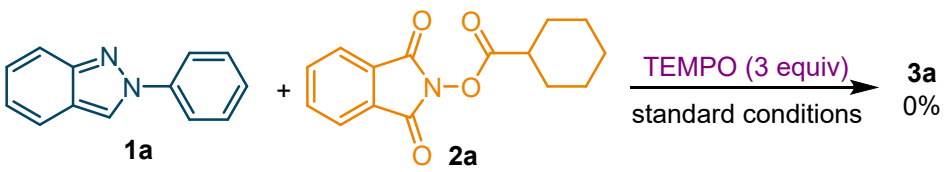

2v

2.2 General experimental procedures for decarboxylative alkylation of 2H-indazoles



In a 10 mL reaction vial with a stirring bar, 2-aryl-2*H*-indazole **1** (0.2 mmol), NHPI ester **2** (3.0 equiv.), NaI (150 mol%) and PPh_3 (20 mol%) were added. The vial was then evacuated and backfilled three times with N_2, followed by adding DMSO (1.5 mL). The mixture was stirred at room temperature with 10 W blue LED irradiation for 12 h under a nitrogen atmosphere. After the reaction was completed, it was quenched with water (5 mL), and then the ethyl acetate (15 mL) was added three times for extraction. The combined organic layers were dried over anhydrous Na_2SO_4 and evaporated under vacuum. The residue was purified by silica gel chromatography to afford the desired product **3**.

2.3 Control experiments



Control experiments with TEMPO: In a 10 mL reaction vial with a stirring bar, 2-phenyl-2*H*-indazole **1a** (0.2 mmol), cyclohexyl NHPI ester **2a** (3.0 equiv.), NaI (150 mol%) and PPh_3 (20 mol%), and 2,2,6,6-tetramethyl-1-piperidinyloxy (TEMPO, 3.0 equiv.) were added. The vial was then evacuated and backfilled three times with N_2, followed by adding DMSO (1.5 mL). The mixture was stirred at room temperature with 10 W blue LED irradiation for 12h under a nitrogen atmosphere. After the reaction was completed, it was quenched with water (5 mL), and then the ethyl acetate (15 mL) was added three times for extraction. No target product **3a** was generated.

2.4 UV-Vis mesurement

Stock solution of **2a** (0.4 mol/L) and the mixture of **2a** (0.4 mol/L), NaI (0.2 mol/L), and PPh_3 (0.027 mol/L) were prepared with the same concentration as the reaction using DMSO as the solvent.

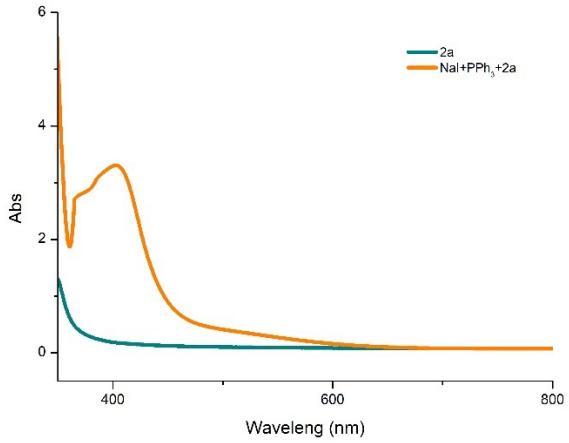
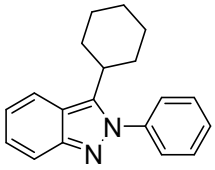


Figure S2. UV/vis absorption spectra of the **2a** and the mixture of **2a**, NaI, and PPh_3 in DMSO

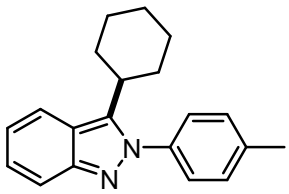
3. Characterization of compounds

*3-cyclohexyl-2-phenyl-2H-indazole **(3a)***[5]



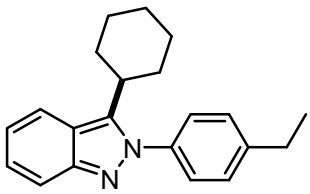
40.3 mg, 73%; White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.6 Hz, 1H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.55–7.47 (m, 5H), 7.31–7.28 (m, 1H), 7.07-7.03 (m, 1H), 3.00–2.93 (m, 1H), 2.04–1.75 (m, 8H), 1.42–1.31 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.0, 141.3, 140.3, 129.3, 129.1, 126.6, 126.5, 121.4, 120.7, 119.7, 118.0, 37.4, 32.7, 26.7, 26.0.

*3-cyclohexyl-2-(p-tolyl)-2H-indazole **(3b)***[5]



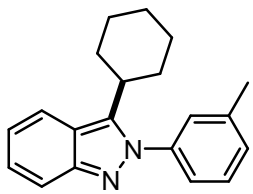
39.3 mg, 68%; White solid; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.6 Hz, 1H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.36–7.32 (m, 4H), 7.30–7.27 (m, 1H), 7.05-7.03 (m, 1H), 3.00–2.94 (m, 1H), 2.47 (s, 3H), 2.04–1.75 (m, 8H), 1.41–1.32 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 148.8, 141.3, 139.1, 137.8, 129.8, 126.3, 126.3, 121.3, 120.5, 119.5, 117.9, 37.4, 32.7, 26.7, 26.0, 21.4.

3-cyclohexyl-2-(4-ethylphenyl)-2H-indazole ***(3c)***[5]



40.7 mg, 67%; Yellow solid; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.5 Hz, 1H), 7.70 (d, *J* = 8.8 Hz, 1H), 7.39–7.34 (m, 4H), 7.30–7.27 (m, 1H), 7.05-7.02 (m, 1H), 3.00–2.96 (m, 1H), 2.77 (q, *J* = 7.6 Hz, 2H), 2.02–1.75 (m, 8H), 1.39–1.29 (m, 5H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 148.9, 145.4, 141.2, 138.0, 128.7, 126.4, 121.4, 120.5, 119.6, 117.9, 37.4, 32.7, 28.8, 26.7, 26.0, 15.6.

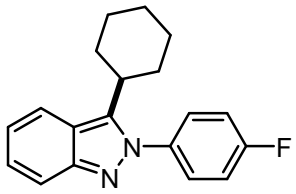
3-cyclohexyl-2-(m-tolyl)-2H-indazole ***(3d)***[5]



31.3 mg, 54%; Yellow solid; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.6 Hz, 1H), 7.71 (d, *J* = 8.7 Hz, 1H), 7.41 (t, *J* = 7.7 Hz, 1H), 7.32–7.23 (m, 3H), 7.24 (d, *J* = 7.7 Hz, 1H), 7.05–7.03 (m, 1H), 3.01–2.96 (m, 1H), 2.46 (s, 3H), 2.02–1.75 (m, 8H), 1.39–

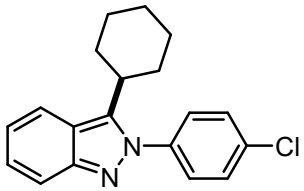
1.30 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 148.9, 141.2, 140.2, 139.5, 129.8, 128.9, 127.3, 126.4, 123.4, 121.4, 120.6, 119.6, 118.0, 37.4, 32.7, 26.7, 26.0, 21.5.

3-cyclohexyl-2-(4-fluorophenyl)-2H-indazole ***(3e)***[5]



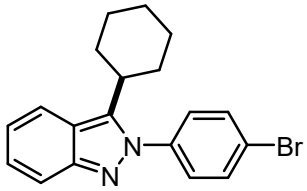
35.9 mg, 61%; White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.6 Hz, 1H), 7.69 (d, *J* = 8.8 Hz, 1H), 7.48–7.43 (m, 2H), 7.32–7.28 (m, 1H), 7.26–7.21 (m, 2H), 7.07–7.03 (m, 1H), 2.95–2.87 (m, 1H), 2.03–1.76 (m, 8H), 1.41–1.31 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.0, 161.6, 149.0, 141.5, 128.4, 128.3, 126.6, 121.3, 120.8, 119.6, 117.9, 116.4, 116.2, 37.5, 32.7, 26.7, 26.0. ^{19}F NMR (376 MHz, $CDCl_3$) δ -111.80.

2-(4-chlorophenyl)-3-cyclohexyl-2H-indazole ***(3f)***[5]



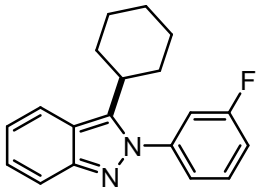
40.9 mg, 66%; Yellow solid; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.5 Hz, 1H), 7.70 (d, *J* = 8.8 Hz, 1H), 7.53–7.51 (m, 2H), 7.44–7.41 (m, 2H), 7.31–7.29 (m, 1H), 7.06–7.04 (m, 1H), 2.96–2.91 (m, 1H), 2.05–1.72 (m, 8H), 1.40–1.30 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 149.2, 141.4, 138.8, 135.1, 129.5, 127.8, 126.7, 121.4, 120.9, 119.7, 118.0, 37.5, 32.7, 26.7, 26.0.

2-(4-bromophenyl)-3-cyclohexyl-2H-indazole ***(3g)***[5]



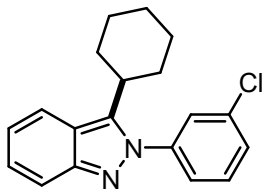
50.4 mg, 71%; White solid; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.6 Hz, 1H), 7.70–7.67 (m, 3H), 7.38–7.35 (m, 2H), 7.31–7.28 (m, 1H), 7.06–7.04 (m, 1H), 2.96–2.91 (m, 1H), 2.02–1.77 (m, 8H), 1.39–1.31 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 149.2, 141.3, 139.3, 132.5, 128.1, 126.7, 123.1, 121.4, 120.9, 119.7, 117.9, 37.5, 32.7, 26.7, 26.0.

*3-cyclohexyl-2-(3-fluorophenyl)-2H-indazole (**3h**)*



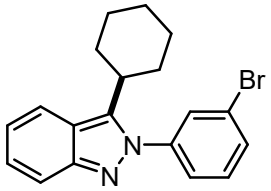
37.0 mg, 63%; Yellow solid; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.5 Hz, 1H), 7.70 (d, *J* = 8.8 Hz, 1H), 7.53–7.49 (m, 1H), 7.32–7.28 (m, 2H), 7.26–7.21 (m, 2H), 7.07-7.04 (m, 1H), 3.01–2.96 (m, 1H), 2.03–1.77 (m, 8H), 1.41–1.32 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.7 (d, *J* = 247.5 Hz), 149.2, 141.6 (d, *J* = 9.0 Hz), 141.3, 130.5 (d, *J* = 9.0 Hz), 126.8, 122.3 (d, *J* = 9.0 Hz), 121.4, 120.9, 119.7, 118.0, 116.2 (d, *J* = 21.0 Hz), 114.4 (d, *J* = 24.0 Hz), 37.5, 32.7, 26.7, 26.0. ^{19}F NMR (376 MHz, $CDCl_3$) δ -110.77.

*2-(3-chlorophenyl)-3-cyclohexyl-2H-indazole (**3i**)*[5]



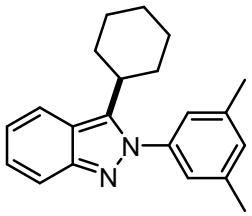
37.2 mg, 60%; Reddish brown solid; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.6 Hz, 1H), 7.69 (d, *J* = 8.8 Hz, 1H), 7.54–7.46 (m, 3H), 7.38-7.36 (m, 1H), 7.31–7.29 (m, 1H), 7.07–7.04 (m, 1H), 2.98–2.93 (m, 1H), 2.03–1.77 (m, 8H), 1.41–1.32 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 149.2, 141.4, 141.3, 135.1, 130.2, 129.4, 127.1, 126.8, 124.7, 121.4, 121.0, 119.7, 118.0, 37.5, 32.7, 26.7, 26.0.

2-(3-bromophenyl)-3-cyclohexyl-2H-indazole ***(3j)***[5]



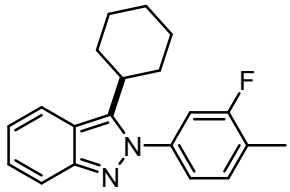
42.6 mg, 60%; White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.6 Hz, 1H), 7.70–7.64 (m, 3H), 7.42–7.40 (m, 2H), 7.32–7.26 (m, 1H), 7.07-7.03 (m, 1H), 3.00–2.92 (m, 1H), 2.04–1.77 (m, 8H), 1.43–1.33 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.2, 141.4, 132.3, 130.4, 129.9, 126.8, 125.1, 122.8, 121.4, 121.0, 119.7, 118.0, 37.5, 32.7, 26.7, 26.0.

3-cyclohexyl-2-(3,5-dimethylphenyl)-2H-indazole (3k)



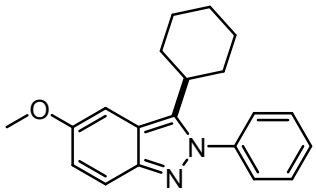
35.9 mg, 59%; White solid; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.85(d, *J* = 8.5 Hz, 1H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.30–7.26 (m, 1H), 7.13 (s, 1H), 7.09 (s, 2H), 7.05–7.02 (m, 1H), 3.03–2.97 (m, 1H), 2.41(s, 6H), 2.03–1.76 (m, 8H), 1.40–1.31 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 148.9, 141.1, 140.1, 139.1, 130.7, 126.3, 124.2, 121.3, 120.5, 119.6, 117.9, 37.4, 32.7, 26.7, 26.0, 21.4. HRMS Calcd for $C_{21}H_{25}N_2$ $[M + H]^+$: m/z 305.2012, Found: 305.2005.

3-cyclohexyl-2-(3-fluoro-4-methylphenyl)-2H-indazole ***(3l)***



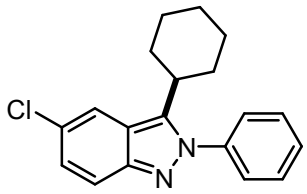
35.7 mg, 58%; White solid; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.6 Hz, 1H), 7.70 (d, *J* = 8.8 Hz, 1H), 7.34 (t, *J* = 8.1 Hz, 1H), 7.31–7.28 (m, 1H), 7.20-7.16 (m, 2H), 7.06–7.03 (m, 1H), 3.00–2.95 (m, 1H), 2.39 (d, *J* = 1.62 Hz, 3H), 2.05–1.76 (m, 8H), 1.40–1.30 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.0 (d, *J* = 244.5 Hz), 149.0, 141.3, 139.1 (d, *J* = 9.0 Hz), 131.7 (d, *J* = 6.0 Hz), 126.6, 126.2 (d, *J* = 18.0 Hz), 121.9 (d, *J* = 3 Hz), 121.4, 120.8, 119.6, 118.0, 113.8 (d, *J* = 25.5 Hz), 37.4, 32.7, 26.7, 26.0, 21.4. ^{19}F NMR (376 MHz, $CDCl_3$) δ -115.00. HRMS Calcd for $C_{22}H_{22}FN_2$ $[M + H]^+$: m/z 309.1762, Found: 309.1772.

3-cyclohexyl-5-methoxy-2-phenyl-2H-indazole ***(3m)***



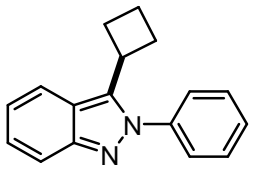
25.7 mg, 42%; Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 10.0 Hz, 1H), 7.55–7.45 (m, 5H), 7.04-7.01 (m, 2H), 3.89 (s, 3H), 2.98–2.90 (m, 1H), 1.97–1.75 (m, 8H), 1.38–1.03 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.1, 145.9, 140.5, 139.9, 129.2, 128.9, 126.5, 121.2, 119.4, 119.2, 97.9, 55.7, 37.2, 32.4, 26.7, 26.0. HRMS Calcd for $C_{20}H_{23}N_2O$ $[M + H]^+$: m/z 307.1805, Found: 307.1837.

5-chloro-3-cyclohexyl-2-phenyl-2H-indazole ***(3n)***



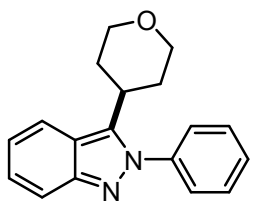
42.2 mg, 68%; Gray solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 1.4 Hz, 1H), 7.64 (d, *J* = 9.2 Hz, 1H), 7.58–7.52 (m, 3H), 7.47–7.45 (m, 2H), 7.22 (dd, *J* = 1.9, 7.2 Hz, 1H), 2.98–2.90 (m, 1H), 1.94–1.75 (m, 8H), 1.42–1.30 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.3, 141.2, 140.0, 129.4, 127.8, 126.5, 126.1, 120.02, 119.97, 119.5, 37.3, 32.7, 26.6, 25.9. HRMS Calcd for $C_{19}H_{20}ClN_2$ $[M + H]^+$: m/z 311.1310, Found: 311.1341.

3-cyclobutyl-2-phenyl-2H-indazole ***(3o)***[5]



33.4 mg, 67%; Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 8.6 Hz, 1H), 7.72 (d, *J* = 8.8 Hz, 1H), 7.54–7.47 (m, 5H), 7.33–7.29 (m, 1H), 7.10–7.06 (m, 1H), 3.99–3.90 (m, 1H), 2.62–2.55 (m, 2H), 2.37–2.30 (m, 2H), 2.10–1.94 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.0, 140.4, 139.3, 129.2, 128.9, 126.5, 126.2, 121.0, 120.6, 118.0, 33.1, 29.3, 19.1.

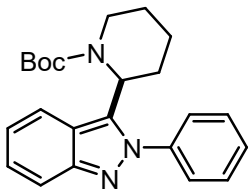
2-phenyl-3-(tetrahydro-2H-pyran-4-yl)-2H-indazole ***(3p)***[5]



40.6 mg, 73%; White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.6 Hz, 1H), 7.72 (d, *J* = 8.8 Hz, 1H), 7.59–7.53 (m, 3H), 7.49–7.46 (m, 2H), 7.34–7.30 (m, 1H),

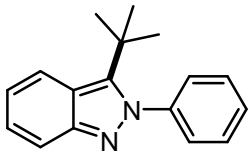
7.11–7.07 (m, 1H), 4.09 (d, *J* = 4.2 Hz, 1H), 4.06 (d, *J* = 4.3 Hz, 1H), 3.44–3.37 (m, 2H), 3.27–3.19 (m, 1H), 2.44–2.33 (m, 2H), 1.79 (dd, *J* = 2.0, 11.2 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.0, 140.1, 139.0, 129.5, 129.4, 126.62, 126.56, 121.3, 120.8, 119.8, 118.2, 68.2, 34.7, 32.2.

tert-butyl (S)-2-(2-phenyl-2H-indazol-3-yl)piperidine-1-carboxylate ***(3q)***



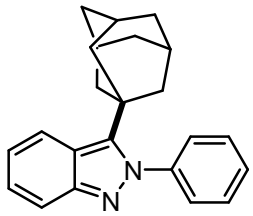
48.3 mg, 64%; White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.8 Hz, 1H), 7.61 (d, *J* = 8.7 Hz, 1H), 7.55–7.45 (m, 5H), 7.30–7.26 (m, 1H), 7.08–7.05 (m, 1H), 5.71–5.68 (m, 1H), 3.90–3.84 (m, 1H), 3.12–3.05 (m, 1H), 2.01–1.94 (m, 1H), 1.73–1.65 (m, 1H), 1.58–1.46 (m, 4H), 1.29 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.1, 129.4, 129.2, 126.4, 125.9, 122.0, 121.0, 120.3, 118.2, 80.3, 51.0, 41.4, 28.6, 28.5, 24.2, 20.0. HRMS Calcd for $C_{23}H_{28}N_3O_2$ $[M + H]^+$: m/z 378.2176, Found: 378.2193.

3-(tert-butyl)-2-phenyl-2H-indazole ***(3r)***[5]



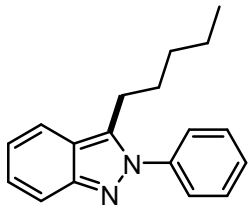
24.0 mg, 48%; White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.8 Hz, 1H), 7.67 (d, *J* = 8.7 Hz, 1H), 7.53–7.42 (m, 5H), 7.30–7.26 (m, 1H), 7.07–7.03 (m, 1H), 1.43 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.6, 144.6, 143.1, 129.5, 128.6, 128.2, 126.1, 122.7, 120.9, 119.8, 118.0, 32.0.

3-((3r,5r,7r)-adamantan-1-yl)-2-phenyl-2H-indazole ***(3s)***[5]



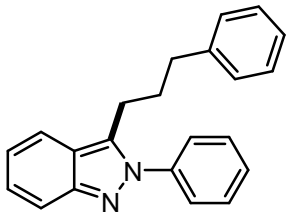
28.9 mg, 44%; White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.8 Hz, 1H), 7.67 (d, *J* = 8.7 Hz, 1H), 7.51–7.41 (m, 5H), 7.29–7.25 (m, 1H), 7.05–7.01 (m, 1H), 2.14 (d, *J* = 2.7 Hz, 6H), 1.99 (s, 3H), 1.73–1.65 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.7, 144.8, 143.5, 129.4, 128.5, 128.3, 126.0, 123.1, 120.6, 119.6, 118.0, 42.7, 37.9, 36.5, 28.7.

3-hexyl-2-phenyl-2H-indazole ***(3t)***[5]



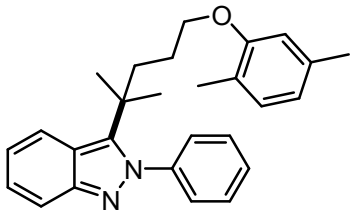
49.5 mg, 89%; Yellow oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.8 Hz, 1H), 7.68 (d, *J* = 8.5 Hz, 1H), 7.56–7.48 (m, 5H), 7.33–7.26 (m, 1H), 7.09–7.06 (m, 1H), 3.03 (t, 2H), 1.68–1.63 (m, 2H), 1.26–1.24 (m, 4H), 0.83–0.81 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.7, 140.2, 137.1, 129.3, 129.0, 126.7, 126.3, 121.2, 121.0, 120.4, 117.7, 31.6, 29.2, 25.4, 22.3, 14.0.

2-phenyl-3-(3-phenylpropyl)-2H-indazole ***(3u)***[5]



20.0 mg, 32%; Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.8 Hz, 1H), 7.62 (d, *J* = 8.5 Hz, 1H), 7.53–7.49 (m, 5H), 7.34–7.30 (m, 1H), 7.27–7.23 (m, 2H), 7.20–7.16 (m, 1H), 7.10–7.05 (m, 3H), 3.07 (t, *J* = 7.6 Hz, 2H), 2.60 (t, *J* = 7.5 Hz, 2H), 2.03–1.95 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.8, 141.3, 140.1, 136.4, 129.3, 129.0, 128.54, 128.45, 126.8, 126.20, 126.15, 121.3, 121.2, 120.3, 117.8, 35.5, 30.9, 24.9.

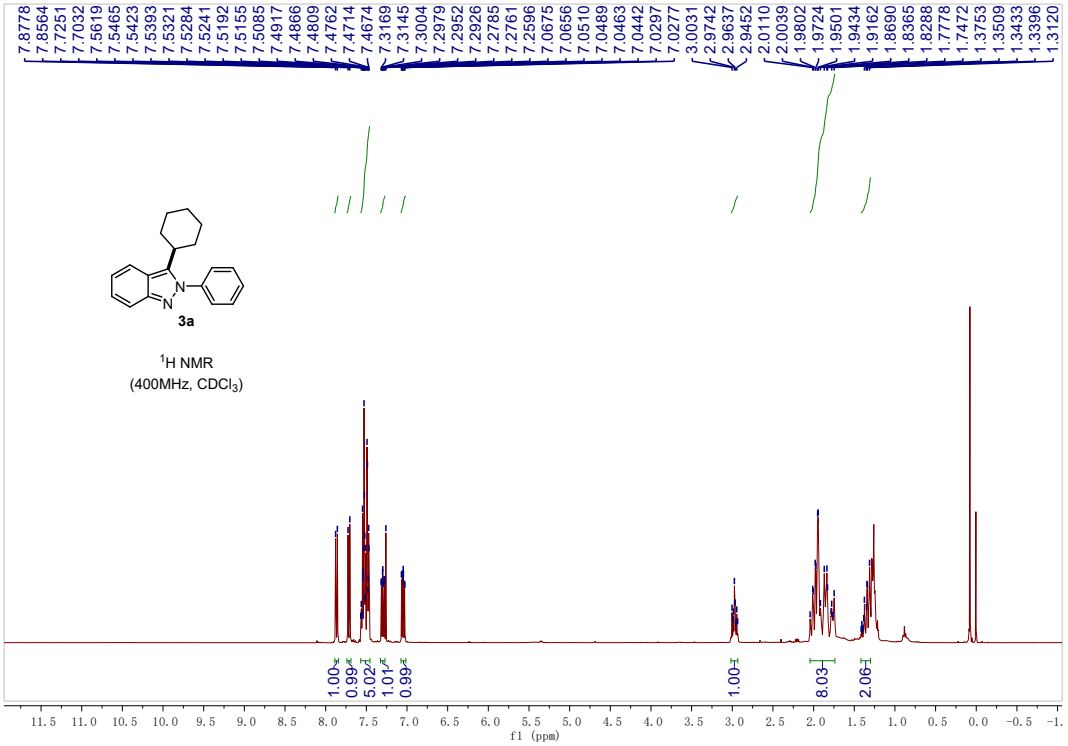
3-(5-(2,5-dimethylphenoxy)-2-methylpentan-2-yl)-2-phenyl-2H-indazole ***(3v)***[5]



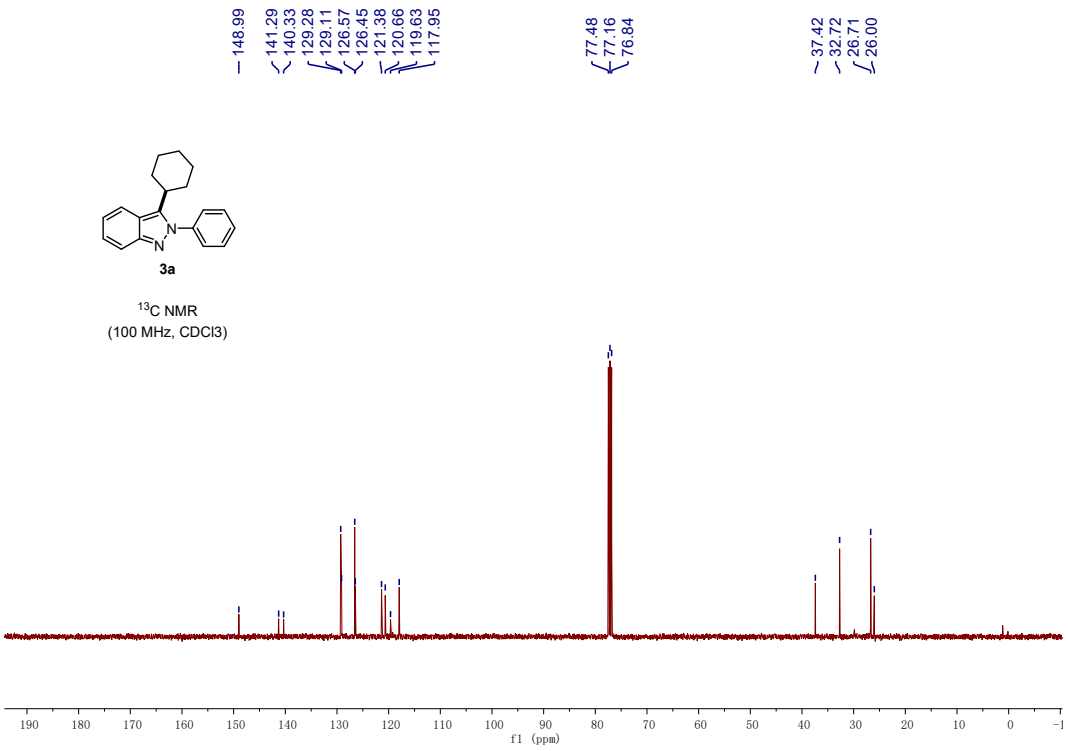
46.2 mg, 58%; White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.8 Hz, 1H), 7.69 (d, *J* = 8.7 Hz, 1H), 7.54–7.43 (m, 5H), 7.32–7.28 (m, 1H), 7.08–7.04 (m, 1H), 6.99 (d, *J* = 7.4 Hz, 1H), 6.65 (d, *J* = 7.5 Hz, 1H), 6.53 (s, 1H), 3.82 (t, *J* = 6.1 Hz, 2H), 2.28 (s, 3H), 2.15 (s, 3H), 1.99–1.94 (m, 2H), 1.67–1.59 (m, 2H), 1.43 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ157.0, 148.6, 143.0, 142.9, 136.6, 130.4, 129.6, 128.7, 128.0, 126.2, 123.6, 122.5, 121.2, 120.9, 120.5, 118.0, 112.0, 67.9, 40.8, 38.2, 30.3, 25.5, 21.5, 16.0.

4. NMR copies of products

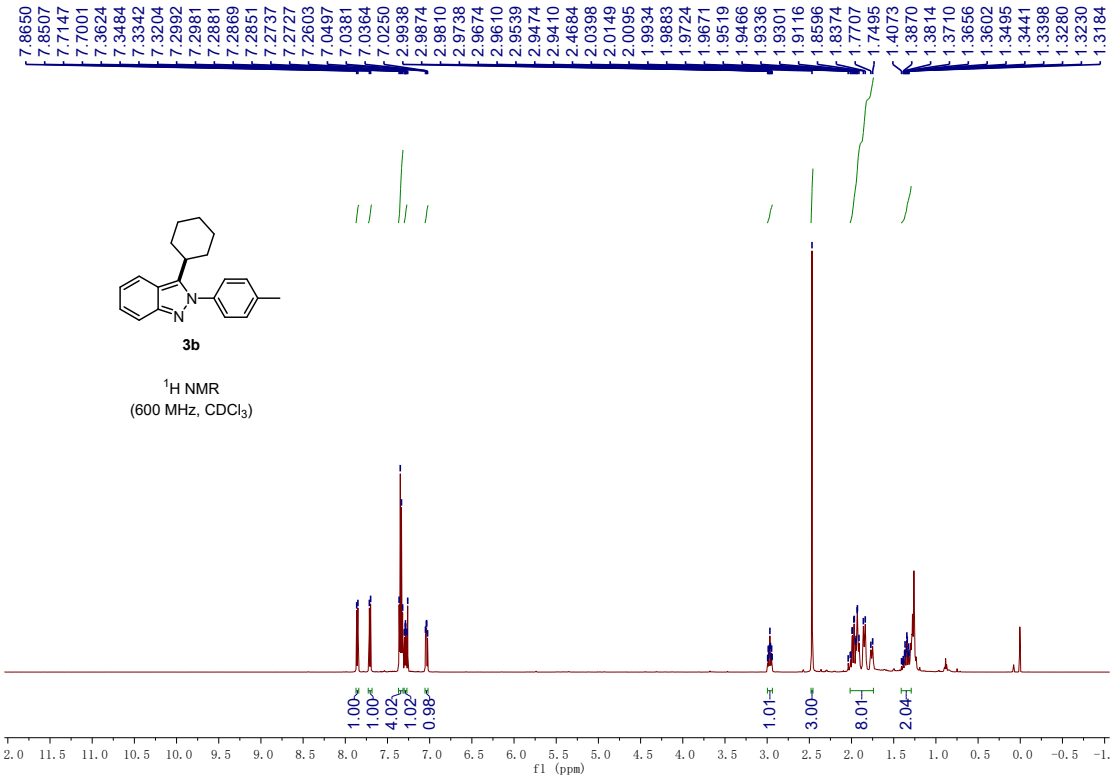
^{1}H NMR spectrum of 3a



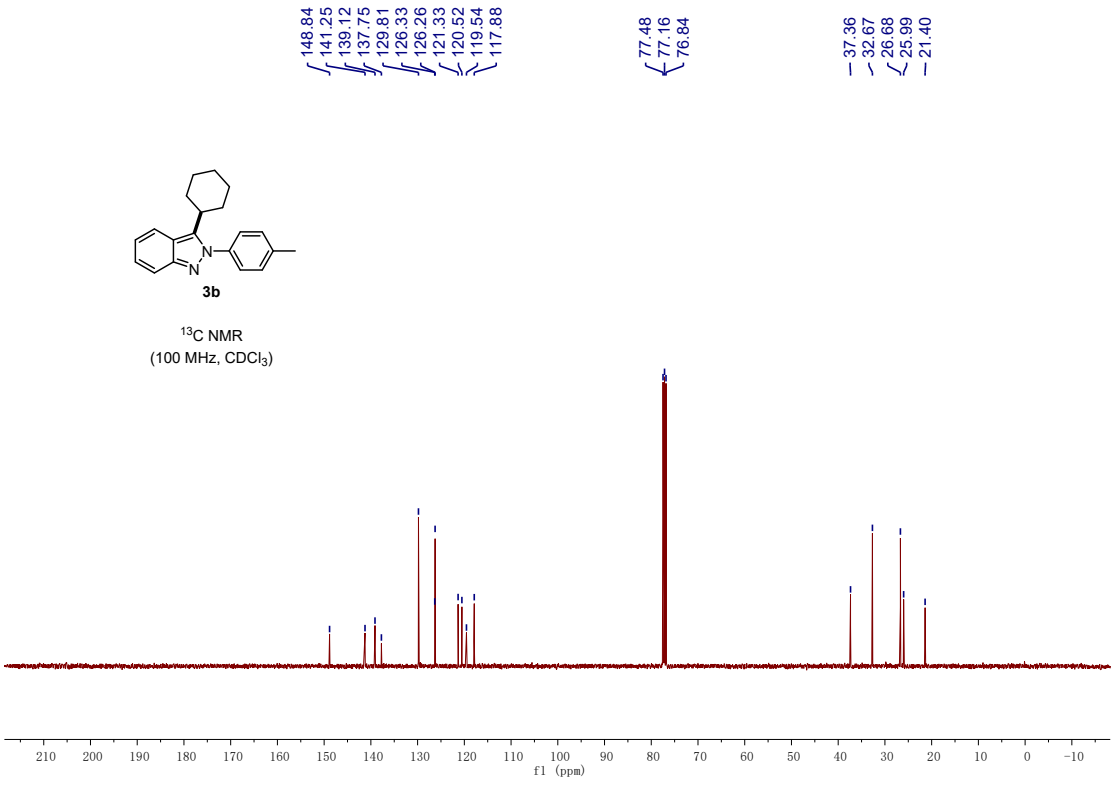
^{13}C NMR spectrum of 3a



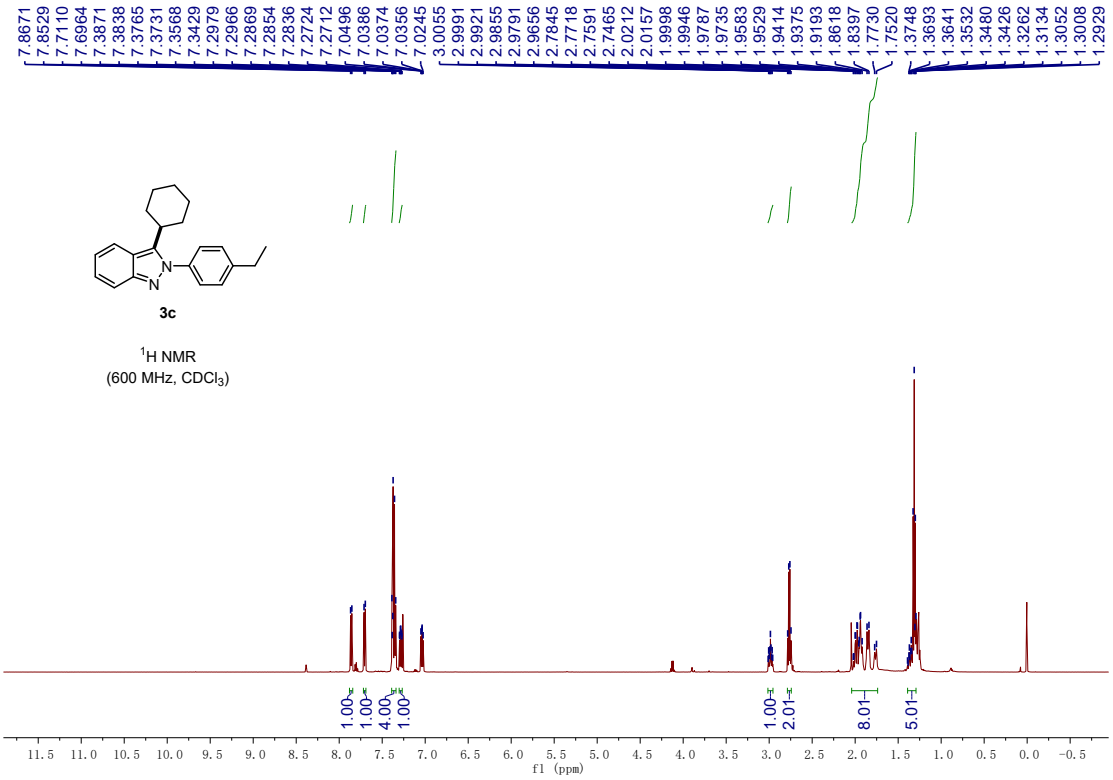
^{1}H NMR spectrum of 3b



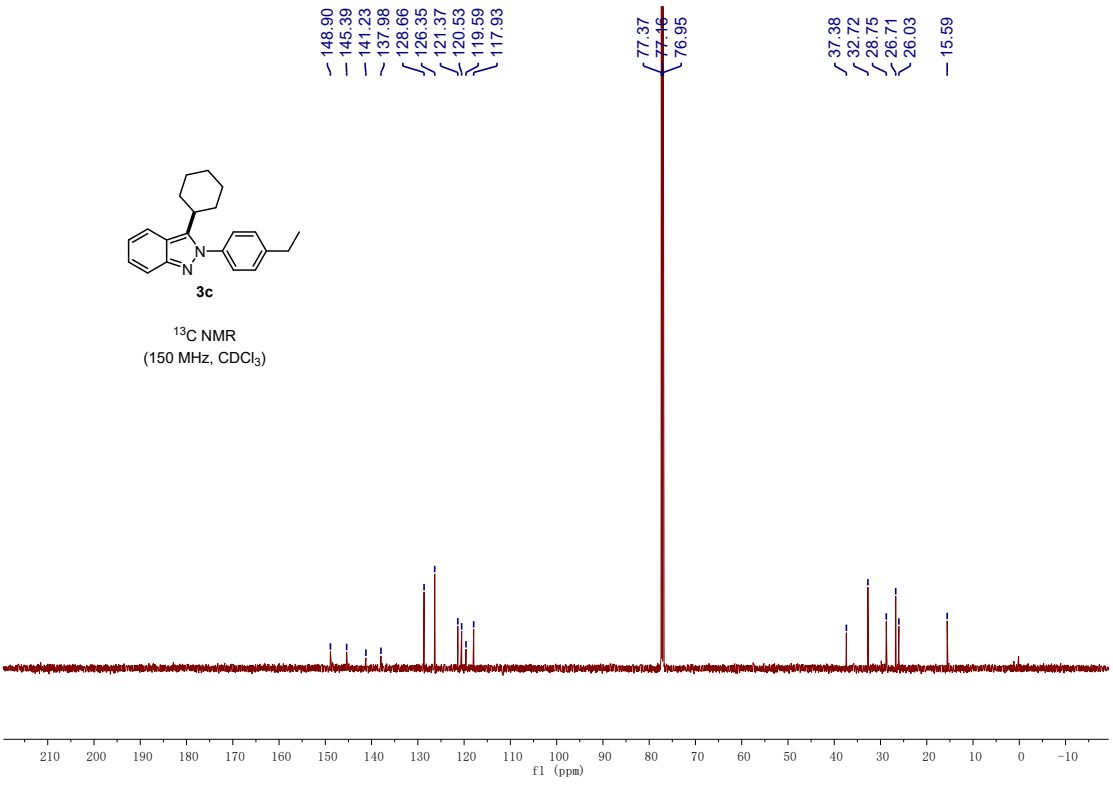
^{13}C NMR spectrum of 3b



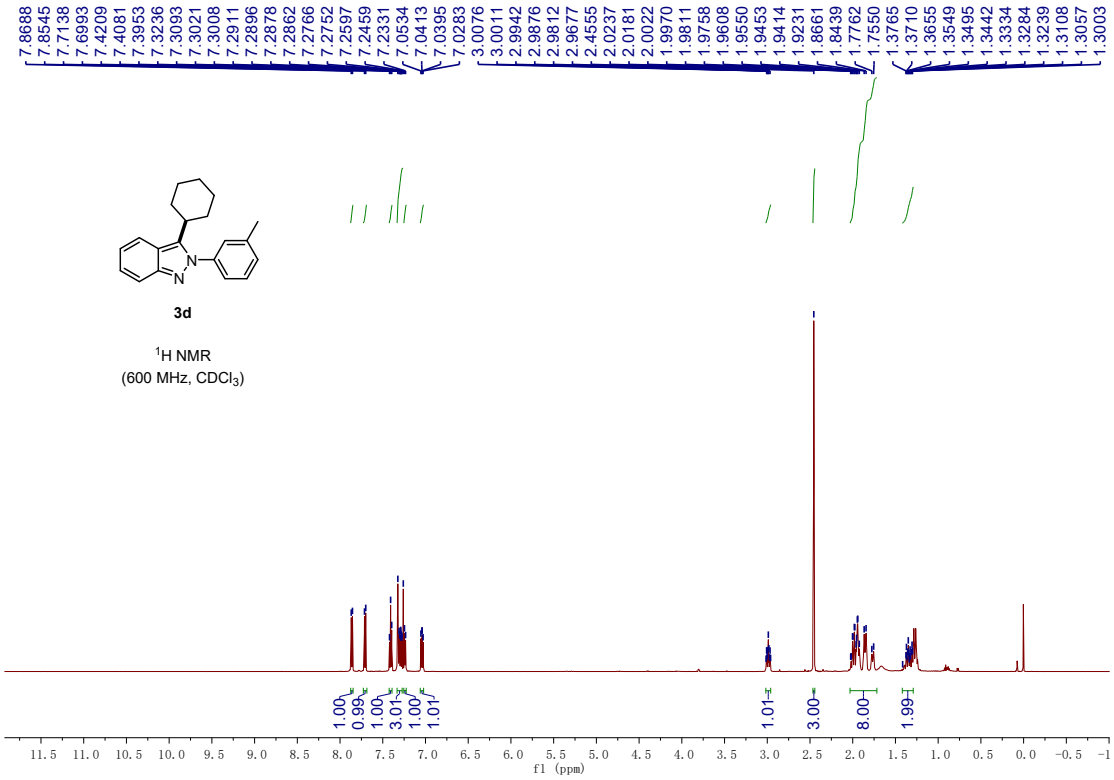
^{1}H NMR spectrum of 3c



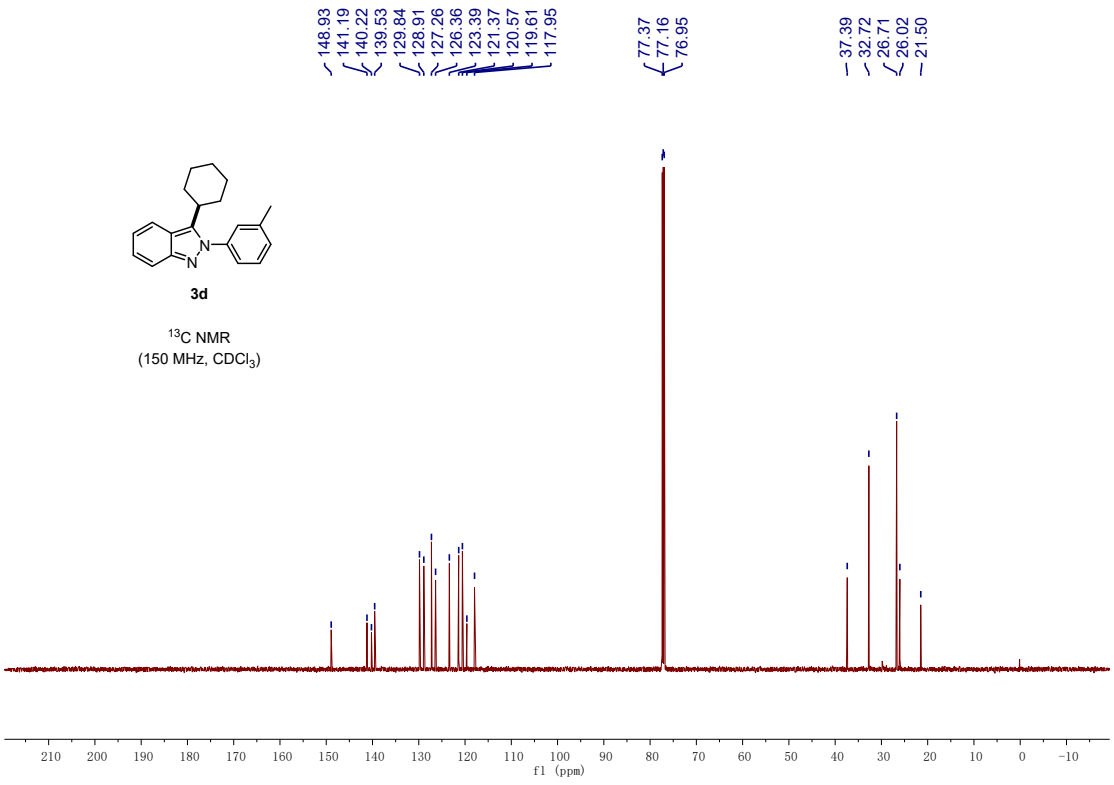
^{13}C NMR spectrum of 3c



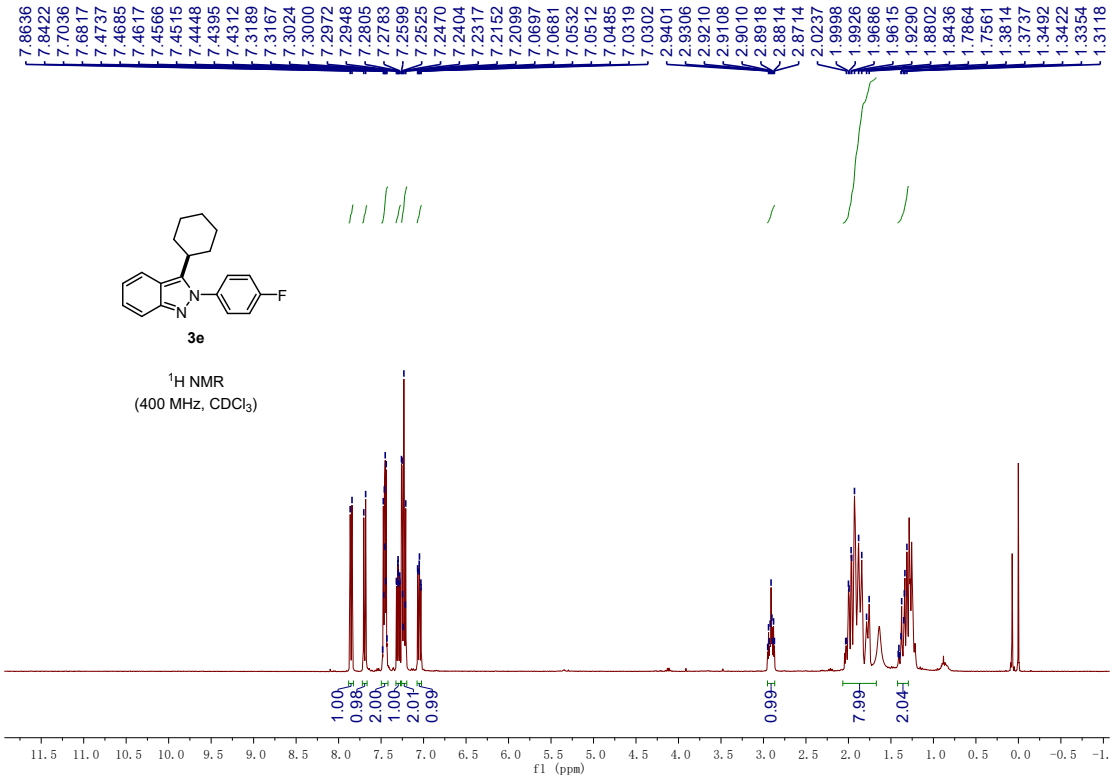
^{1}H NMR spectrum of 3d



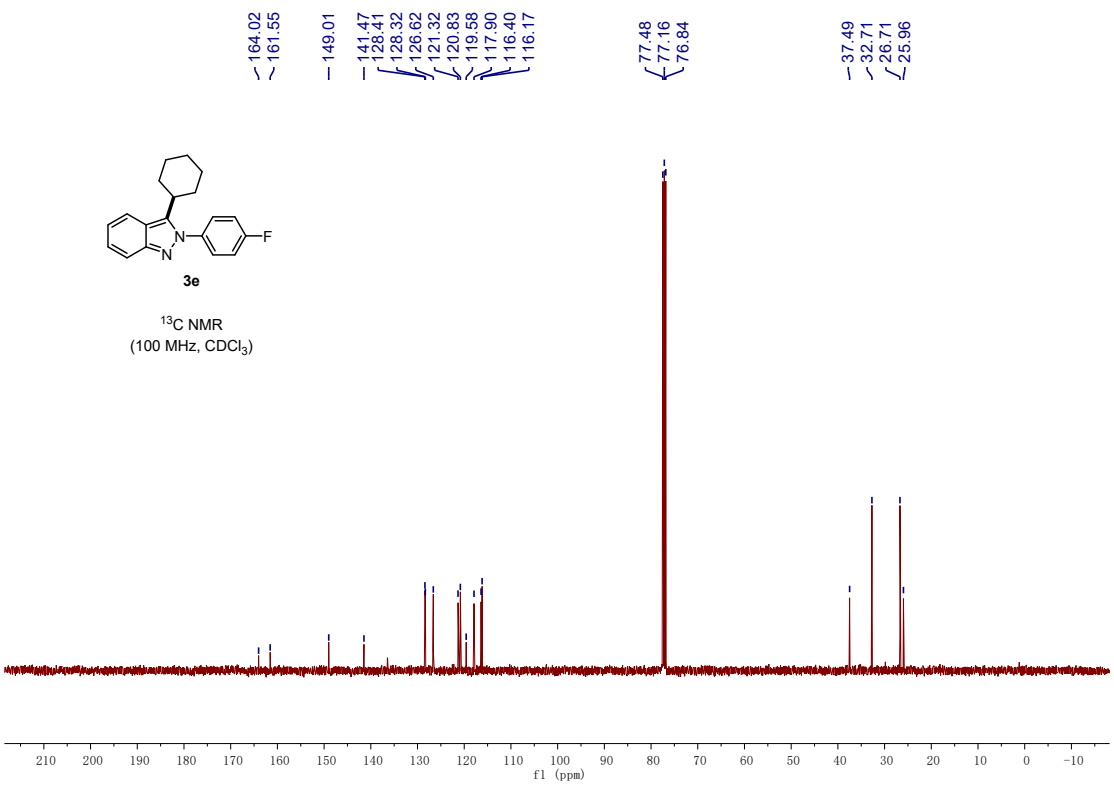
^{13}C NMR spectrum of 3d



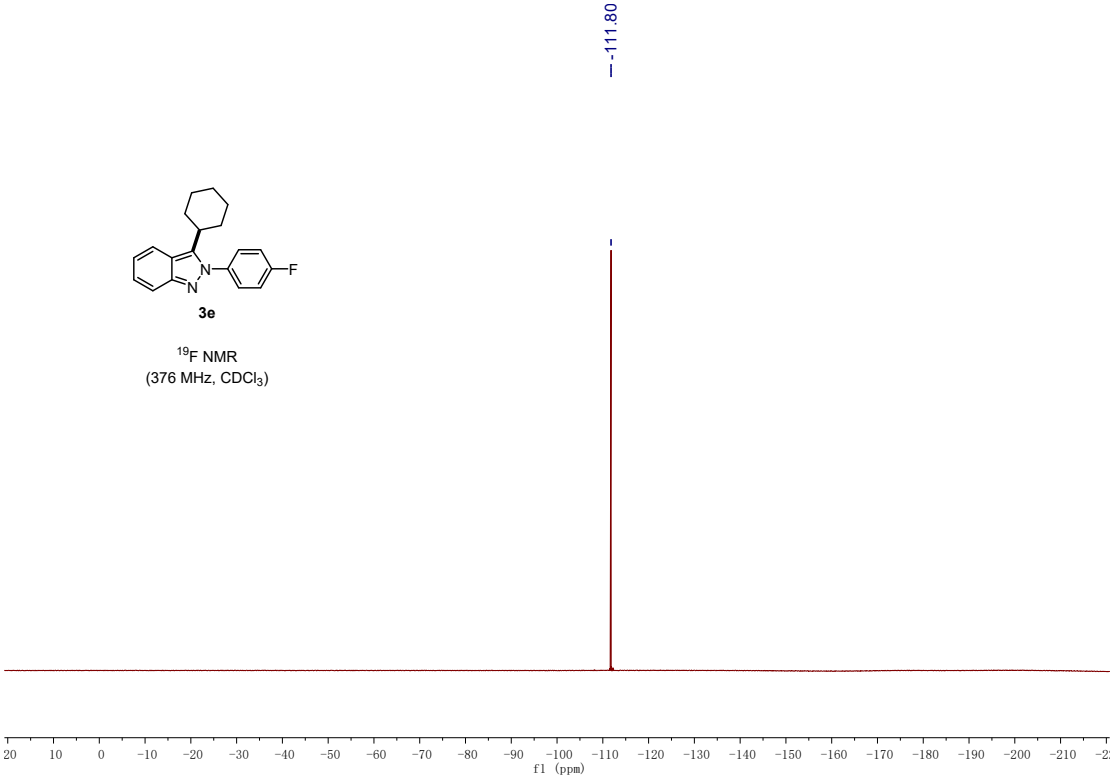
^{1}H NMR spectrum of 3e



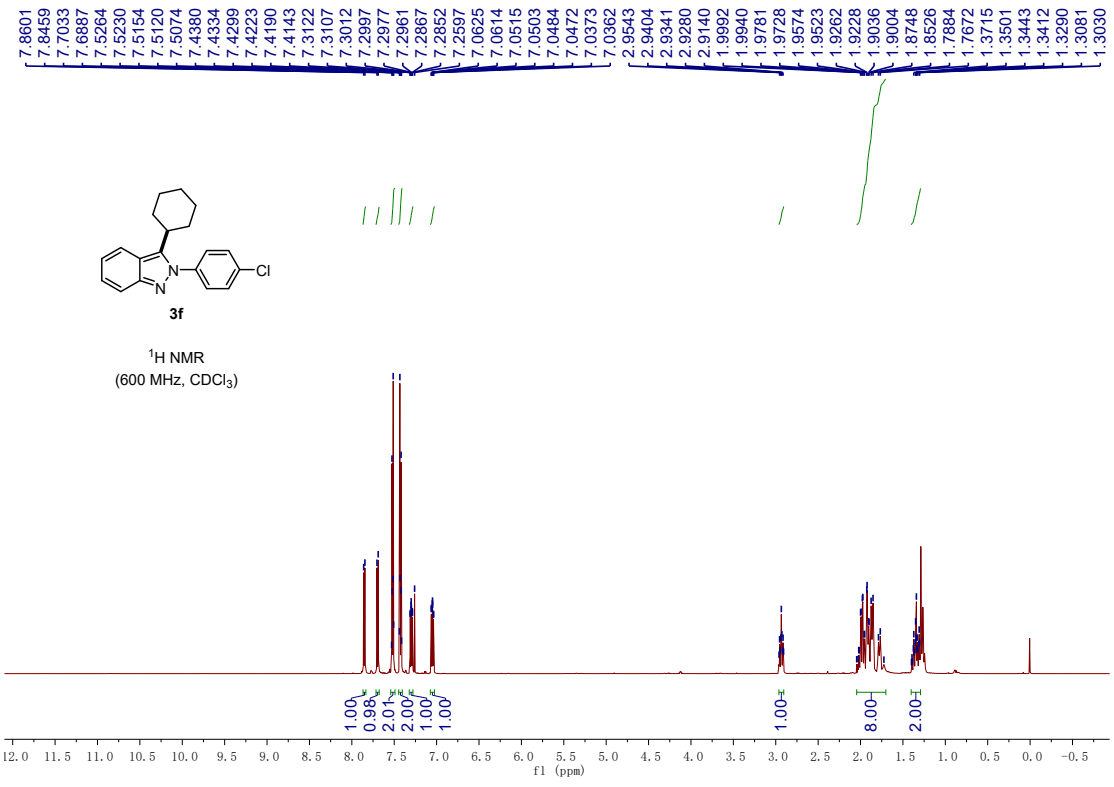
^{13}C NMR spectrum of 3e



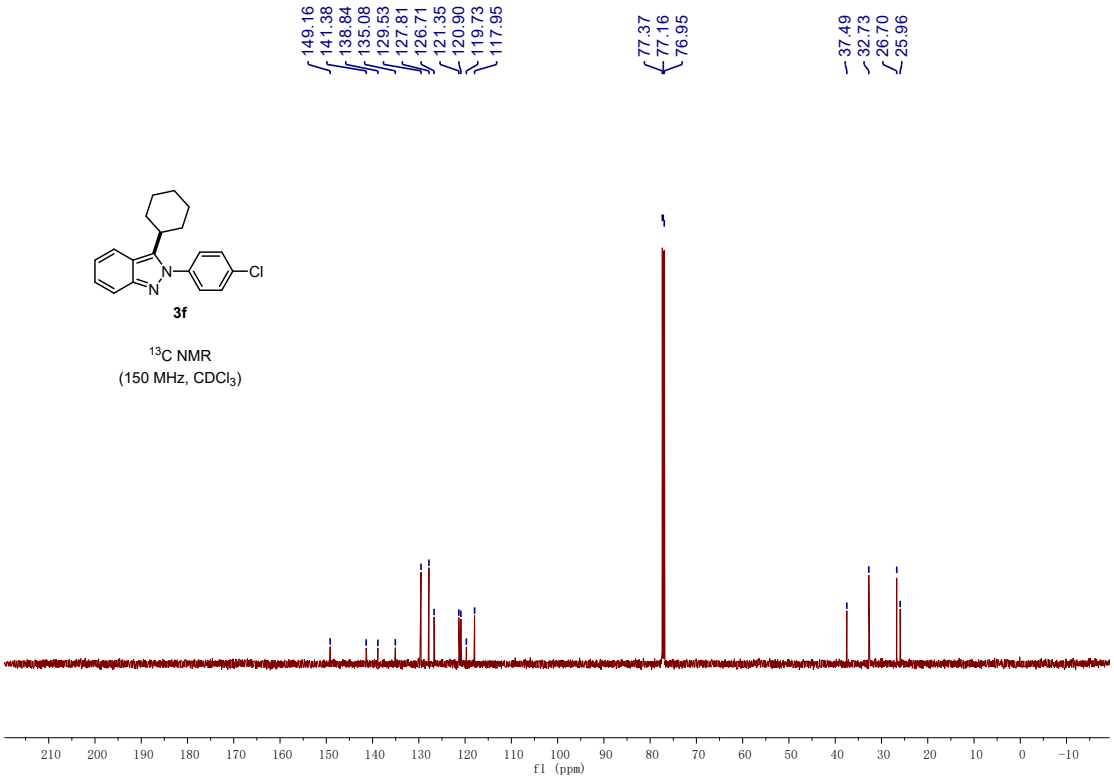
^{19}F NMR spectrum of 3e



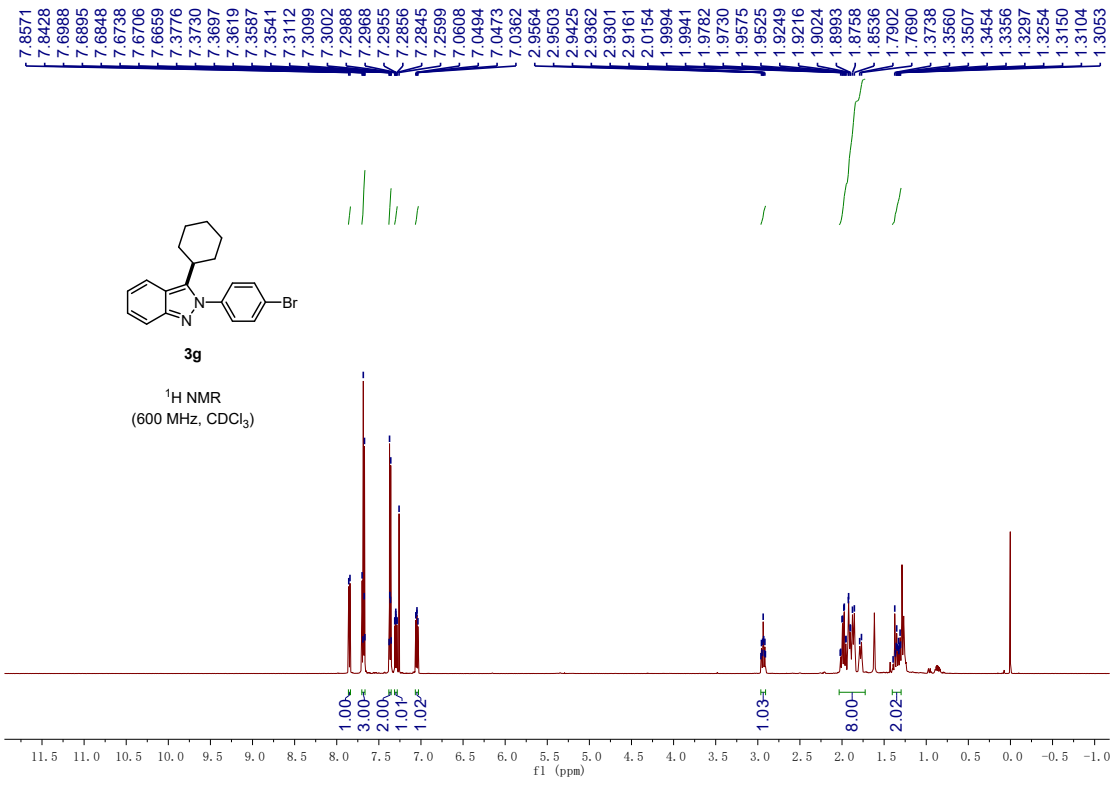
^{1}H NMR spectrum of 3f



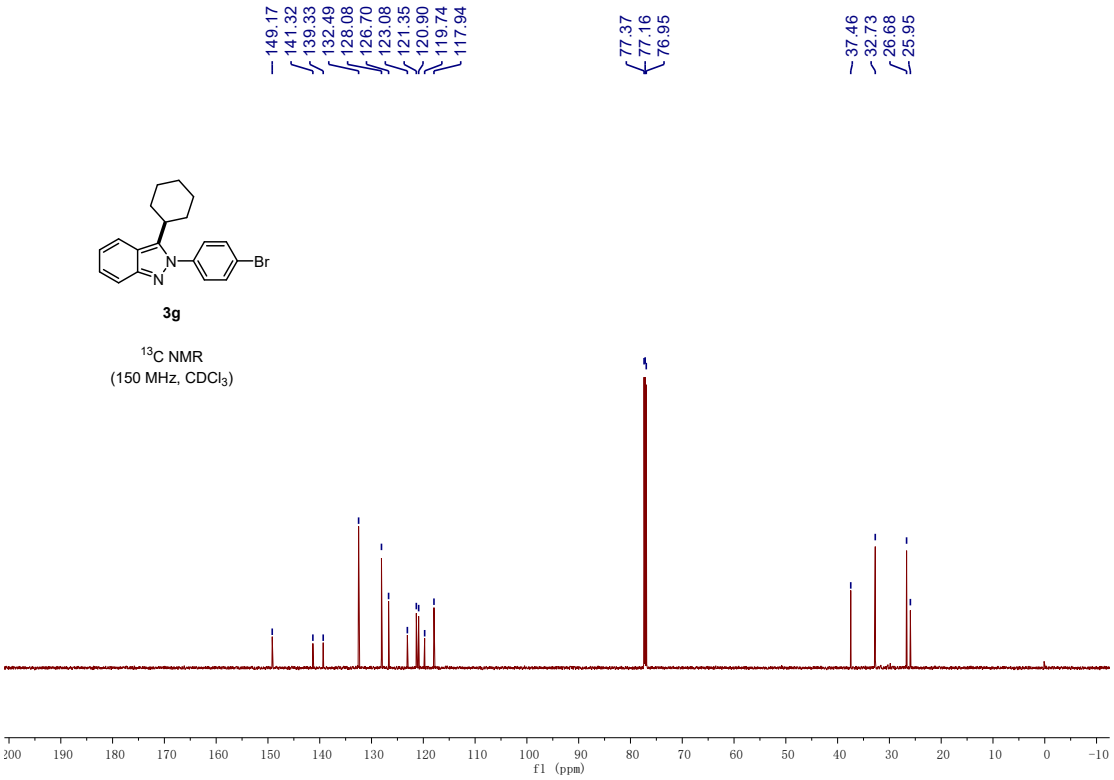
^{13}C NMR spectrum of 3f



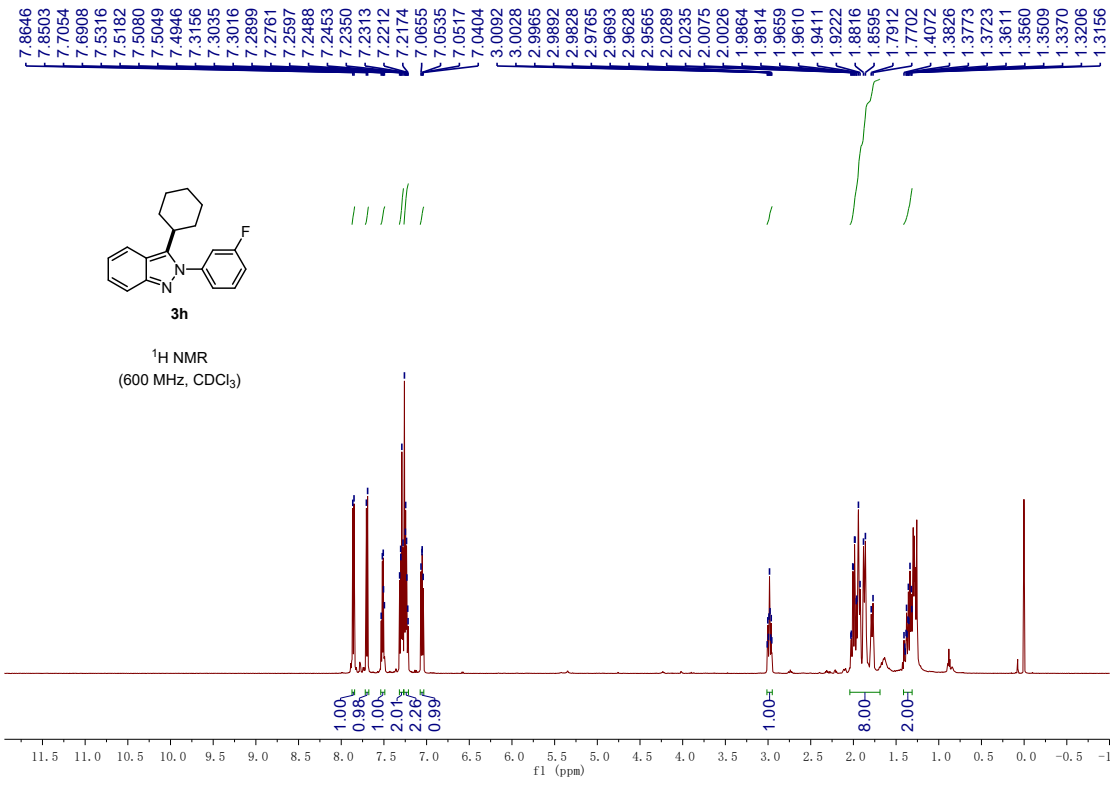
^{1}H NMR spectrum of 3g



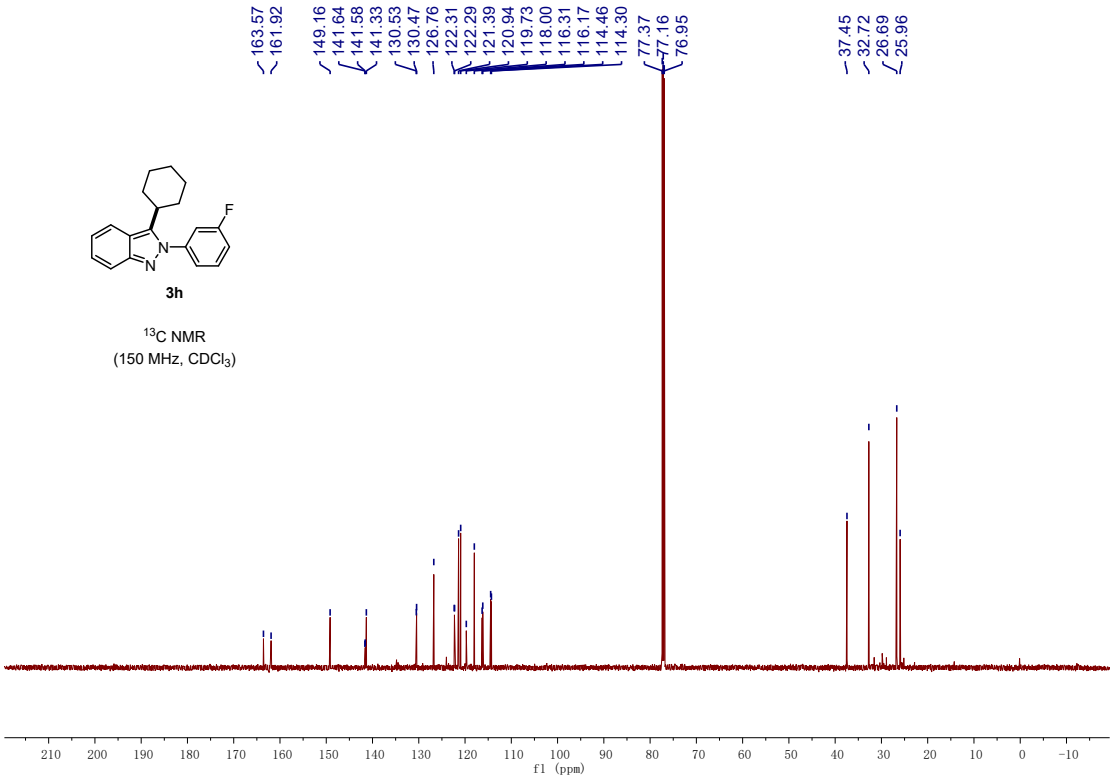
^{13}C NMR spectrum of 3g



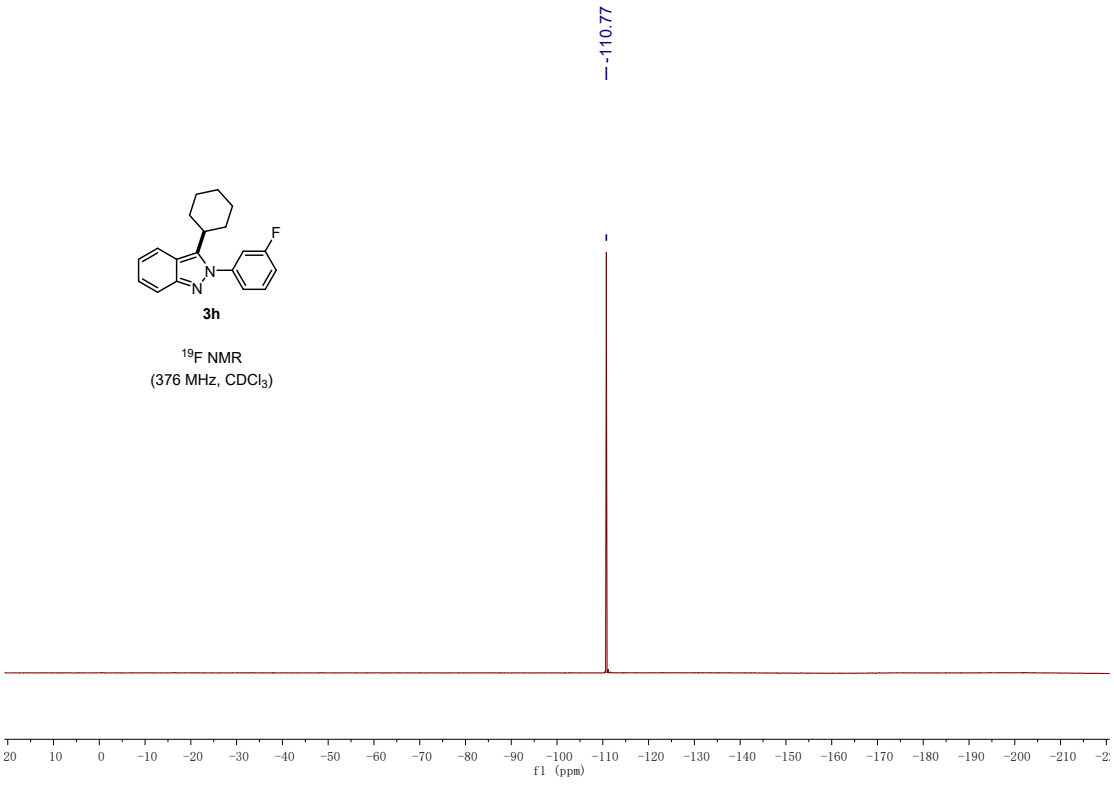
^{1}H NMR spectrum of 3h



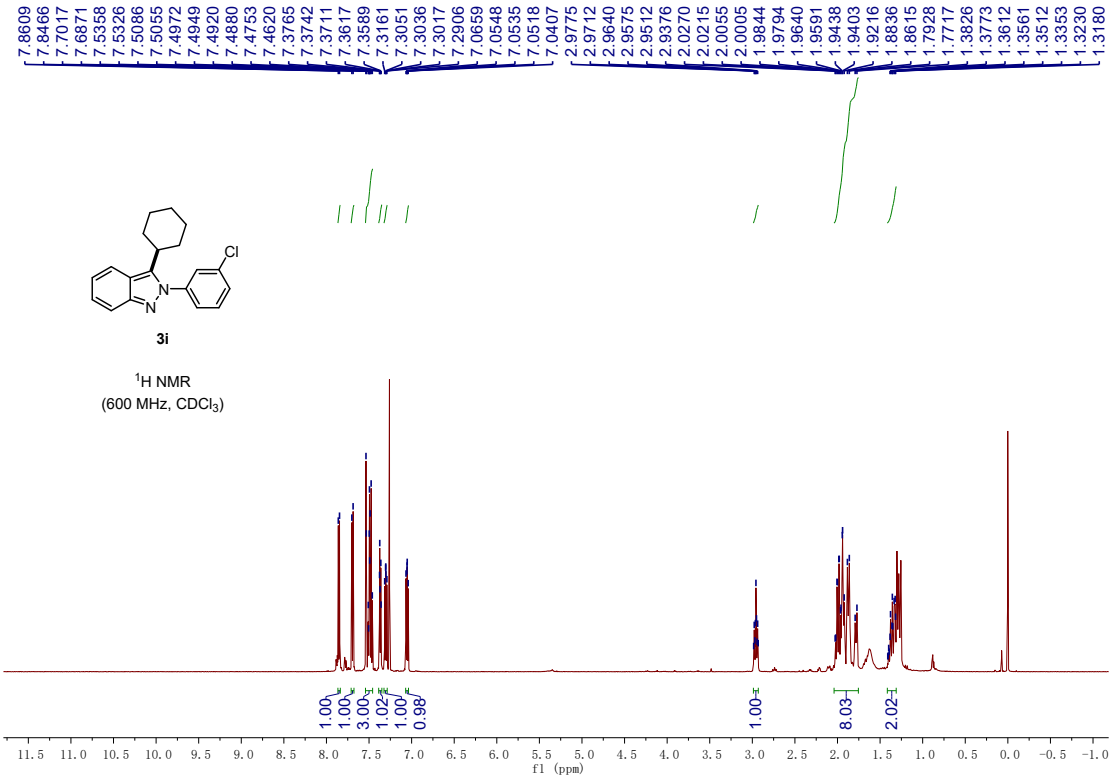
^{13}C NMR spectrum of 3h



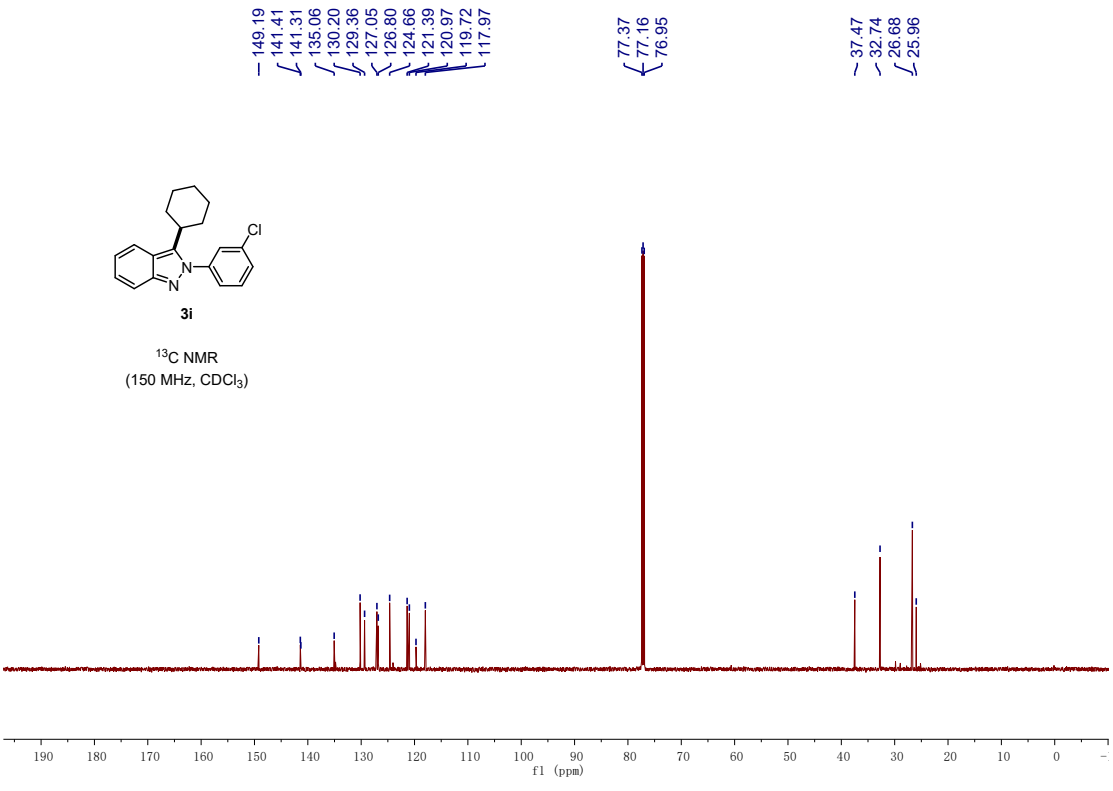
^{19}F NMR spectrum of 3h



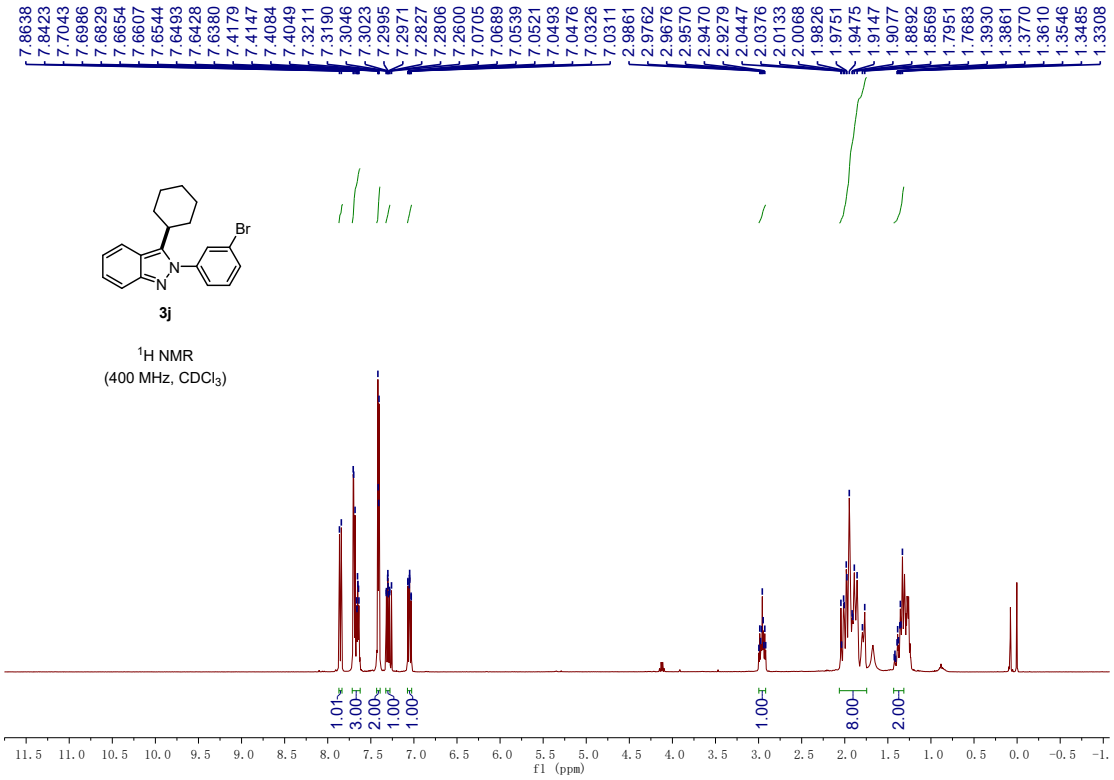
^{1}H NMR spectrum of 3i



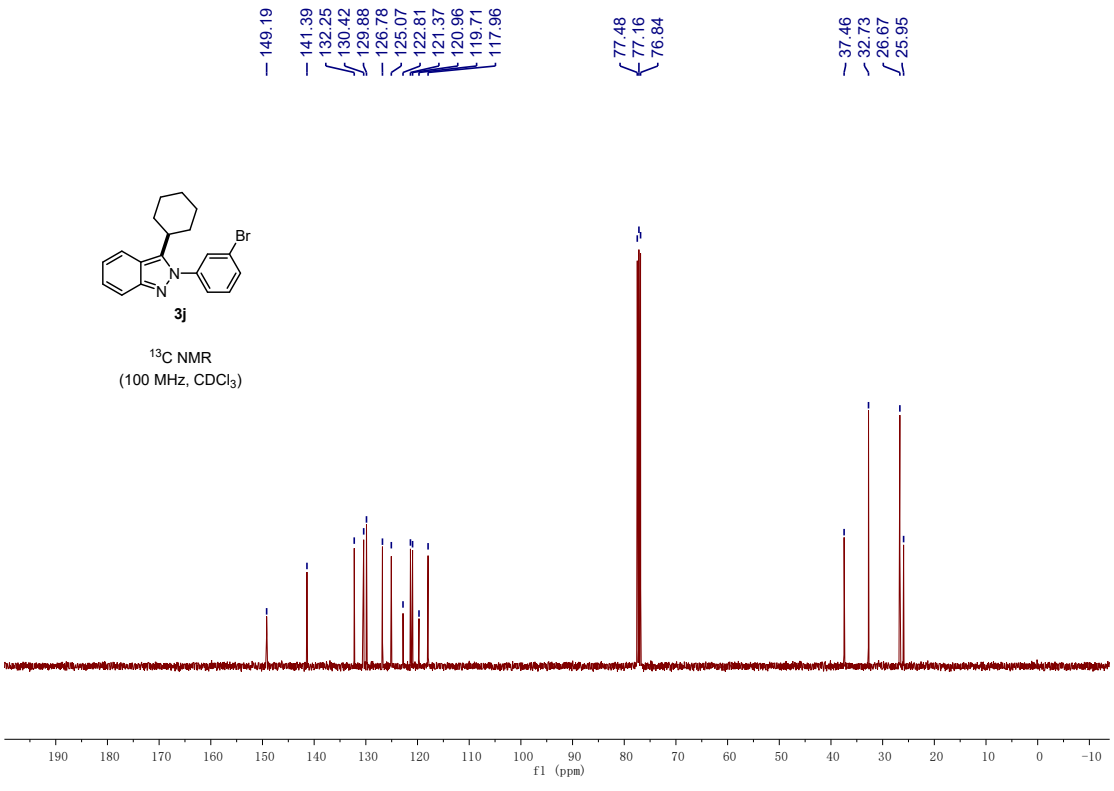
^{13}C NMR spectrum of 3i



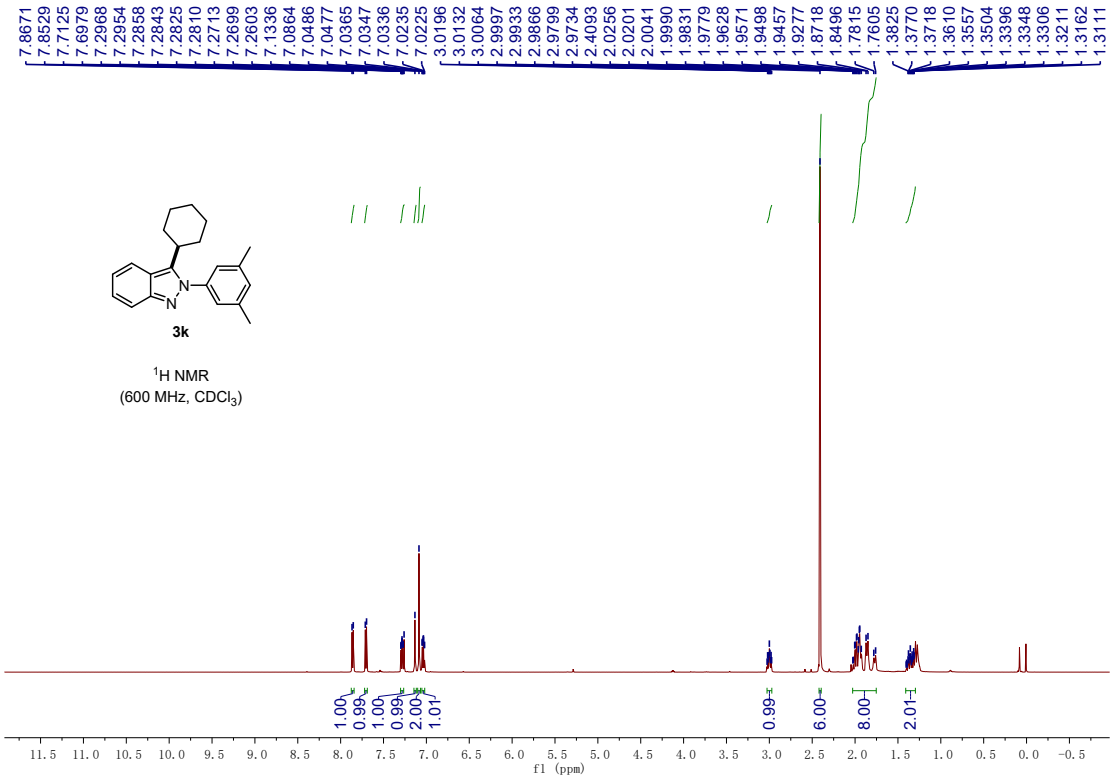
^{1}H NMR spectrum of 3j



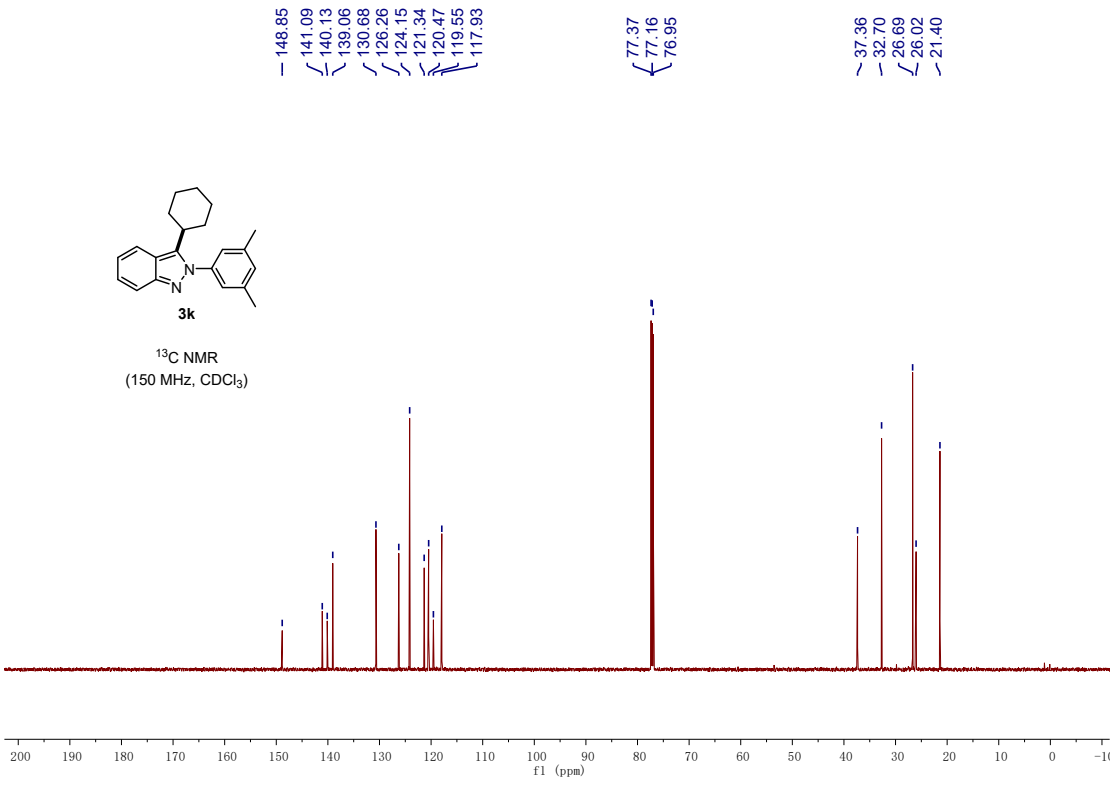
^{13}C NMR spectrum of 3j



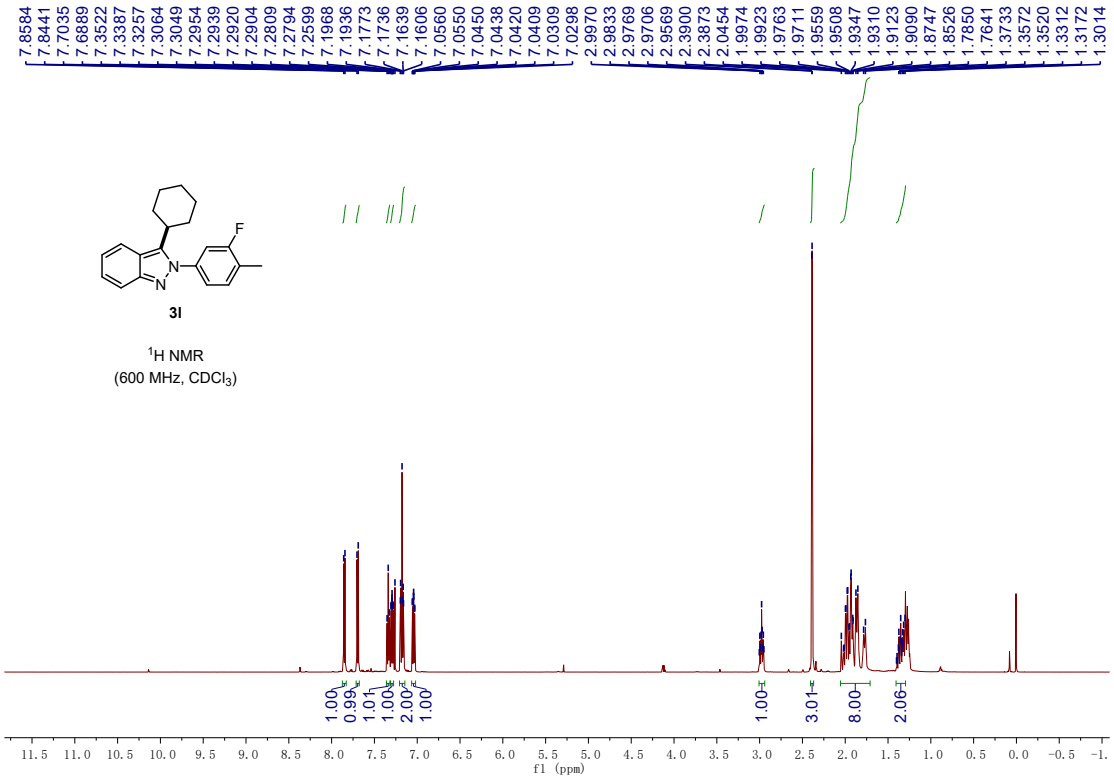
^{1}H NMR spectrum of 3k



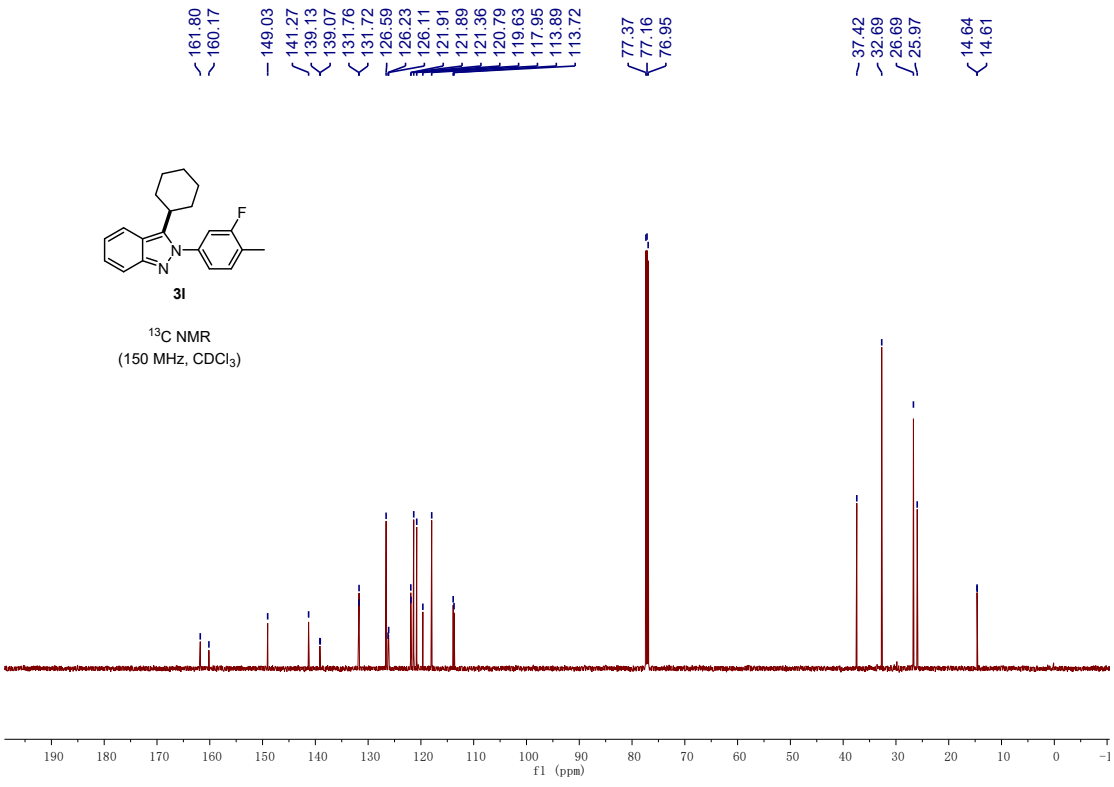
^{13}C NMR spectrum of 3k



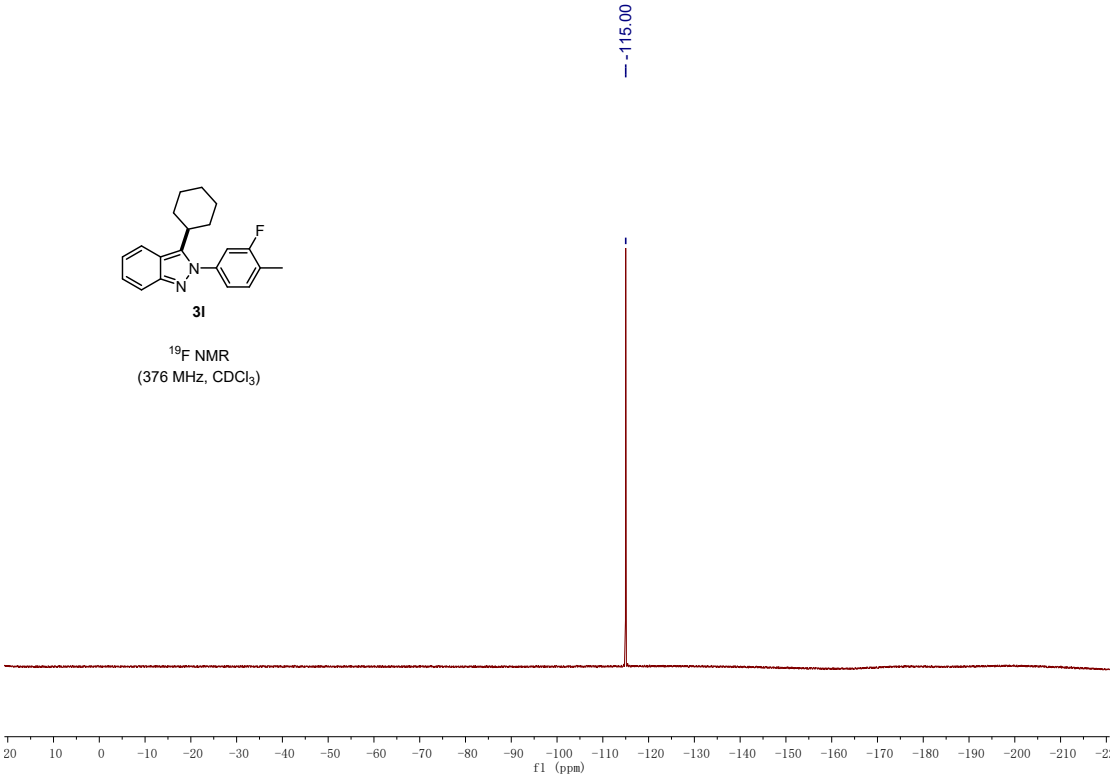
^{1}H NMR spectrum of 3l



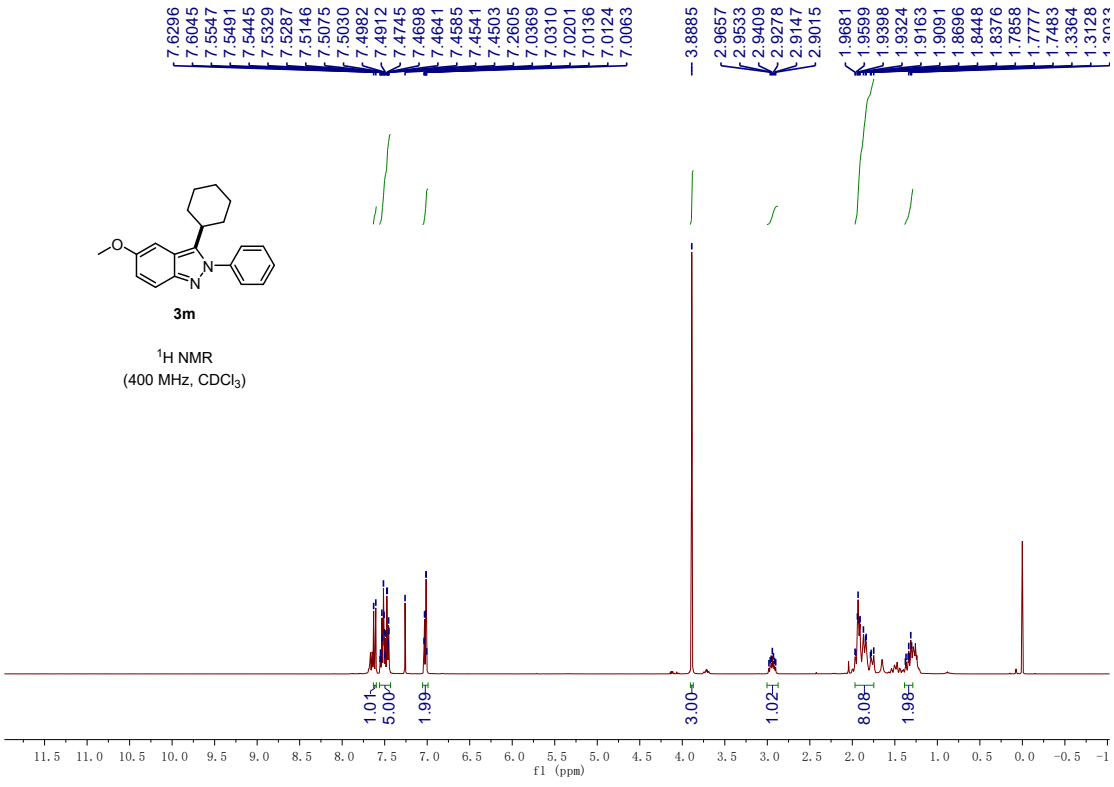
^{13}C NMR spectrum of 3l



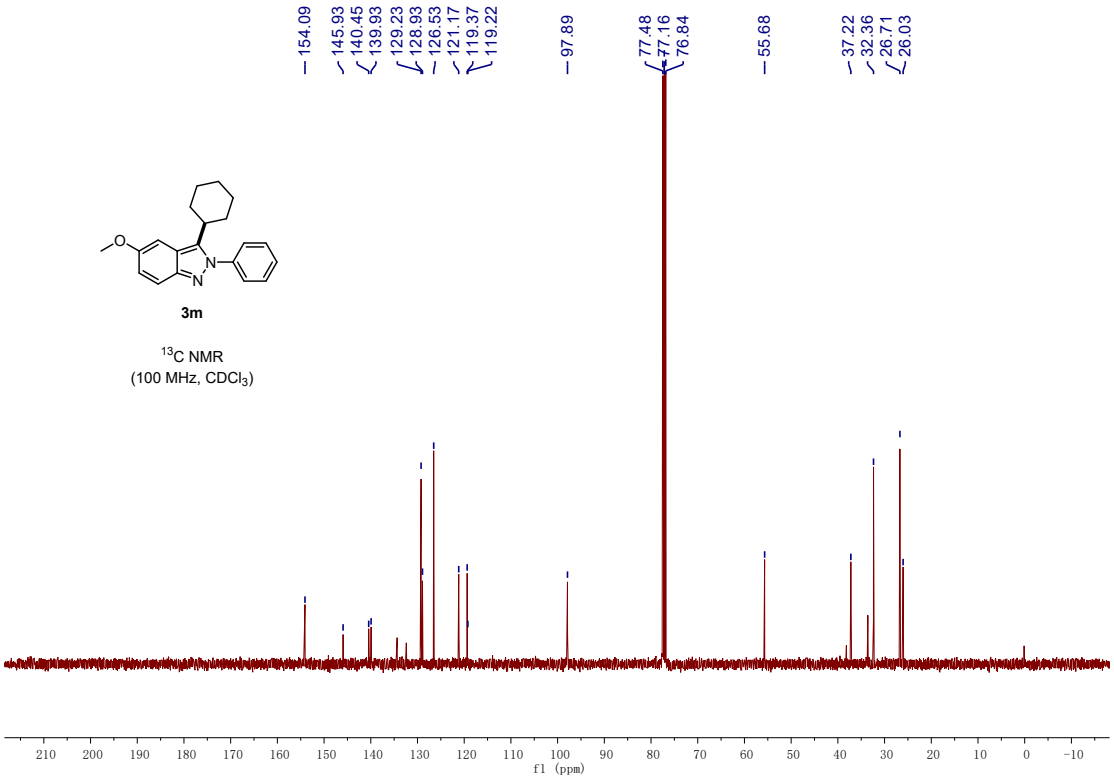
^{19}F NMR spectrum of 3l



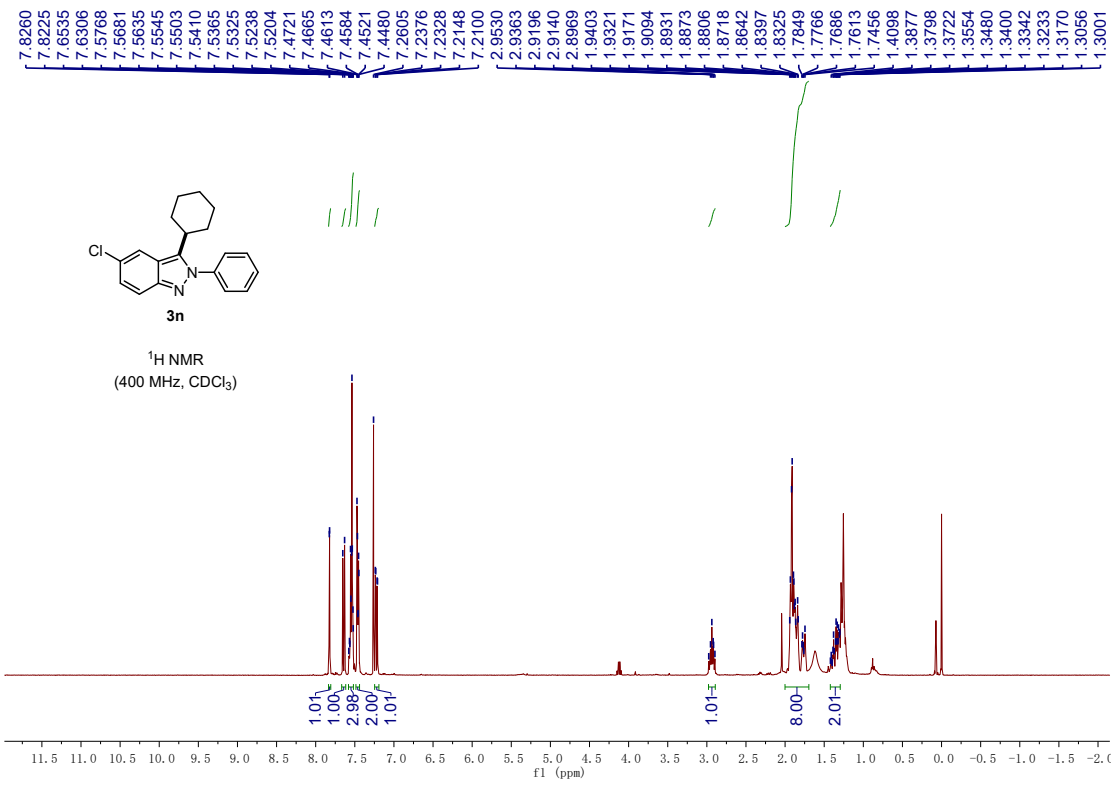
^{1}H NMR spectrum of 3m



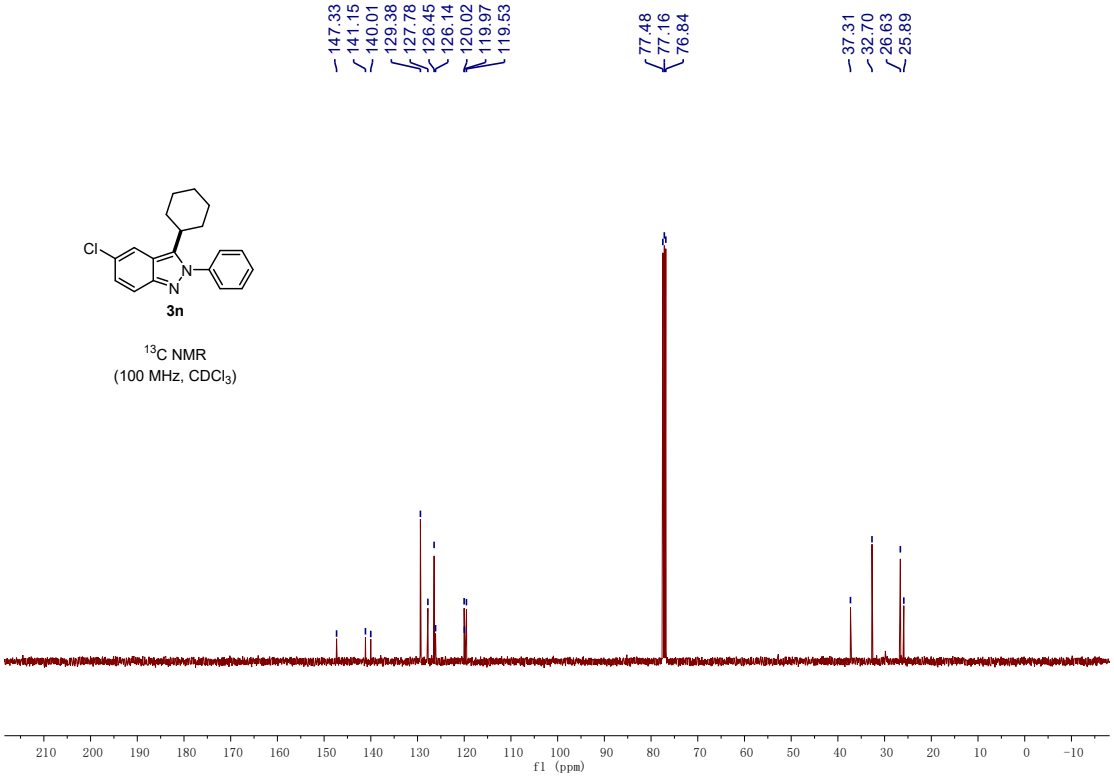
^{13}C NMR spectrum of 3m



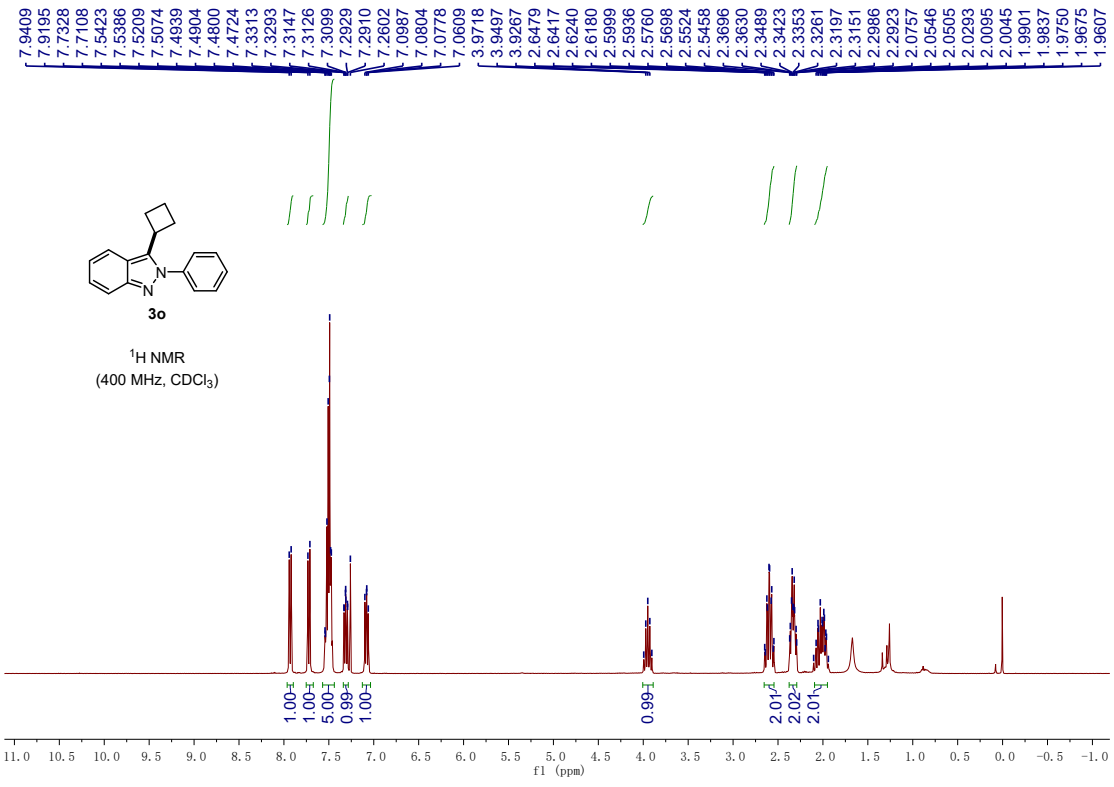
^{1}H NMR spectrum of 3n



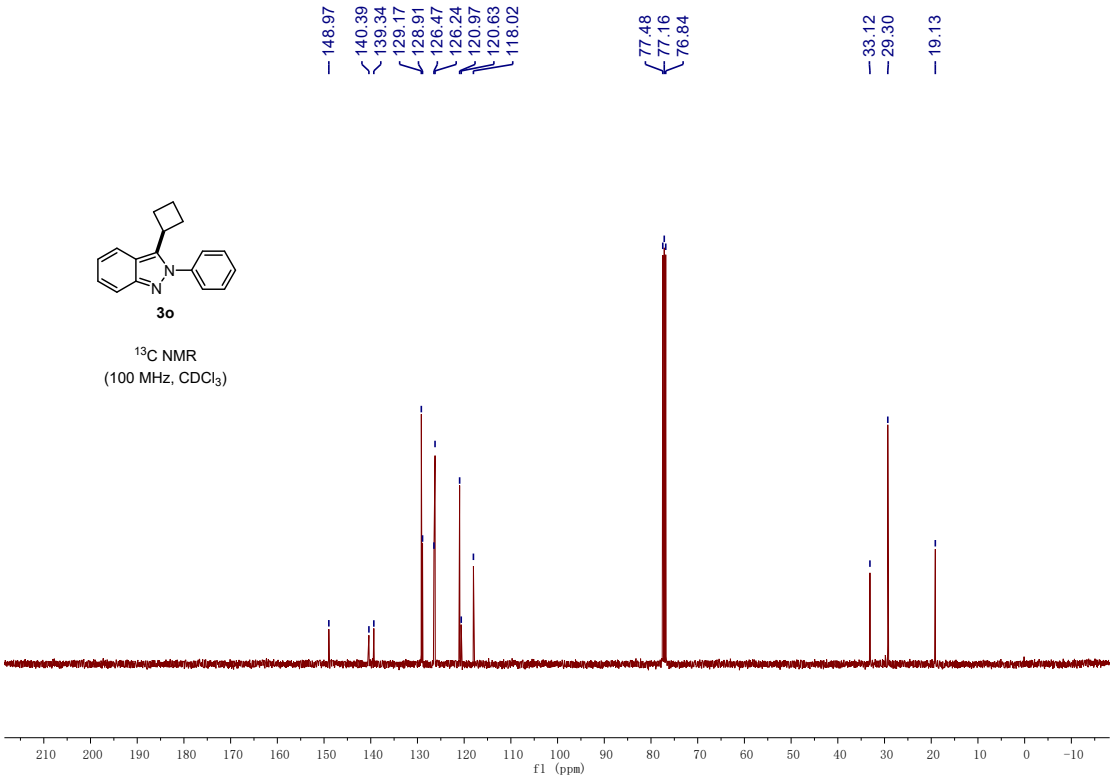
^{13}C NMR spectrum of 3n



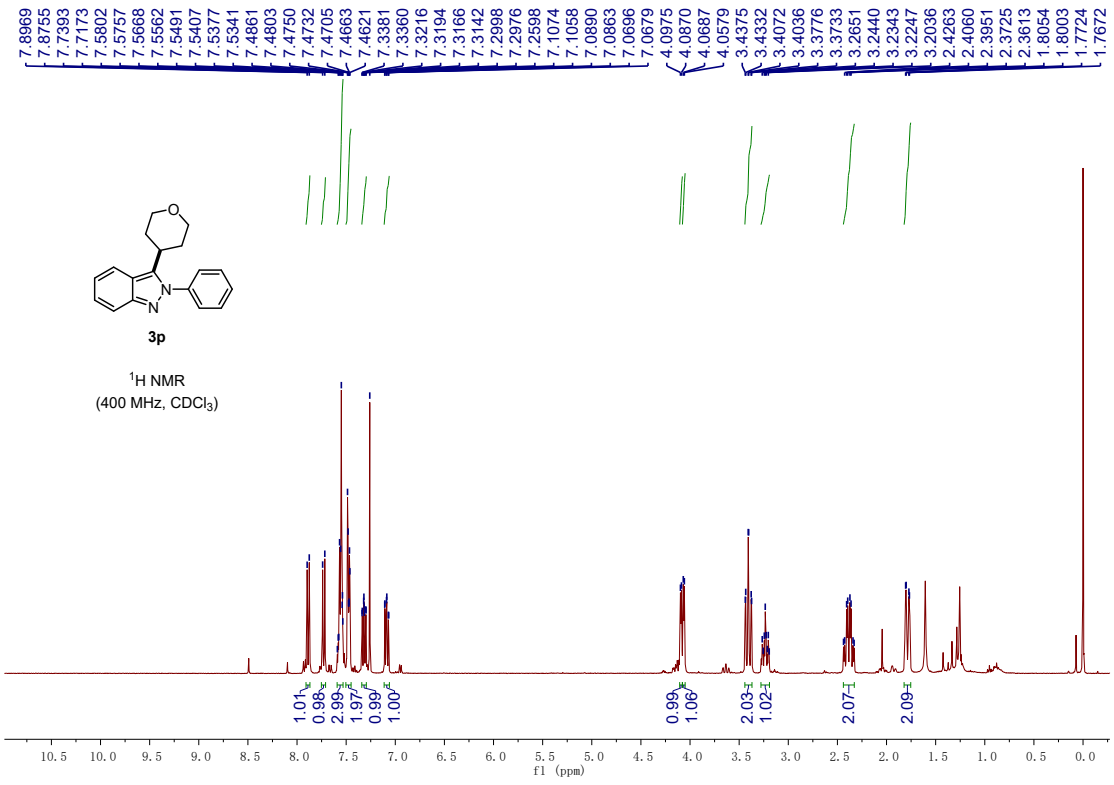
^{1}H NMR spectrum of 3o



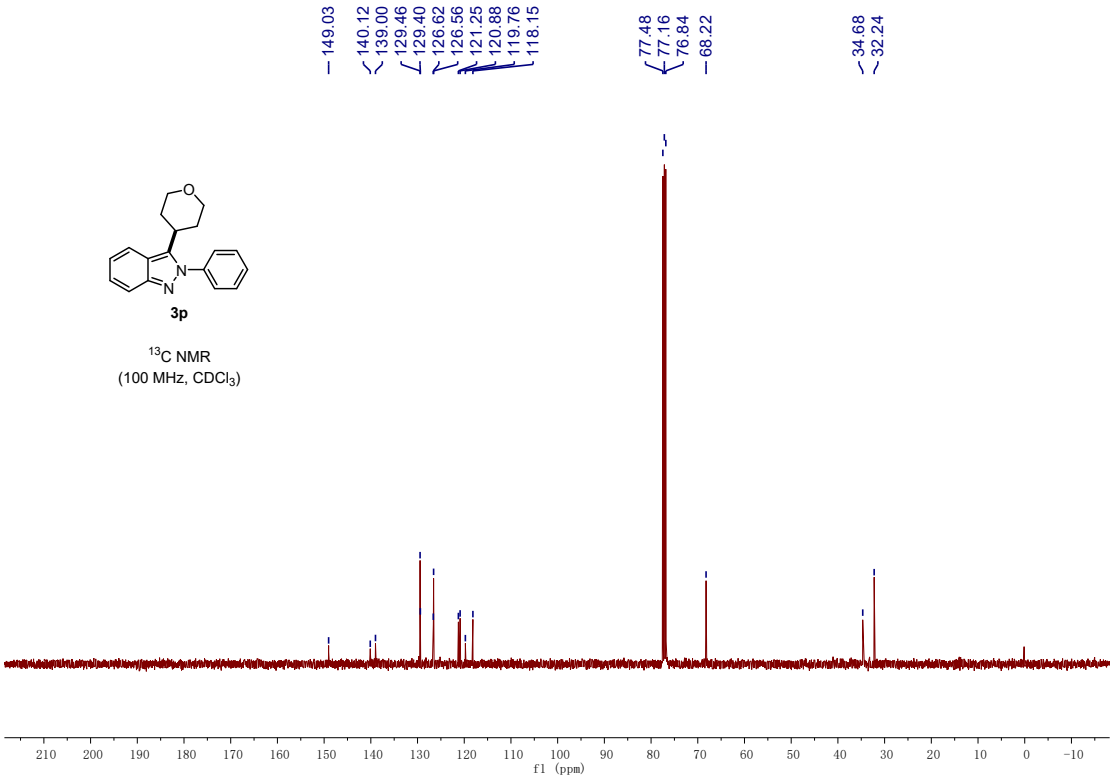
^{13}C NMR spectrum of 3o



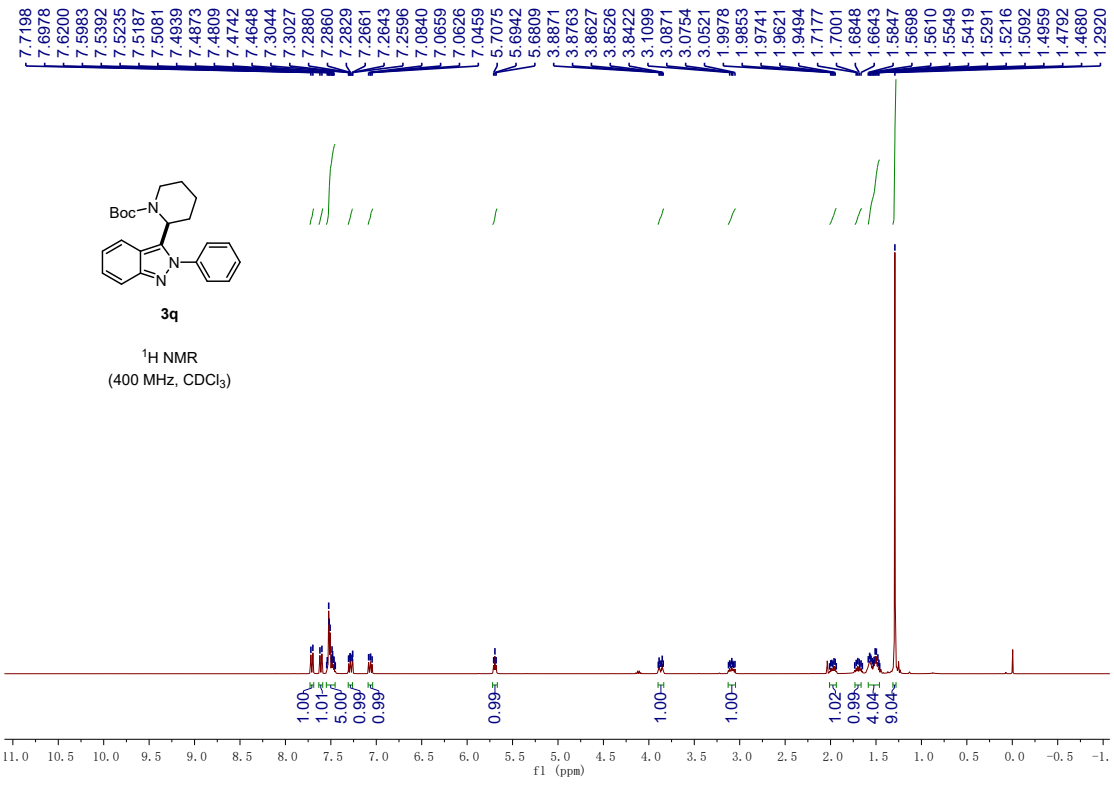
^{1}H NMR spectrum of 3p



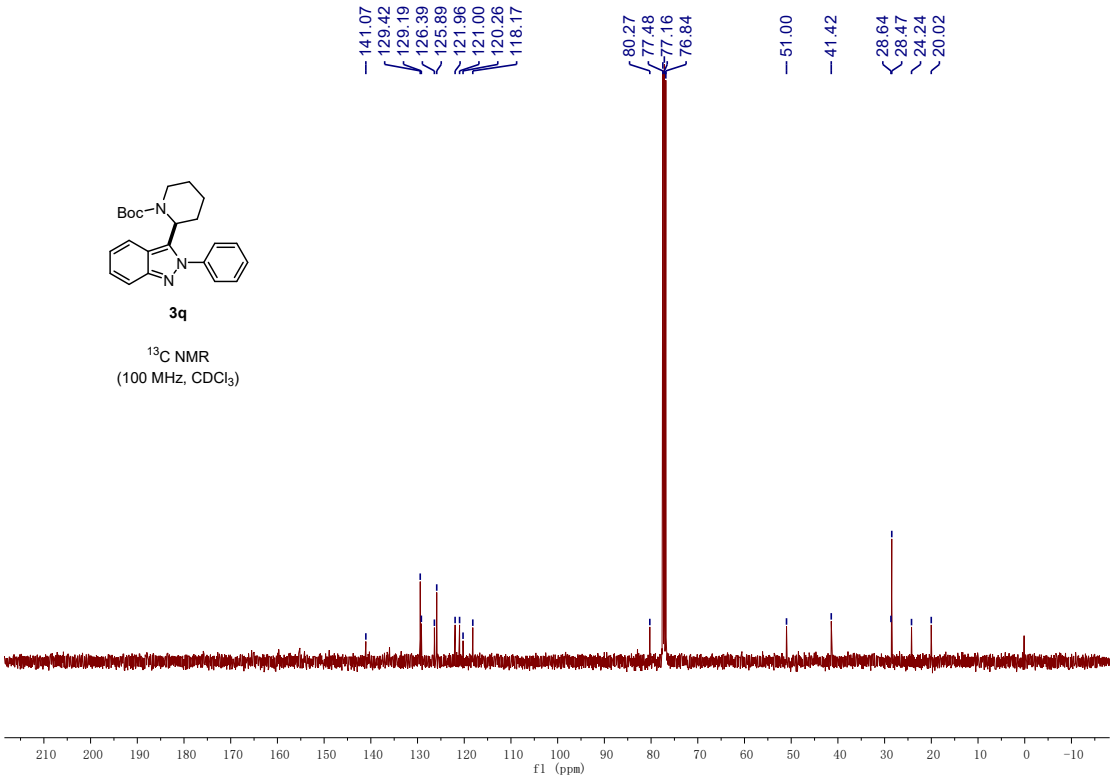
^{13}C NMR spectrum of 3p



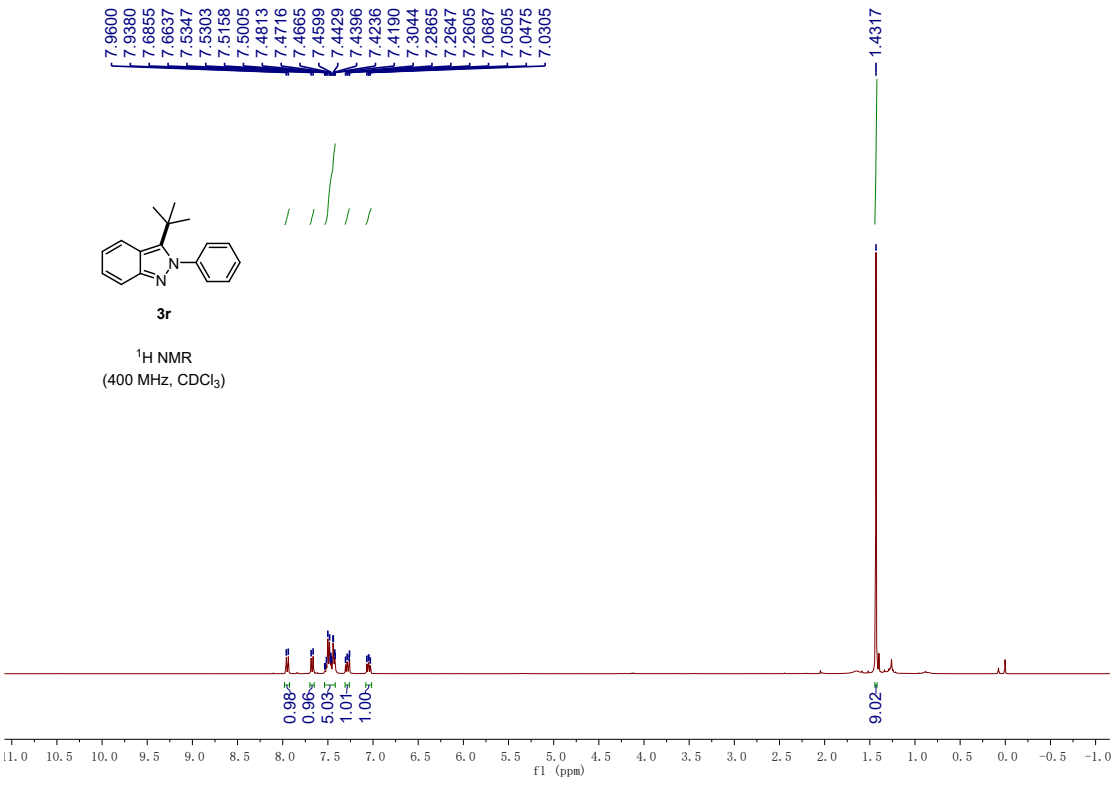
^{1}H NMR spectrum of 3q



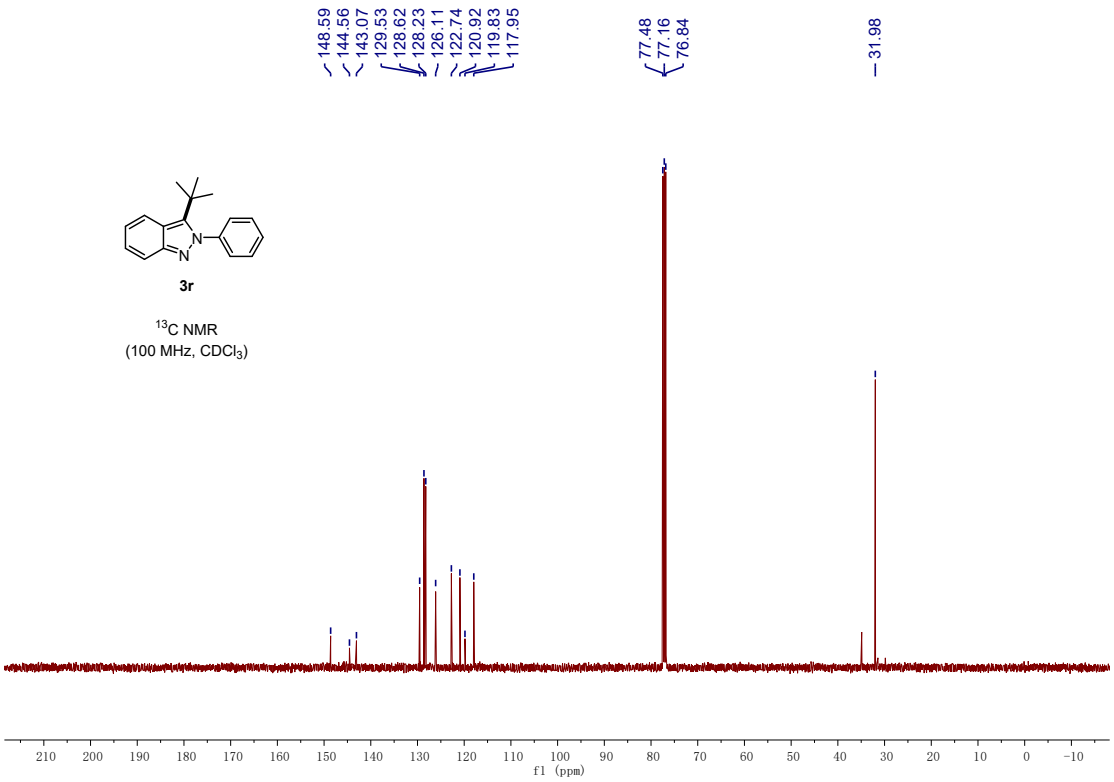
^{13}C NMR spectrum of 3q



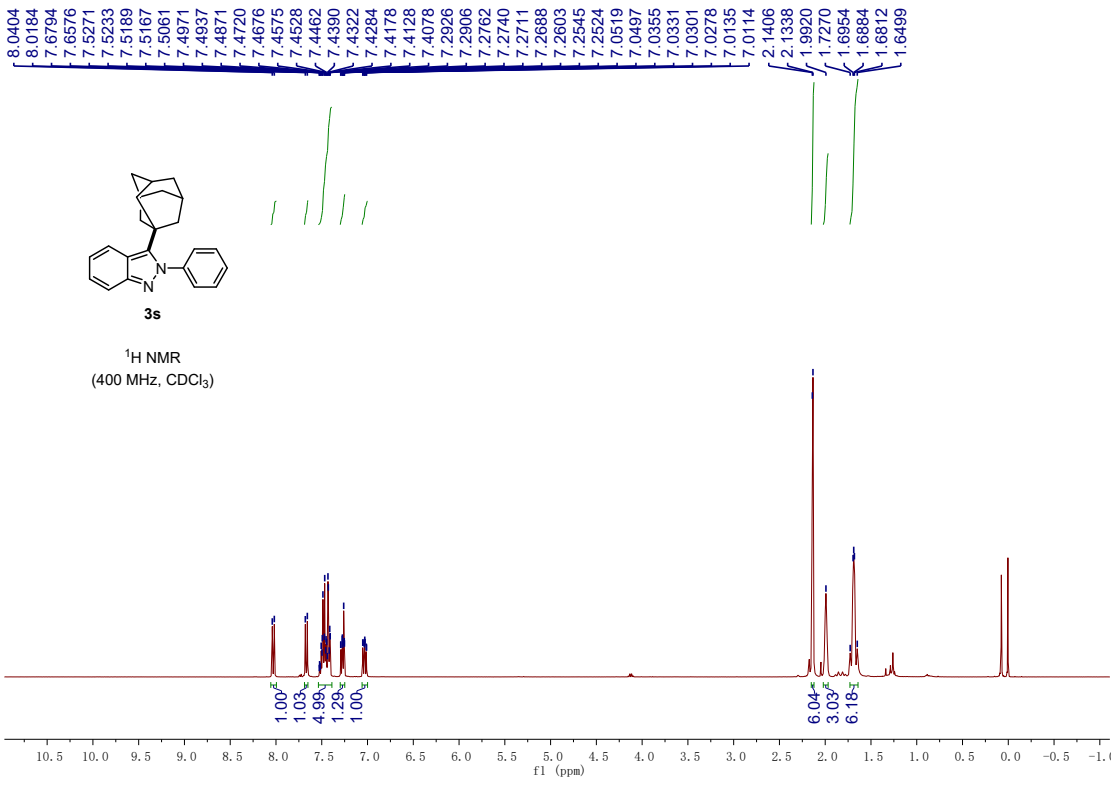
^{1}H NMR spectrum of 3r



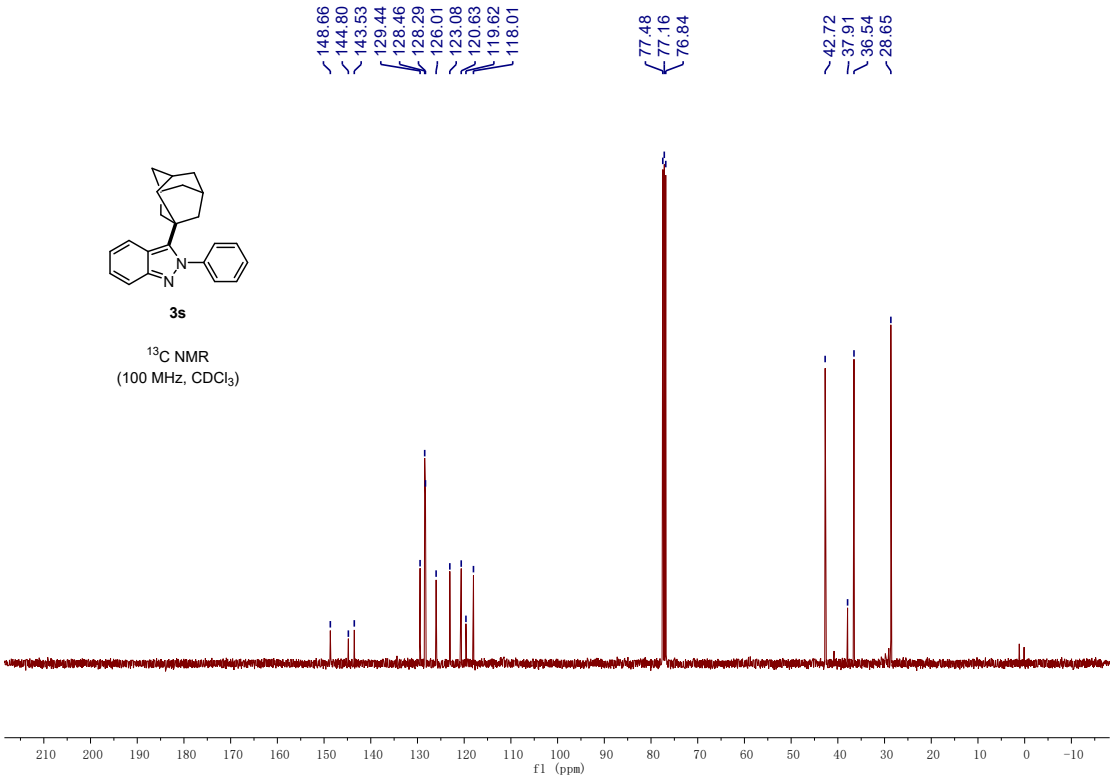
^{13}C NMR spectrum of 3r



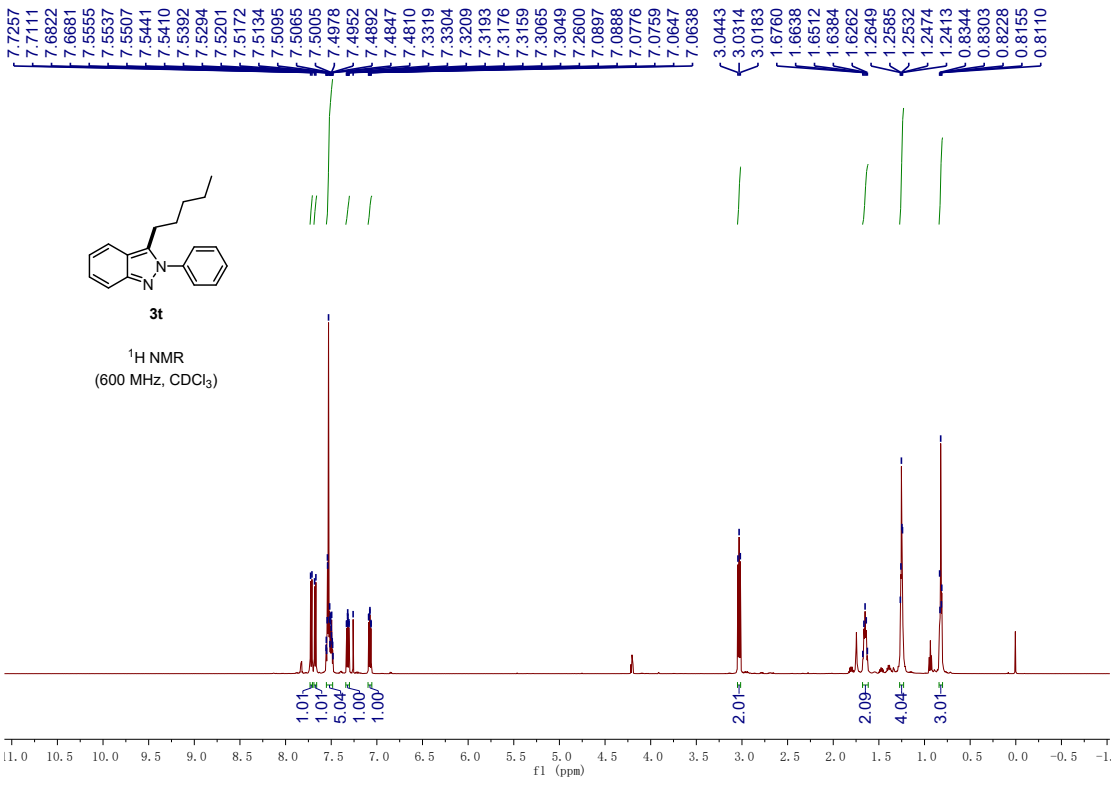
^{1}H NMR spectrum of 3s



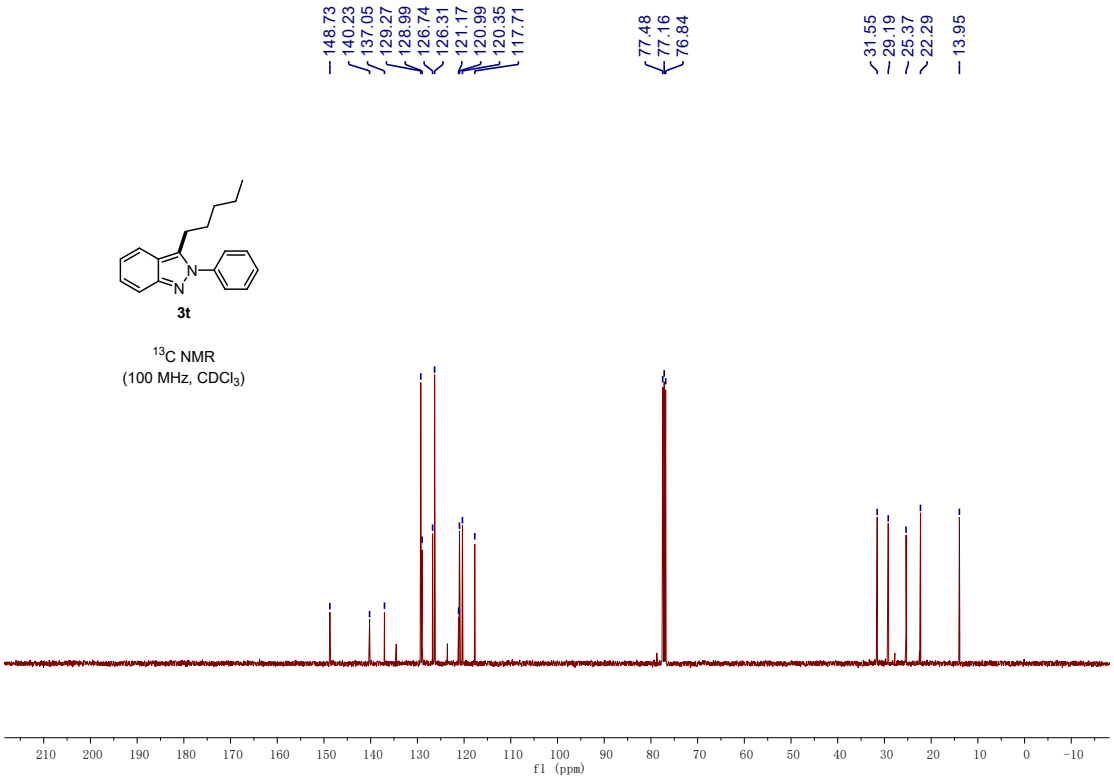
^{13}C NMR spectrum of 3s



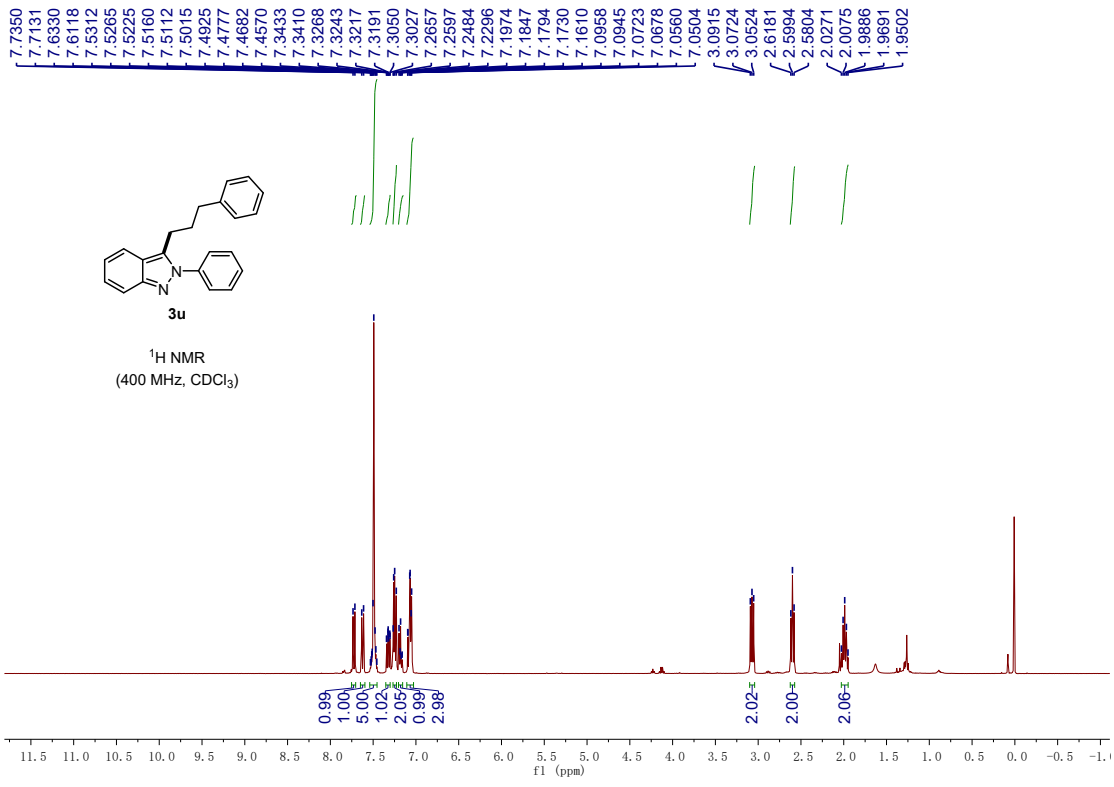
^{1}H NMR spectrum of 3t



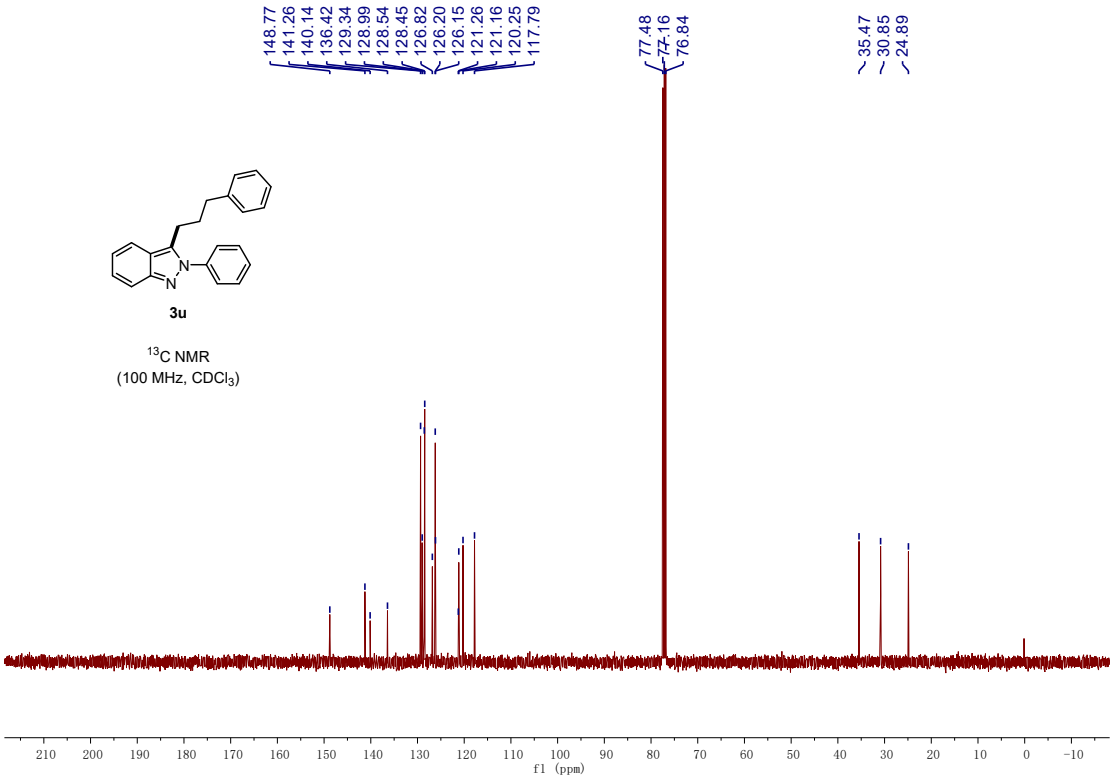
^{13}C NMR spectrum of 3t



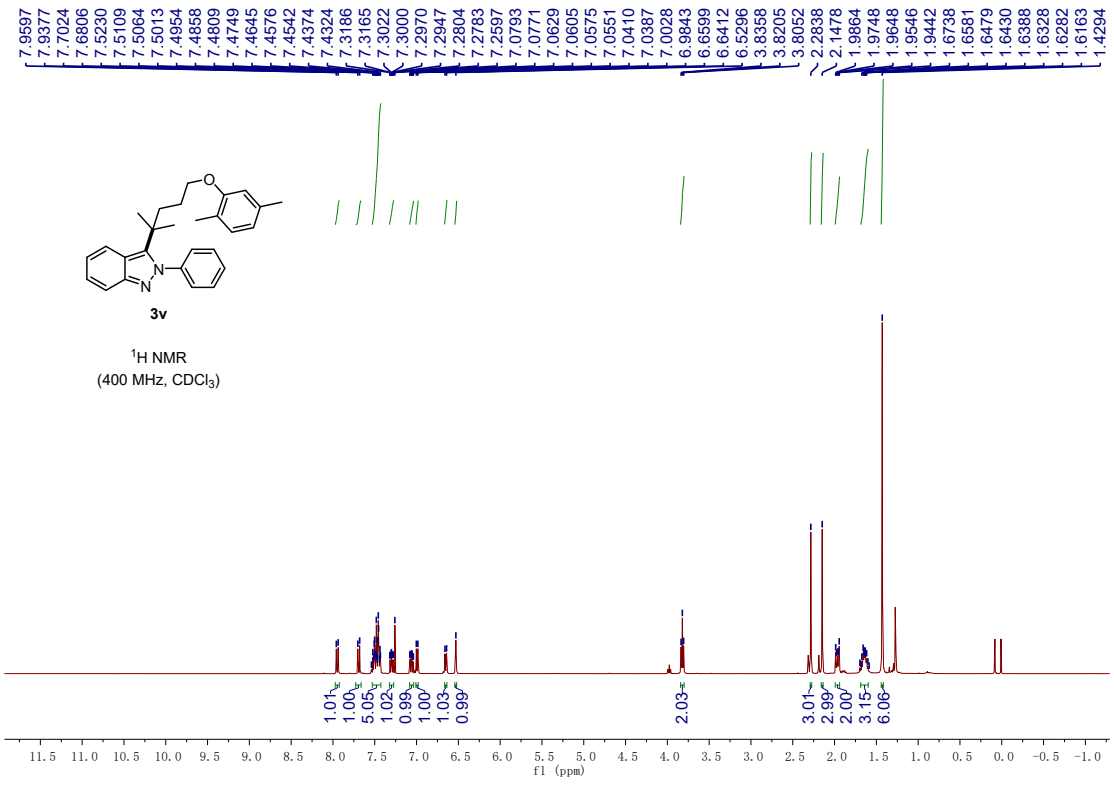
^{1}H NMR spectrum of 3u



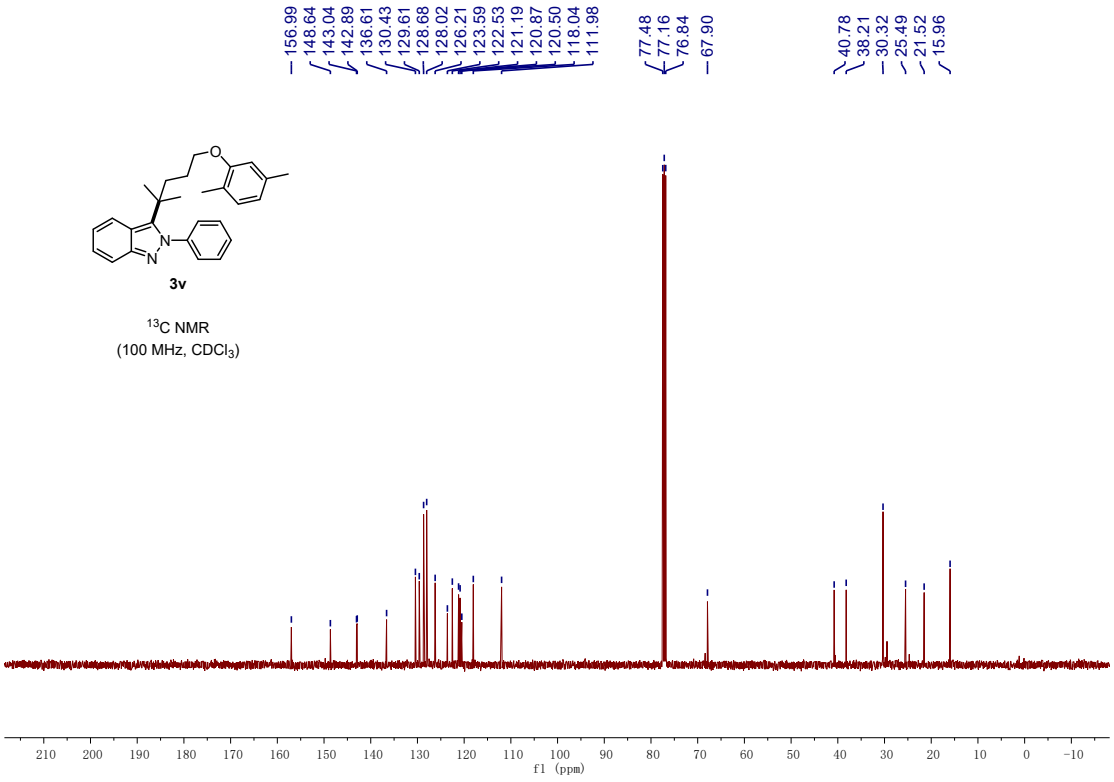
^{13}C NMR spectrum of 3u



^{1}H NMR spectrum of 3v



^{13}C NMR spectrum of 3v



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