Supporting Information for

Efficient synthesis of 2-aryl-2H-indazoles by base-catalyzed benzyl C–H deprotonation and cyclization

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Table of Contents

1. General information…….S2

2. General procedure for the preparation of unsymmetrical azoxybenzenes…….....S2

3. General experimental procedure……..S3

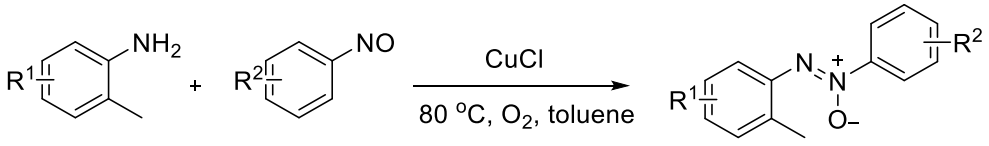
4. Characterization of products in details……S3

5. ^{1}H, ^{13}C and ^{19}F NMR spectra of products…….....S15

1. General information

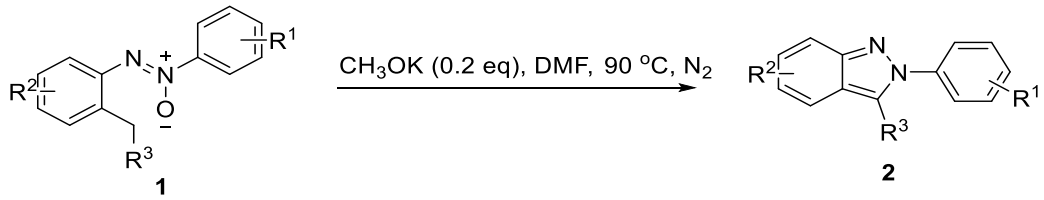
All reagents and solvents were purchased from TCI, Sigma-Aldrich, Alfa Aesar, Acros and Meryer. All reactions were conducted using standard Schlenk techniques. Column chromatography was performed using EM silica gel 60 (300−400 mesh). ^{1}H NMR and ^{13}C NMR spectra were measured on Bruker AVANCE spectrometer (400 MHz or 500 MHz for ^{1}H, 125 MHz for ^{13}C), using DMSO-d_6 or $CDCl_3$ as the solvent with tetramethylsilane (TMS) as the internal standard at room temperature. Chemical shifts were reported in ppm. ^{1}H NMR spectra were referenced to $CDCl_3$ (7.26 ppm) or DMSO-d_6 (2.50 ppm), and ^{13}C-NMR spectra were referenced to $CDCl_3$ (77.0 ppm) or DMSO-d_6 (39.5 ppm). Peak multiplicities were designated by the following abbreviations: s, singlet; d, doublet; t, triplet; m, multiplet. Chemical shifts are given in δ relative to TMS, the coupling constants J are given in Hz. Analysis of crude reaction mixture was done on the Varian 4000 GC/MS and Agilent 7890A/5975C. High-resolution mass spectra were recorded on a micrOTOF-Q II 10410 mass spectrometer. Unless otherwise noted, all reagents and solvents were obtained commercially and used without further purification.

2. General procedure for the preparation of unsymmetrical azoxybenzenes



A 50 mL Schlenk tube equipped with a stir bar was charged with substituted *o*-toluidine (30.0 mmol), nitrosobenzene (32.0 mmol), CuCl (6.0 mmol), pyridine (15.0 mmol) and toluene (30 mL). The reaction mixture was stirred at 80 °C for 24 h under O_2. After the reaction completed, the solvent was then removed under reduced pressure. The residue was then purified by flash chromatography on silica gel to provide the unsymmetrical azoxybenzenes.

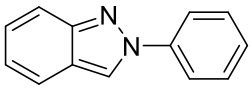
3. General experimental procedure



A 25 mL Schlenk tube equipped with a stir bar was charged with **1** (0.3 mmol), CH_3OK (0.06 mmol) and DMF (2 mL). The reaction mixture was stirred at 90 °C for 8 h under N_2. After the reaction completed, water (20.0 mL) was added, and the reaction solution was extracted by 50.0 mL of ethyl acetate in three times, then concentrated with ethyl acetate layer under reduced pressure. The residue was then purified by flash chromatography on silica gel to provide the product **2**.

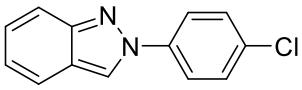
4. Characterization of products in details

2-phenyl-2H-indazole (2a)[1]



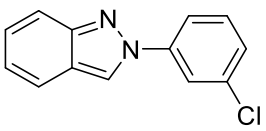
White solid (57 mg, 98% yield); EtOAc/PE = 1/15. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.33 (s, 1H), 7.87-7.85 (m, 2H), 7.80-7.78 (m, 1H), 7.67-7.65 (m, 1H), 7.48-7.45 (m, 2H), 7.36-7.29 (m, 2H), 7.10-7.07 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.8, 140.6, 129.6, 127.9, 126.8, 122.8, 122.5, 121.1, 120.4, 120.3, 118.0.

2-(4-chlorophenyl)-2H-indazole (2b)[1]



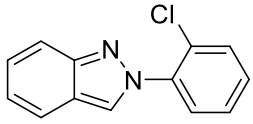
White solid (60 mg, 88% yield); EtOAc/PE = 1/15. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (s, 1H), 7.79-7.74 (m, 3H), 7.64-7.62 (m, 1H), 7.44-7.40 (m, 2H), 7.32-7.28 (m, 1H), 7.10-7.06 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.9, 139.0, 133.5, 129.6, 127.1, 122.9, 122.7, 121.9, 120.4, 120.2, 117.9.

2-(3-chlorophenyl)-2H-indazole (2c)[1]



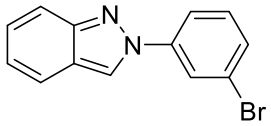
White solid (46 mg, 67% yield); EtOAc/PE = 1/15. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (s, 1H), 7.98 (s, 1H), 7.80-7.77 (m, 2H), 7.71-7.69 (m, 1H), 7.48-7.44 (m, 1H), 7.38-7.32 (m, 2H), 7.15-7.13 (m,1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.0, 141.5, 135.5, 130.6, 127.9, 127.2, 122.9, 122.8, 121.3, 120.4, 120.3, 118.8, 118.0.

2-(2-chlorophenyl)-2H-indazole (2d)[1]



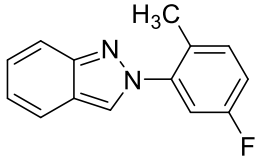
Yellow oil (49 mg, 72% yield); EtOAc/PE = 1/15. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (s, 1H), 7.87-7.73 (m, 3H), 7.63-7.61 (m, 1H), 7.50-7.38 (m, 3H), 7.21-7.17 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.4, 138.6, 130.6, 129.9, 128.9, 128.5, 127.6, 126.9, 125.1, 122.4, 122.0, 120.5, 117.9.

2-(3-bromophenyl)-2H-indazole (2e)[2]



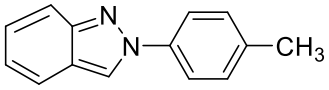
White solid (57 mg, 70% yield); EtOAc/PE = 1/15. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (s, 1H), 8.11 (s, 1H), 7.81-7.75 (m, 2H), 7.68-7.66 (m, 1H), 7.51-7.49 (m, 1H), 7.37-7.30 (m, 2H), 7.13-7.09 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.0, 141.5, 130.8, 127.2, 124.1, 123.2, 122.9, 122.8, 120.4, 120.3, 119.2, 118.0.

2-(5-fluoro-2-methylphenyl)-2H-indazole (2f)



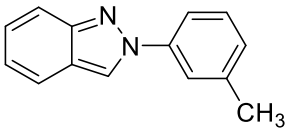
Yellow oil (64 mg, 95% yield); EtOAc/PE = 1/15. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (s, 1H), 7.80-7.78 (m, 1H), 7.73-7.71 (m, 1H), 7.36-7.28 (m, 2H), 7.21-7.07 (m, 3H), 2.21 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.8 (d, J = 245.0), 149.4, 140.9 (d, J = 8.8Hz), 132.4 (d, J = 8.8Hz), 129.4 (d, J = 3.8Hz), 126.7, 124.2, 122.4, 122.1, 120.4, 118.0, 116.1 (d, J = 21.3Hz), 114.0 (d, J = 23.8), 17.4. ^{19}F NMR (470 MHz, $CDCl_3$) δ -115.7 (s, 1F). HRMS (ESI): calculated for $C_{14}H_{11}FN_2Na$ $[M+Na]^+$ 249.0804, found 249.0800.

2-(p-tolyl)-2H-indazole (2g)[3]



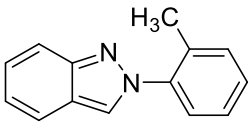
White solid (57 mg, 91% yield); EtOAc/PE = 1/15. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (s, 1H), 7.80-7.73 (m, 3H), 7.67-7.65 (m, 1H), 7.32-7.25 (m, 3H), 7.10-7.06 (m, 1H), 2.38 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.7, 138.3, 137.9, 130.1, 126.7, 122.8, 122.3, 120.8, 120.4, 120.3, 117.9, 21.0.

2-(m-tolyl)-2H-indazole (2h)[2]



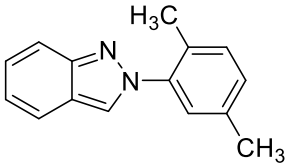
Yellow oil (57 mg, 92% yield); EtOAc/PE = 1/15. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (s, 1H), 7.80-7.78 (m, 1H), 7.74 (s, 1H), 7.68-7.61 (m, 2H), 7.38-7.29 (m, 2H), 7.18-7.16 (m, 1H), 7.11-7.07 (m,1H), 2.43 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.8, 140.5, 139.7, 129.3, 128.7, 126.8, 122.8, 122.4, 121.8, 120.4, 120.3, 118.0, 117.9, 21.4.

2-(o-tolyl)-2H-indazole (2i)[2]



White solid (59 mg, 94% yield); EtOAc/PE = 1/15. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (s, 1H), 7.81-7.79 (m, 1H), 7.74-7.72 (m, 1H), 7.43-7.30 (m, 5H), 7.15-7.11 (m, 1H), 2.23 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.3, 140.4, 134.0, 131.3, 129.2, 126.6, 126.5, 126.4, 124.3, 122.2, 122.0, 120.3, 117.9, 17.9.

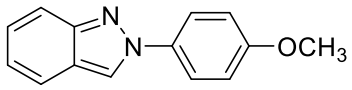
2-(2,5-dimethylphenyl)-2H-indazole (2j)[4]



White solid (58 mg, 87% yield); EtOAc/PE = 1/15. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.81-7.78 (m, 1H), 7.72-7.70 (m, 1H), 7.34-7.30 (m, 1H), 7.25-7.16 (m, 3H), 7.13-7.10 (m, 1H), 2.36 (s, 3H), 2.18 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ

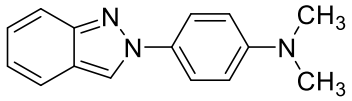
149.3, 140.2, 136.5, 131.1, 130.5, 129.9, 127.2, 126.3, 124.3, 122.1, 122.0, 120.3, 117.9, 20.8, 17.5.

2-(4-methoxyphenyl)-2H-indazole (2k)[1]



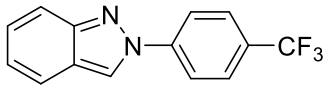
Yellow solid (58 mg, 87% yield); EtOAc/PE = 1/10. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (s, 1H), 7.79-7.77 (m, 3H), 7.69-7.67 (m, 1H), 7.33-7.29 (m, 1H), 7.12-7.08 (m, 1H), 7.02-7.00 (m, 2H), 3.84 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.3, 149.6, 134.1, 126.6, 122.7, 122.4, 122.2, 120.3, 120.2, 117.8, 114.7, 55.6.

4-(2H-indazol-2-yl)-N,N-dimethylaniline (2l)[5]



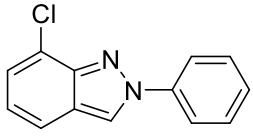
Yellow solid (64 mg, 90% yield); EtOAc/PE = 1/10. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (s, 1H), 7.79-7.77 (m, 1H), 7.73-7.67 (m, 3H), 7.31-7.27 (m, 1H), 7.10-7.07 (m, 1H), 6.80-6.77 (m, 2H), 2.99 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.1, 149.4, 130.7, 126.1, 122.7, 122.1, 121.9, 120.1, 119.9, 117.6, 112.6, 40.6.

2-(4-(trifluoromethyl)phenyl)-2H-indazole (2m)[3]



White solid (38 mg, 49% yield); EtOAc/PE = 1/15. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.46 (s, 1H), 8.07-8.05 (m, 2H), 7.80-7.77 (m, 3H), 7.72-7.70 (m, 1H), 7.36-7.33 (m, 1H), 7.15-7.12 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.2, 143.0, 129.9, 129.6, 127.5, 126.8 (q, J = 3.8Hz),124.9, 123.1, 122.7, 120.8, 120.5, 120.4, 118.1. ^{19}F NMR (470 MHz, $CDCl_3$) δ -62.4 (s, 1F).

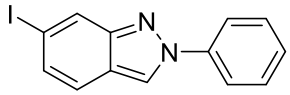
7-chloro-2-phenyl-2H-indazole (2n)[1]



White oil (64 mg, 94% yield); EtOAc/PE = 1/15. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (s, 1H), 7.87-7.85 (m, 2H), 7.57-7.55 (m, 1H), 7.48-7.44 (m, 2H), 7.38-7.30 (m, 2H),

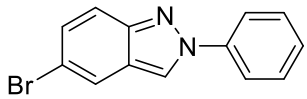
7.00-6.96 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 147.3, 140.2, 129.5, 128.3, 126.1, 124.0, 123.2, 122.7, 121.7, 121.3, 119.3.

6-iodo-2-phenyl-2H-indazole (2o)



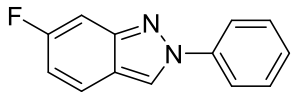
White solid (84 mg, 88% yield); mp 97.3-97.4 ºC; EtOAc/PE = 1/15. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (s, 1H), 8.22 (s, 1H), 7.86-7.84 (m, 2H), 7.53-7.49 (m, 2H), 7.45-7.38 (m, 2H), 7.34-7.32 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.9, 140.2, 131.2, 129.6, 128.2, 127.2, 121.8, 121.5, 121.0, 120.9, 92.3. HRMS (ESI): calculated for $C_{13}H_9IN_2Na$ $[M+Na]^+$ 342.9708, found 342.9734.

5-bromo-2-phenyl-2H-indazole (2p)[1]



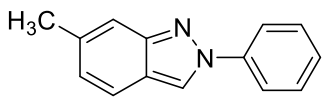
White solid (75 mg, 92% yield); EtOAc/PE = 1/15. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (s, 1H), 7.86-7.82 (m, 3H), 7.67-7.64 (m, 1H), 7.52-7.48 (m, 2H), 7.41-7.34 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.1, 140.2, 130.5, 129.6, 128.2, 123.9, 122.5, 120.9, 119.8, 119.7, 116.0.

6-fluoro-2-phenyl-2H-indazole (2q)[1]



Yellow solid (60 mg, 95% yield); EtOAc/PE = 1/15. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (s, 1H), 7.85-7.83 (m, 2H), 7.65-7.62 (m, 1H), 7.51-7.47 (m, 2H), 7.39-7.35 (m, 2H), 6.93-6.88 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.1 (d, J = 242.5Hz), 149.7 (d, J = 12.5Hz), 140.3, 129.6, 128.0, 122.3 (d, J = 10.0Hz), 120.9, 120.8, 120.1, 114.3 (d, J = 28.8Hz), 101.0 (d, J = 23.8Hz). ^{19}F NMR (470 MHz, $CDCl_3$) δ -112.9 (s, 1F).

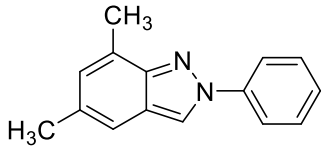
6-methyl-2-phenyl-2H-indazole (2r)[6]



White solid (56 mg, 90% yield); EtOAc/PE = 1/15. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (s, 1H), 7.84-7.82 (m, 2H), 7.54-7.52 (m, 2H), 7.47-7.43 (m, 2H), 7.34-7.30 (m,

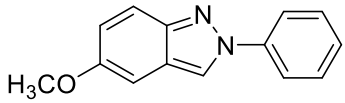
1H), 6.93-6.91 (m, 1H), 2.44 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.5, 140.6, 136.7, 129.5, 127.6, 125.5, 121.3, 120.8, 120.2, 119.9, 116.3, 22.3.

5,7-dimethyl-2-phenyl-2H-indazole (2s)[7]



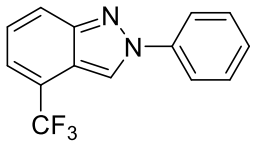
Yellow solid (65 mg, 98% yield); EtOAc/PE = 1/15. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (s, 1H), 7.86-7.84 (m, 2H), 7.48-7.44 (m, 2H), 7.35-7.31 (m, 1H), 7.22 (s, 1H), 6.90 (s, 1H), 2.64 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.3, 140.9, 132.1, 129.5, 128.8, 127.7, 127.5, 123.0, 121.0, 119.6, 115.8, 21.8, 17.0.

5-methoxy-2-phenyl-2H-indazole (2t)[1]



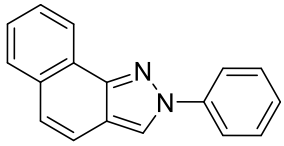
White solid (64 mg, 95% yield); EtOAc/PE = 1/10. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (s, 1H), 7.84-7.82 (m, 2H), 7.69-7.67 (m, 1H), 7.49-7.45 (m, 2H), 7.35-7.32 (m, 1H), 7.04-7.01 (m, 1H), 6.84-6.83 (m, 1H), 3.81 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.6, 146.8, 140.6, 129.5, 127.5, 122.8, 122.1, 120.5, 119.3, 119.2, 96.4, 55.3.

2-phenyl-4-(trifluoromethyl)-2H-indazole (2u)



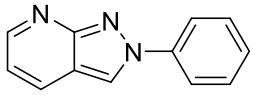
White solid (77 mg, 98% yield); mp 84.1-84.4 °C; EtOAc/PE = 1/15. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (s, 1H), 7.97-7.89 (m, 3H), 7.53-7.49 (m, 2H), 7.44-7.32 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.7, 140.2, 129.6, 128.5, 124.2 (q, J = 270.0Hz), 125.3, 122.5 (q, J = 33.8Hz), 122.2, 121.2, 120.8 (q, J = 3.8Hz), 119.9, 118.1. ^{19}F NMR (470 MHz, $CDCl_3$) δ -62.6 (s, 1F). HRMS (ESI): calculated for $C_{14}H_9F_3N_2Na$ $[M+Na]^+$ 285.0616, found 285.0622.

2-phenyl-2H-benzo[g]indazole (2v)[8]



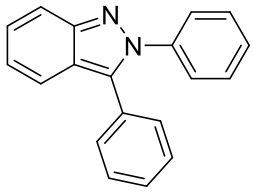
Yellow solid (61 mg, 83% yield); EtOAc/PE = 1/15. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71-8.69 (m, 1H), 8.34 (s, 1H), 7.94-7.92 (m, 2H), 7.82-7.79 (m, 1H), 7.62-7.49 (m, 5H), 7.39-7.34 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 147.6, 140.7, 132.8, 129.5, 128.4, 127.3, 127.0, 126.7, 125.8, 124.6, 122.7, 121.1, 120.5, 120.1, 118.3.

2-phenyl-2H-pyrazolo[3,4-b]pyridine (2w)[9]



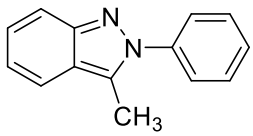
White solid (55 mg, 94% yield); EtOAc/PE = 1/2. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74-8.73 (m, 1H), 8.44 (s, 1H), 8.09-8.06 (m, 1H), 7.98-7.96 (m, 2H), 7.54-7.50 (m, 2H), 7.43-7.39 (m, 1H), 7.08-7.05 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.9, 152.4, 140.2, 129.9, 129.6, 128.4, 120.9, 120.0, 118.5, 115.0.

2,3-diphenyl-2H-indazole (2x)[10]



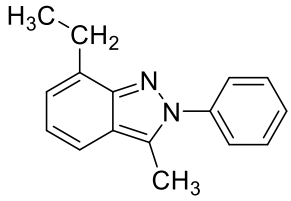
White solid (75 mg, 92% yield); EtOAc/PE = 1/15. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.81-7.80 (m, 1H), 7.71-7.69 (m, 1H), 7.44-7.42 (m, 2H), 7.36-7.33 (m, 9H), 7.14-7.11 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.1, 140.3, 135.4, 130.0, 129.7, 129.0, 128.8, 128.3, 128.2, 127.0, 126.1, 122.5, 121.8, 120.5, 117.8.

3-methyl-2-phenyl-2H-indazole (2y)[11]



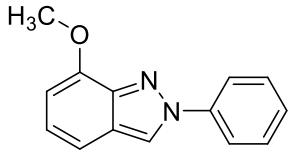
Yellow solid (32 mg, 52% yield); EtOAc/PE = 1/15. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73-7.71 (m, 1H), 7.63-7.61 (m, 1H), 7.58-7.51 (m, 4H), 7.49-7.45 (m, 1H), 7.33-7.30 (m, 1H), 7.09-7.06 (m, 1H), 2.64 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.7, 140.0, 131.9, 129.2, 128.6, 126.8, 125.8, 121.7, 120.9, 120.0, 117.6, 11.1.

7-ethyl-3-methyl-2-phenyl-2H-indazole (2z)[7]



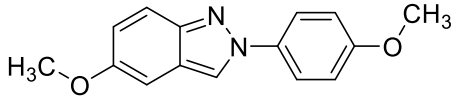
White solid (63 mg, 89% yield); EtOAc/PE = 1/15. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57-7.51 (m, 4H), 7.47-7.45 (m, 2H), 7.12-7.10 (m, 1H), 7.05-7.01 (m, 1H), 3.09 (q, 2H, J = 7.6Hz), 2.61 (s, 3H), 1.41 (t, 3H, J = 7.6Hz); ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.3, 140.2, 133.7, 132.0, 129.2, 128.5, 126.0, 123.6, 121.6, 121.3, 117.4, 24.3, 13.9, 11.1.

7-methoxy-2-phenyl-2H-indazole (2aa)[12]



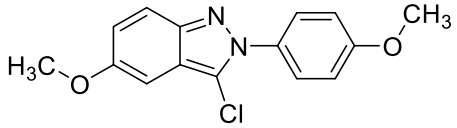
colorless oil (65 mg, 97% yield); EtOAc/PE = 1/10. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (s, 1H), 7.90-7.88 (m, 2H), 7.46-7.42 (m, 2H), 7.34-7.30 (m, 1H), 7.23-7.21 (m, 1H), 7.00-6.97 (m, 1H), 6.55-6.54 (m, 1H), 4.00 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.4, 143.4, 140.4, 129.4, 127.8, 124.4, 123.1, 121.0, 120.3, 112.4, 103.2, 55.5.

5-methoxy-2-(4-methoxyphenyl)-2H-indazole (2bb)[13]



White solid (67 mg, 88% yield); EtOAc/PE = 1/10. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.78 (s, 1H), 7.96-7.94 (m, 2H), 7.63-7.61 (m, 1H), 7.13-7.11 (m, 2H), 7.01-6.97 (m, 2H), 3.83 (s, 3H), 3.80 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 158.5, 154.6, 145.5, 133.6, 122.4, 121.3, 121.2, 119.9, 118.7, 114.6, 96.9, 55.5, 55.1.

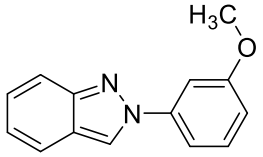
3-chloro-5-methoxy-2-(4-methoxyphenyl)-2H-indazole (2cc)[13]



White solid (59 mg, 68% total yield); EtOAc/PE = 1/10. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60-7.56 (m, 3H), 7.05-7.02 (m, 3H), 6.75-6.74 (m, 1H), 3.87 (s, 6H); ^{13}C NMR

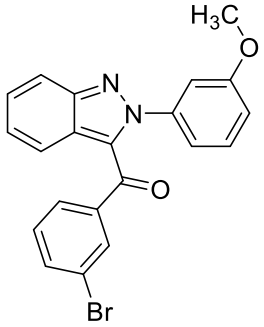
(125 MHz, $CDCl_3$) δ 159.9, 155.8, 145.2, 131.7, 126.9, 122.7, 119.6, 119.5, 118.1, 114.2, 94.7, 55.6, 55.5.

2-(3-methoxyphenyl)-2H-indazole (2dd)[1]



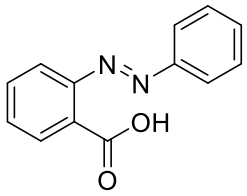
Colorless oil (61 mg, 91% yield); EtOAc/PE = 1/10. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.32 (s, 1H), 7.79-7.77 (m, 1H), 7.66-7.64 (m, 1H), 7.50-7.49 (m, 1H), 7.39-7.28 (m, 3H), 7.09-7.06 (m, 1H), 6.90-6.88 (m, 1H), 3.84 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.6, 149.7, 141.7,130.3, 126.9, 122.8, 122.5, 120.6, 120.5, 117.9, 113.9, 112.9, 106.8, 55.6.

(3-bromophenyl)(2-(3-methoxyphenyl)-2H-indazol-3-yl)methanone (2ee)



White solid (84 mg, 69% total yield); EtOAc/PE = 1/10. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90-7.88 (m, 2H), 7.74-7.72 (m, 1H), 7.67-7.65 (m, 1H), 7.48-7.46 (m, 1H), 7.41-7.38 (m, 1H), 7.30-7.21 (m, 3H), 7.11 (s, 1H), 7.02-7.00 (m, 1H), 6.92-6.90 (m, 1H), 3.80 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 184.4, 160.1, 148.6, 141.3, 139.5, 136.2, 132.5, 131.8, 130.2, 129.8, 128.2, 127.3, 125.6, 124.3, 122.8, 120.4, 118.7, 118.0, 115.3, 111.2, 55.6.

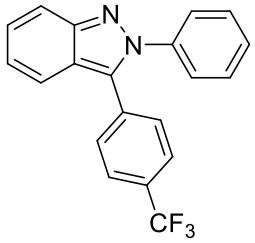
(E) -2-(phenyldiazenyl)benzoic acid (3a)



White solid (7mg, 10% yield); mp 175.6-176.2 °C; EtOAc/PE = 1/2. ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.66 (s, 1H), 7.94-7.93 (m, 2H), 7.77-7.75 (m, 1H), 7.63-7.60 (m, 1H), 7.53-7.50 (m, 2H), 7.38-7.37 (m, 1H), 7.27-7.20 (m, 2H). ^{13}C NMR (125 MHz,

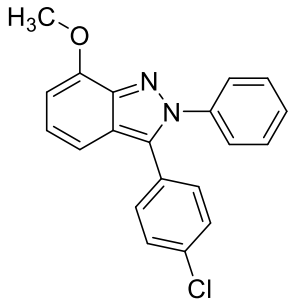
DMSO-d_6) δ 160.2, 146.6, 137.6, 132.5, 129.0. 124.8, 123.4, 121.8, 118.9, 118.1, 112.6. HRMS (ESI): calculated for $C_{13}H_{10}N_2O_2Na$ $[M+Na]^+$ 249.0640, found 249.0646.

2-phenyl-3-(4-(trifluoromethyl)phenyl)-2H-indazole (A)[14]



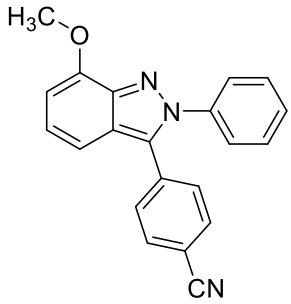
White solid (94 mg, 93% total yield); EtOAc/PE = 1/15. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89-7.87 (m, 1H), 7.75-7.72 (m, 1H), 7.70-7.68 (m, 2H), 7.52-7.50 (m, 2H), 7.47-7.41 (m, 6H), 7.24-7.20 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.1, 139.9, 133.6, 133.5, 130.1 (q, J = 32.5Hz), 129.9, 129.3, 128.7, 127.2, 126.1, 125.8 (q, J = 3.8Hz), 125.0, 123.3, 122.9, 122.0, 119.9, 118.1.

3-(4-chlorophenyl)-7-methoxy-2-phenyl-2H-indazole (B)[15]



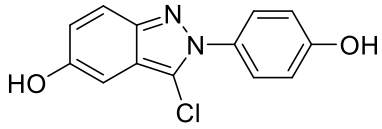
White solid (80 mg, 80% total yield); EtOAc/PE = 1/10. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41-7.32 (m, 7H), 7.26-7.20 (m, 3H), 7.06-7.02 (m, 1H), 6.62-6.60 (m, 1H), 4.03 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.5, 142.6, 139.9, 134.3, 134.2, 130.8, 129.1, 129.0, 128.5, 128.4, 126.2, 123.6, 123.3, 111.9, 103.4, 55.5.

4-(7-methoxy-2-phenyl-2H-indazol-3-yl)benzonitrile (C)[15]



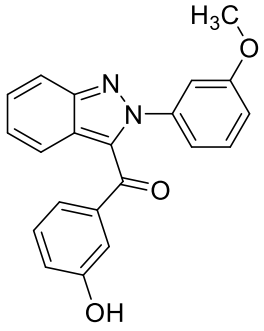
White solid (79 mg, 81% total yield); EtOAc/PE = 1/10. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66-7.64 (m, 2H), 7.45-7.40 (m, 7H), 7.26-7.24 (m, 1H), 7.13-7.10 (m, 1H), 6.66-6.65 (m, 1H), 4.05 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.6, 142.6, 139.6, 134.5, 133.2, 132.4, 130.0, 129.2, 128.8, 126.2, 124.5, 123.4, 118.4, 111.6, 111.4, 103.6, 55.6.

3-chloro-2-(4-hydroxyphenyl)-2H-indazol-5-ol (D)[13]



White solid (42 mg, 54% total yield); EtOAc/PE = 1/2. ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.04 (s, 1H), 9.62 (s, 1H), 7.58-7.56 (m, 1H), 7.48-7.47 (m, 2H), 7.02-6.95 (m, 3H), 6.73 (s, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 163.2, 158.1, 149.1, 134.9, 132.2, 127.4, 124.7, 124.5, 121.0, 120.7, 102.3.

(3-hydroxyphenyl)(2-(3-methoxyphenyl)-2H-indazol-3-yl)methanone (E)[16]



White solid (59 mg, 57% total yield); EtOAc/PE = 1/3. ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.90 (s, 1H), 7.91-7.90 (m, 1H), 7.46-7.31 (m, 4H), 7.28-7.17 (m, 4H), 7.11-7.03 (m, 3H), 3.79 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 185.5, 159.5,

157.5, 147.7, 141.1, 138.5, 132.2, 129.9, 127.1, 125.0, 123.3, 120.9, 120.5, 120.2, 118.2, 117.7, 115.5, 114.7, 111.1, 55.5.

Reference:

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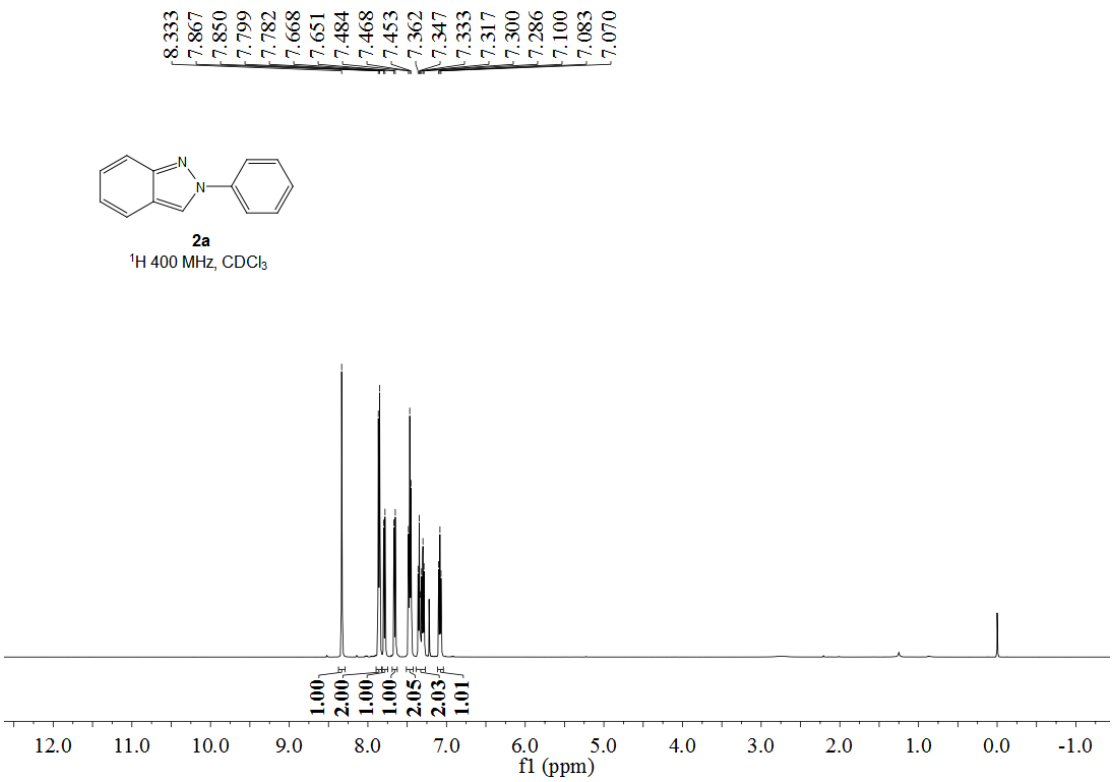
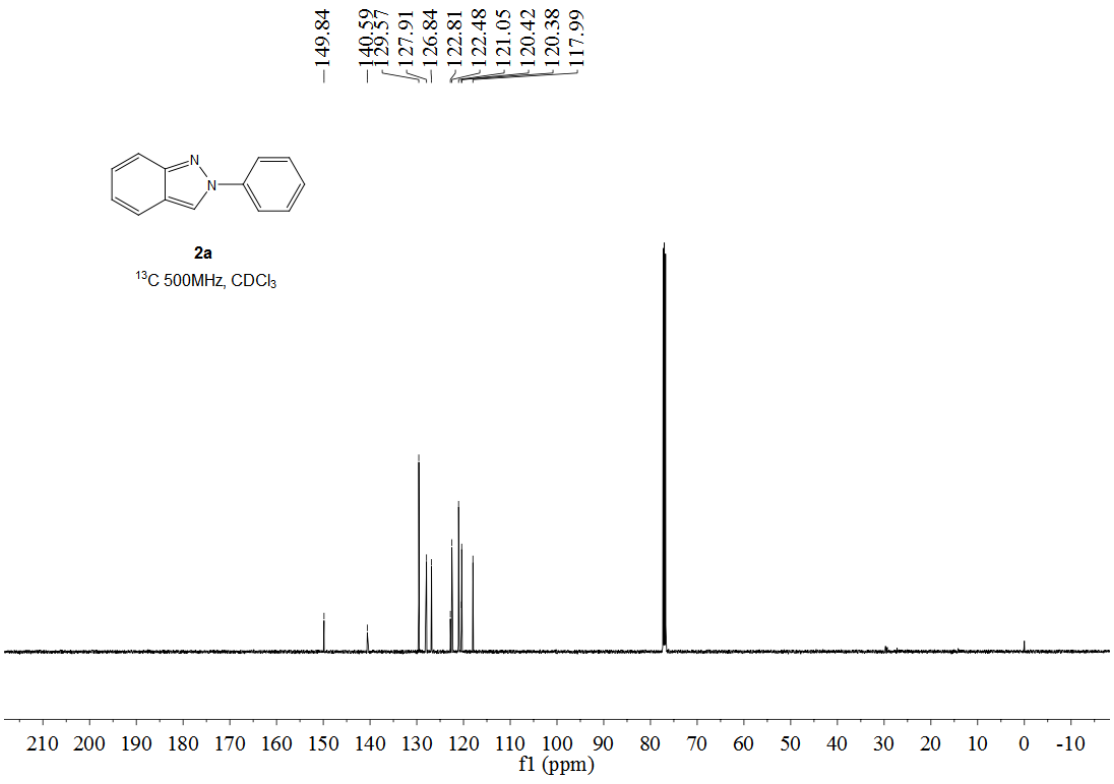
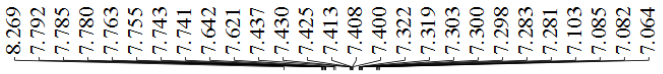
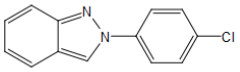
5. ^{1}H, ^{13}C and ^{19}F NMR spectra of products



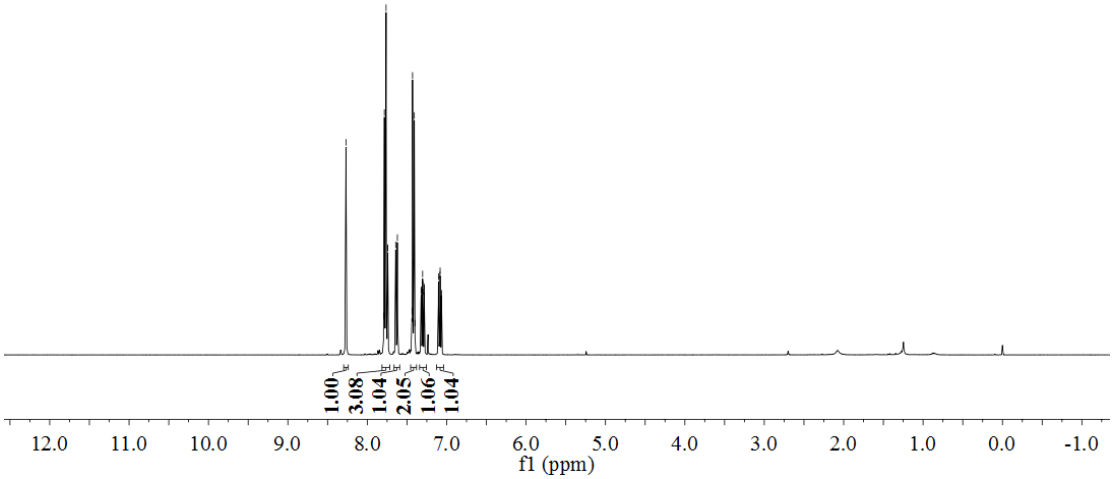


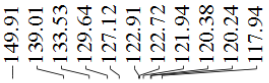


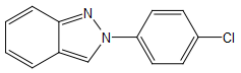


2b

^{1}H 400 MHz, $CDCl_3$

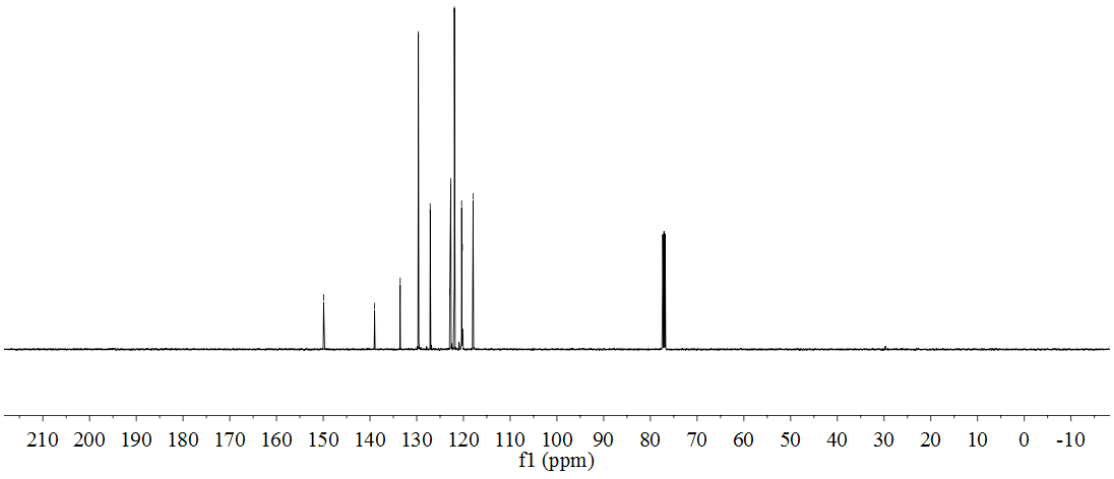


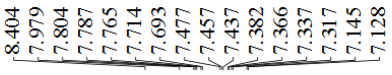


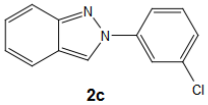


2b

^{13}C 500MHz, $CDCl_3$

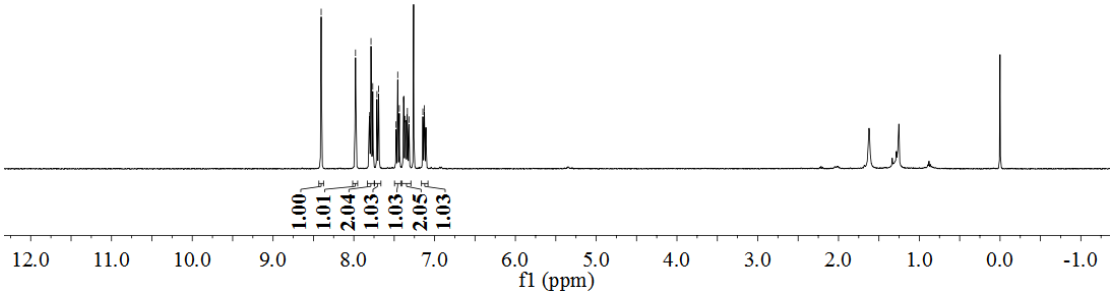


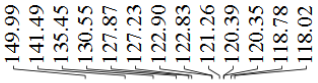


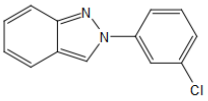


2c

^{1}H 400 MHz, $CDCl_3$

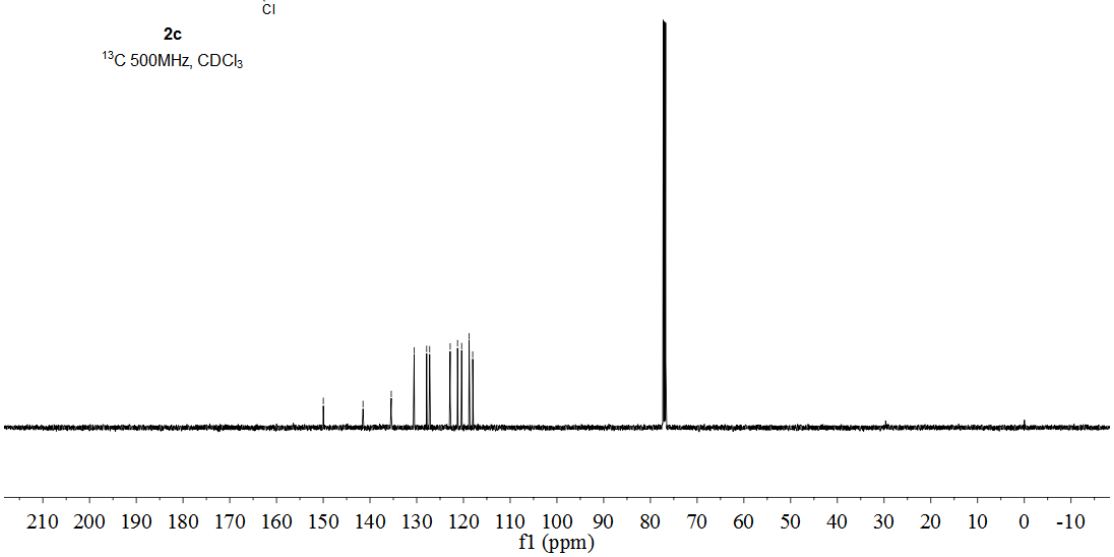


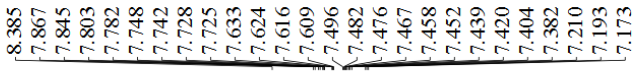


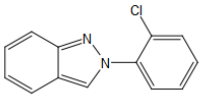


2c

^{13}C 500MHz, $CDCl_3$

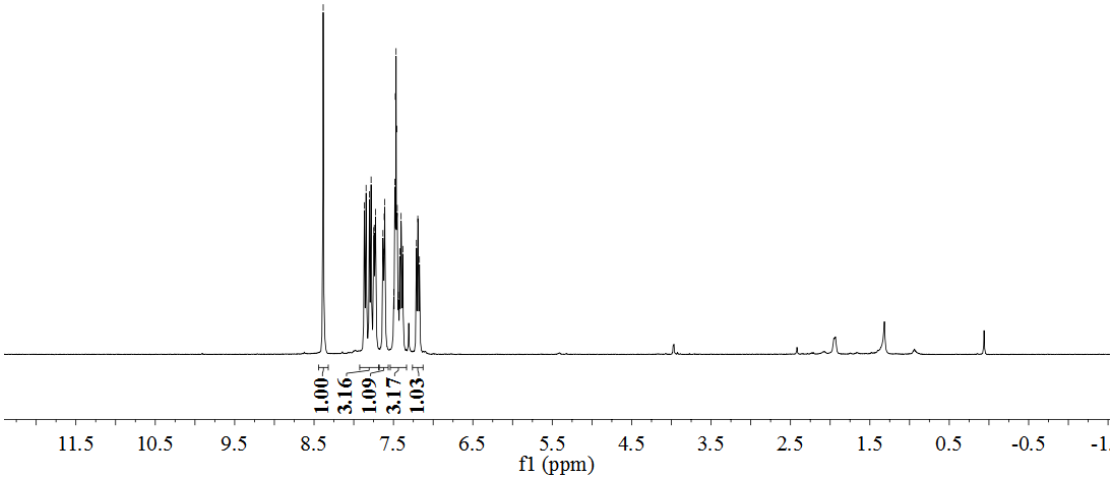


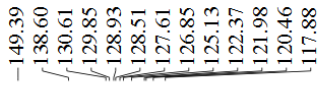


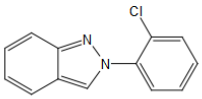


2d

^{1}H 400 MHz, $CDCl_3$

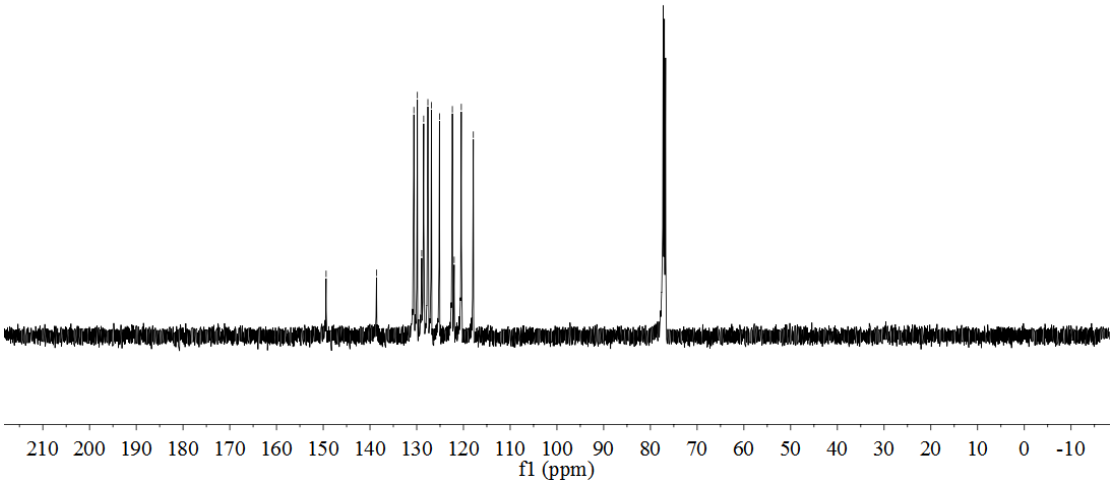


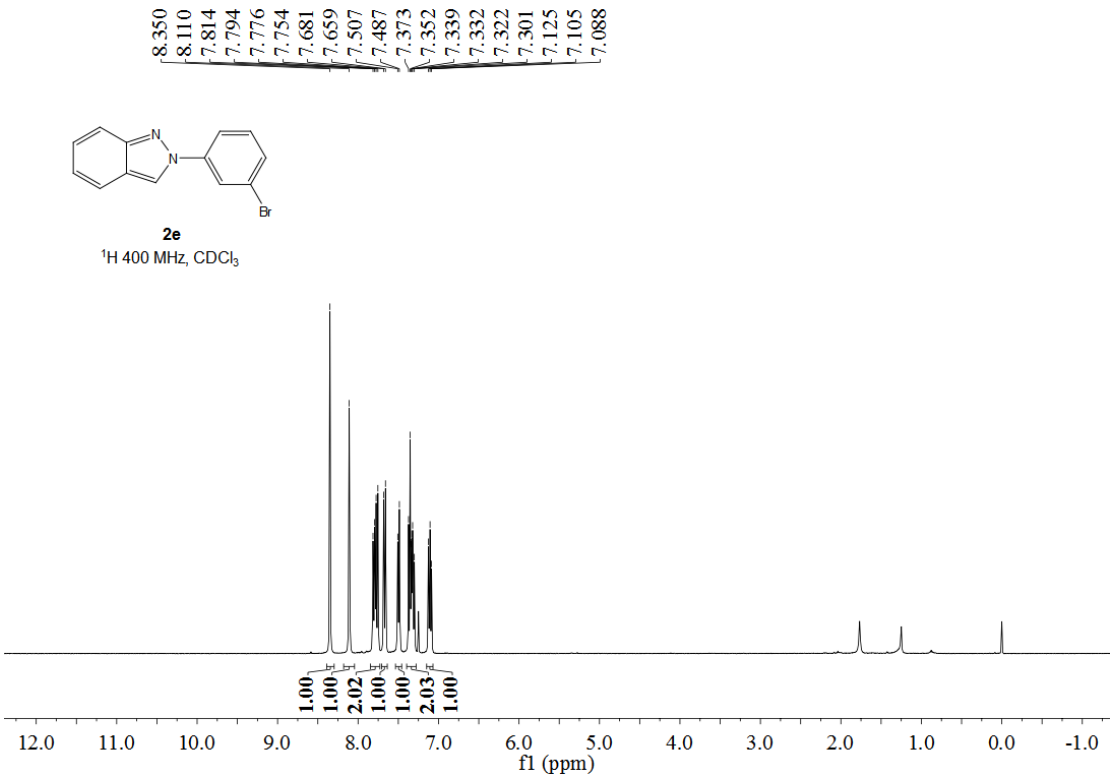


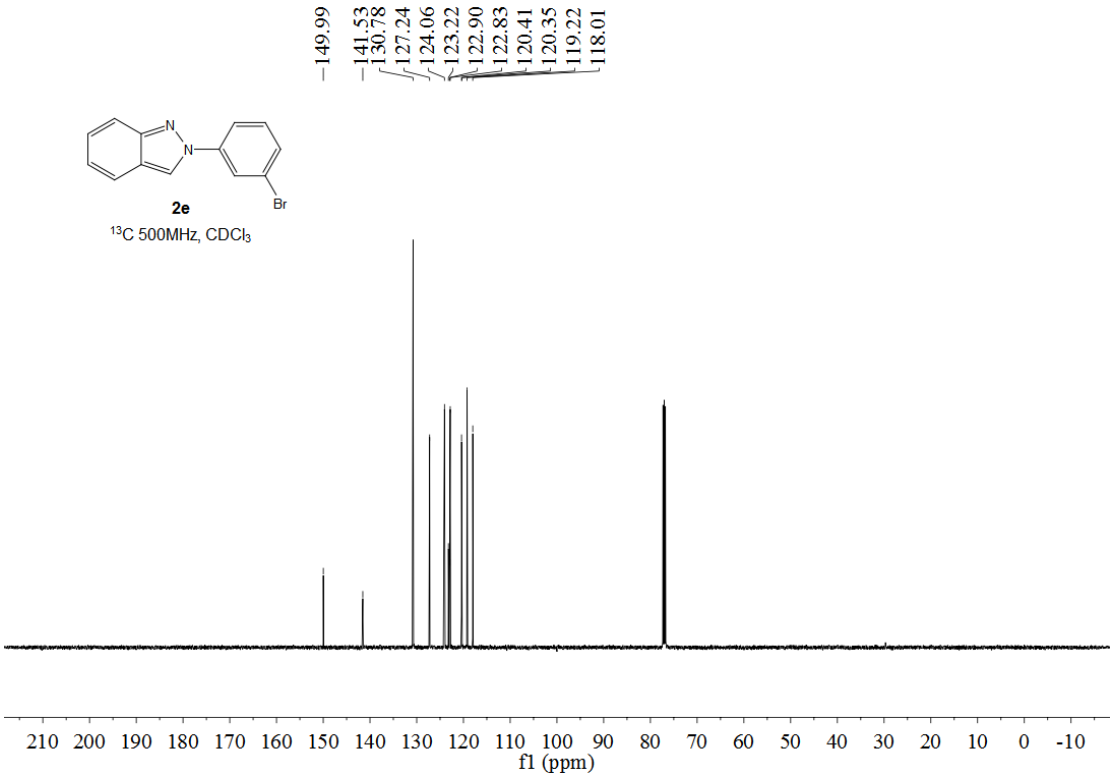


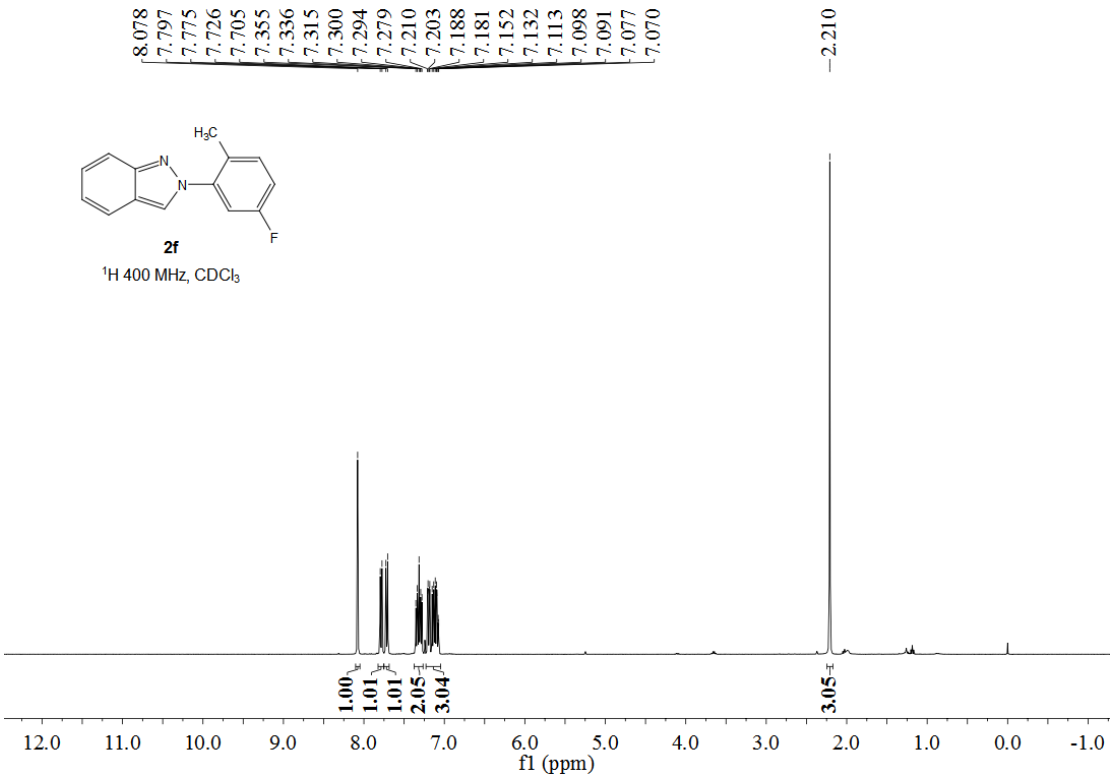
2d

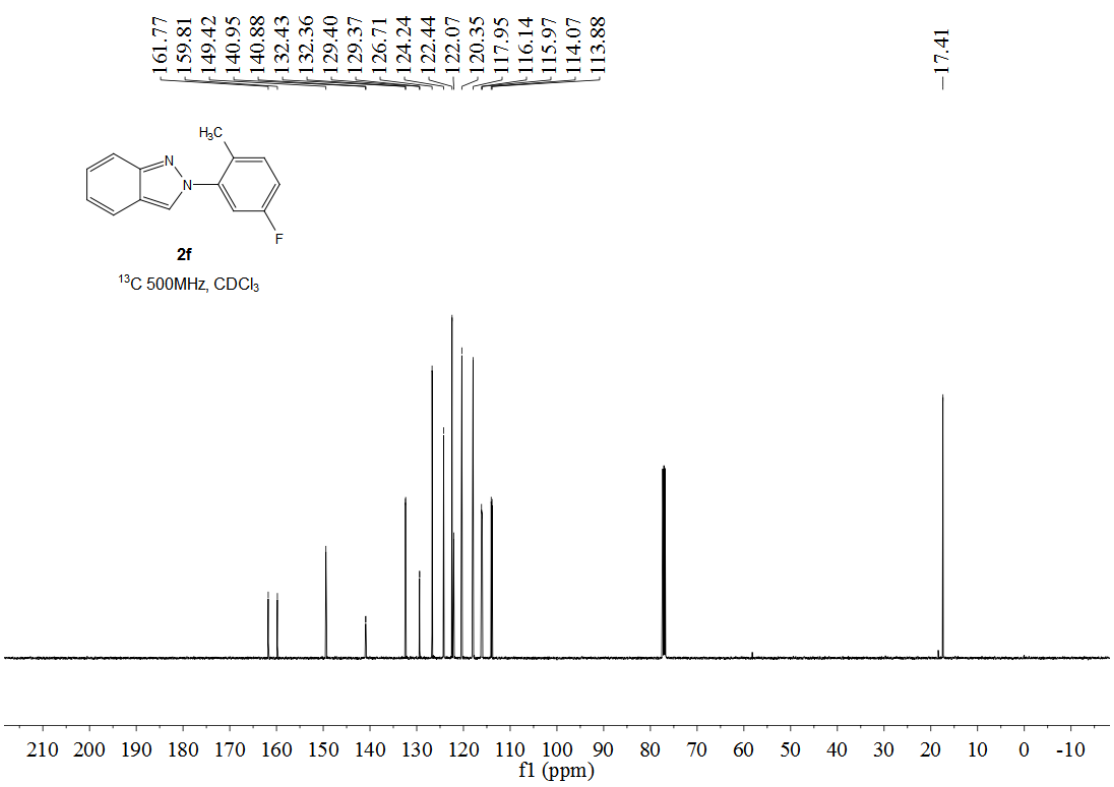
^{13}C 500MHz, $CDCl_3$

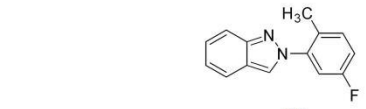



8.350
8.110
7.814
7.794
7.776
7.754
7.681
7.659
7.507
7.487
7.373
7.352
7.339
7.332
7.322
7.301
7.125
7.105
7.088
N
N
Br
2e
1H 400 MHz, CDCl3
1.00
1.00
2.02
1.00
1.00
2.03
1.00
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)


149.99
141.53
130.78
127.24
124.06
123.22
122.90
122.83
120.41
120.35
119.22
118.01
N
N
Br
2e
13C 500MHz, CDCl3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

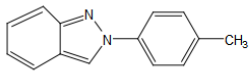

8.078
7.797
7.775
7.726
7.705
7.355
7.336
7.315
7.300
7.294
7.279
7.210
7.203
7.188
7.181
7.152
7.132
7.113
7.098
7.091
7.077
7.070
2.210
H3C
N
N
F
2f
1H 400 MHz, CDCl3
1.00
1.01
1.01
2.05
3.04
3.05
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)


161.77
159.81
149.42
140.95
140.88
132.43
132.36
129.40
129.37
126.71
124.24
122.44
122.07
120.35
117.95
116.14
115.97
114.07
113.88
17.41
H3C
N
N
F
2f
13C 500MHz, CDCl3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



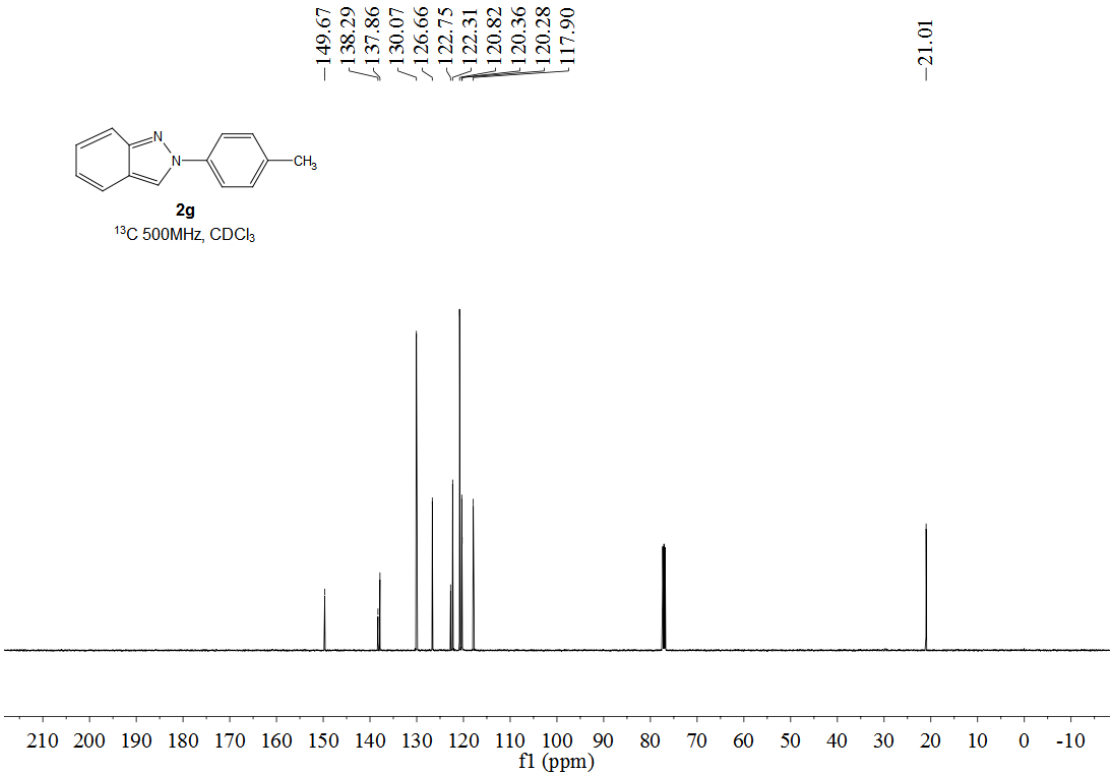
2f

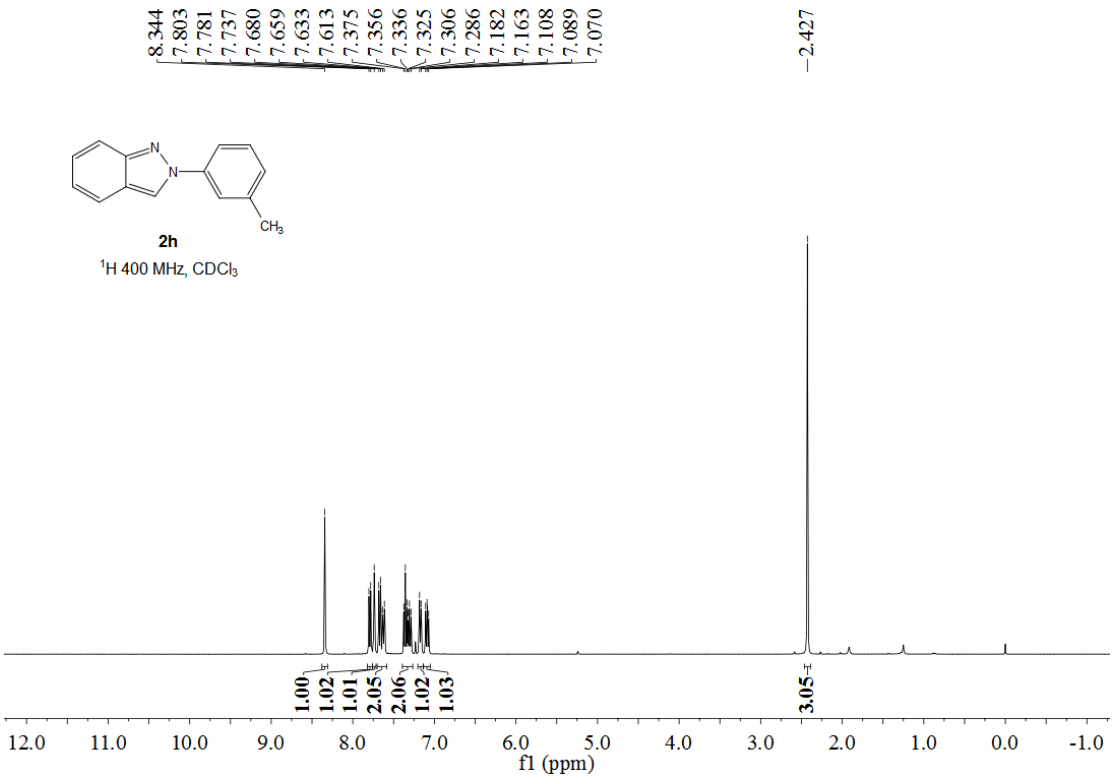
^{19}F 470MHz, $CDCl_3$

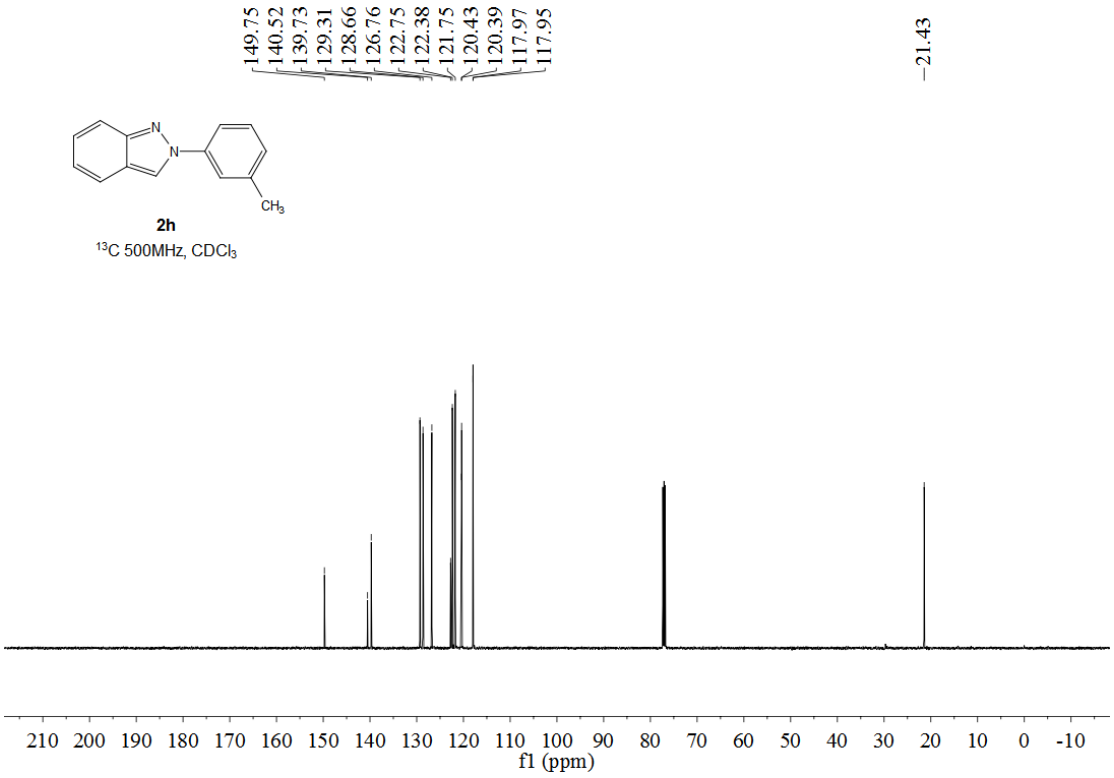


2g

^{1}H 400 MHz, $CDCl_3$

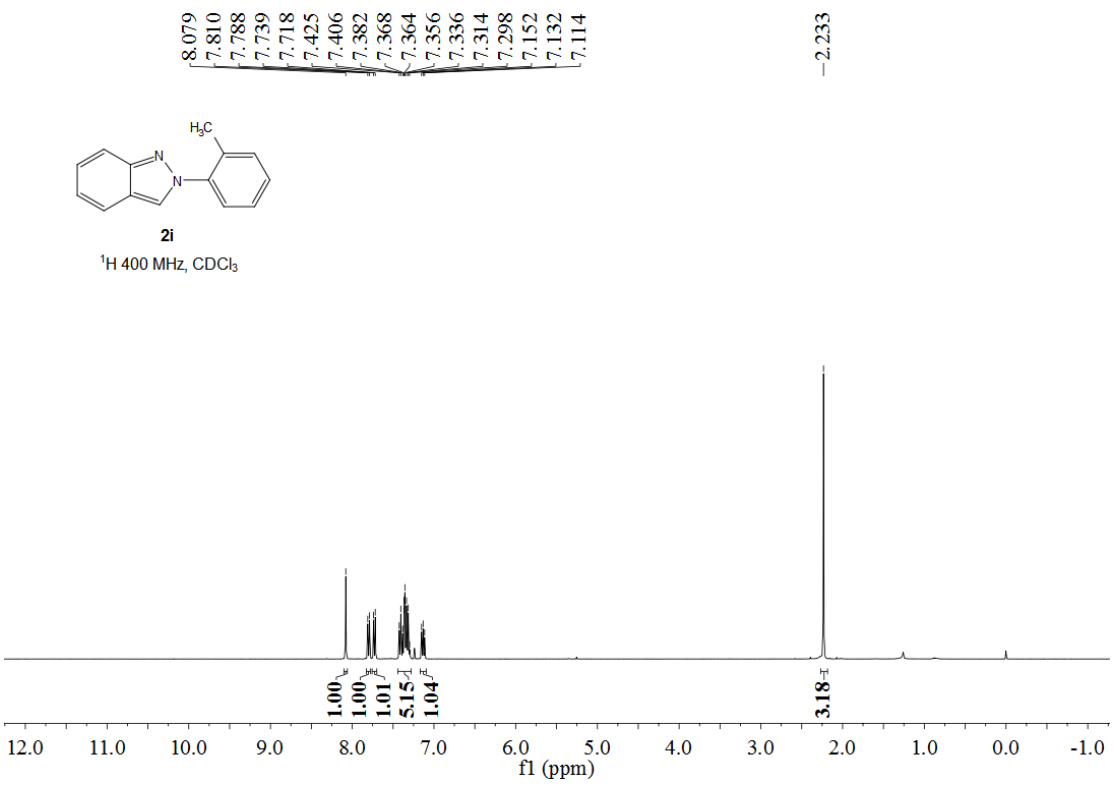

149.67
138.29
137.86
130.07
126.66
122.75
122.31
120.82
120.36
120.28
117.90
21.01
N
N
CH3
2g
13C 500MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.344
7.803
7.781
7.737
7.680
7.659
7.633
7.613
7.375
7.356
7.336
7.325
7.306
7.286
7.182
7.163
7.108
7.089
7.070
2.427
N
N
CH3
2h
1H 400 MHz, CDCl3
1.00
1.02
1.01
2.05
2.06
1.02
1.03
3.05
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0
f1 (ppm)



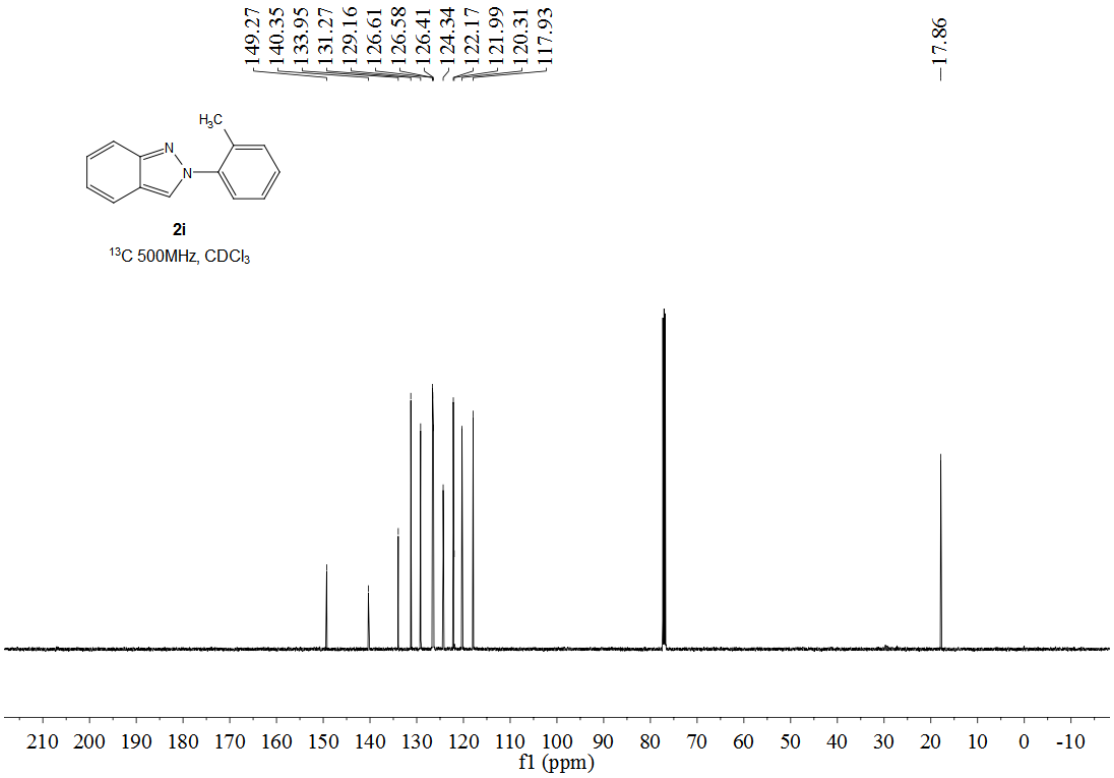
2h

^{13}C 500MHz, $CDCl_3$



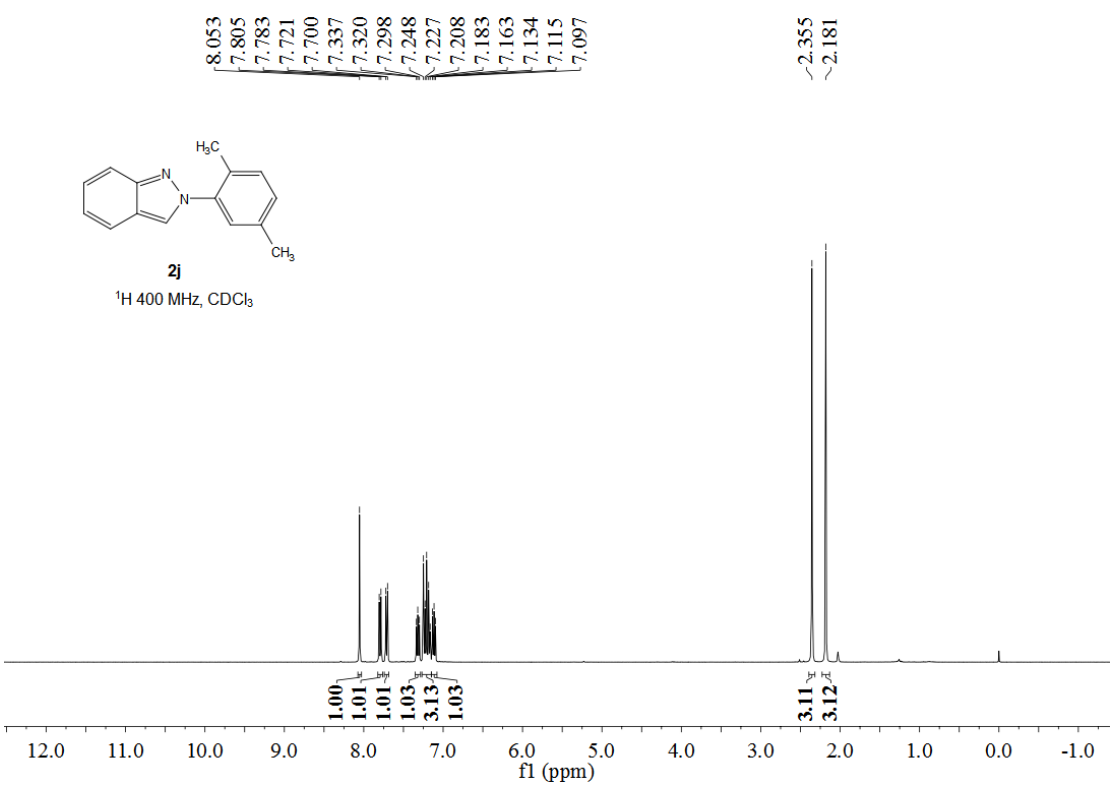
2i

^{1}H 400 MHz, $CDCl_3$



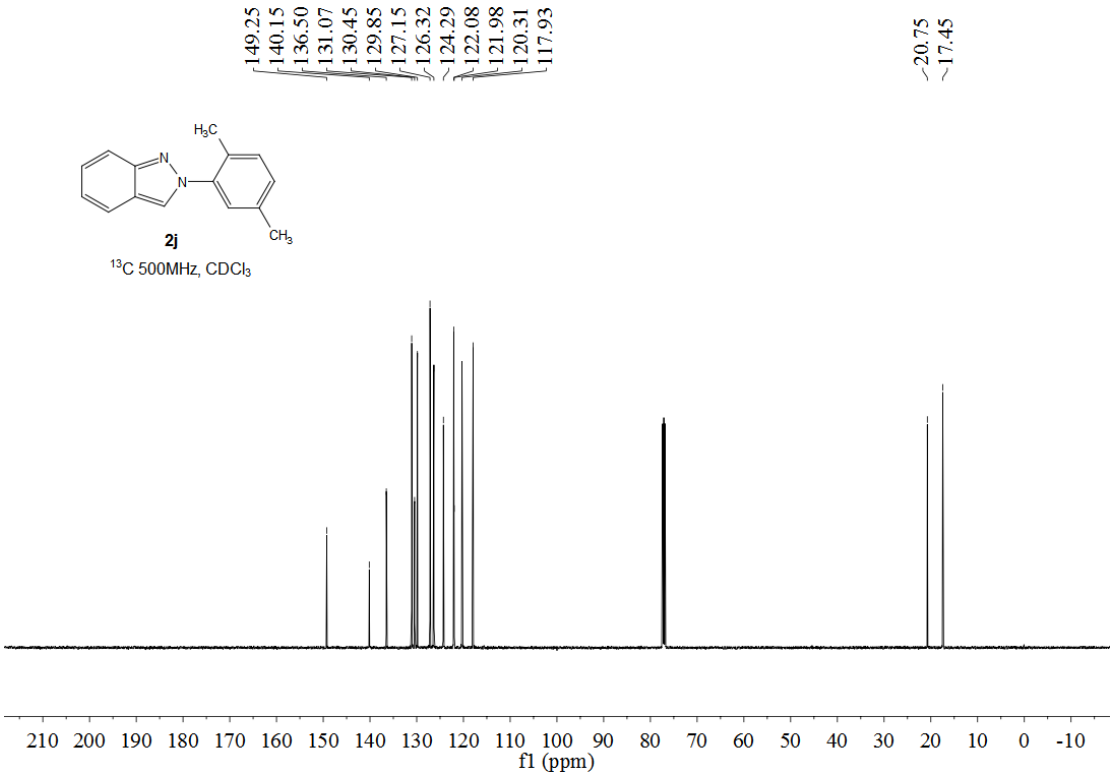
2i

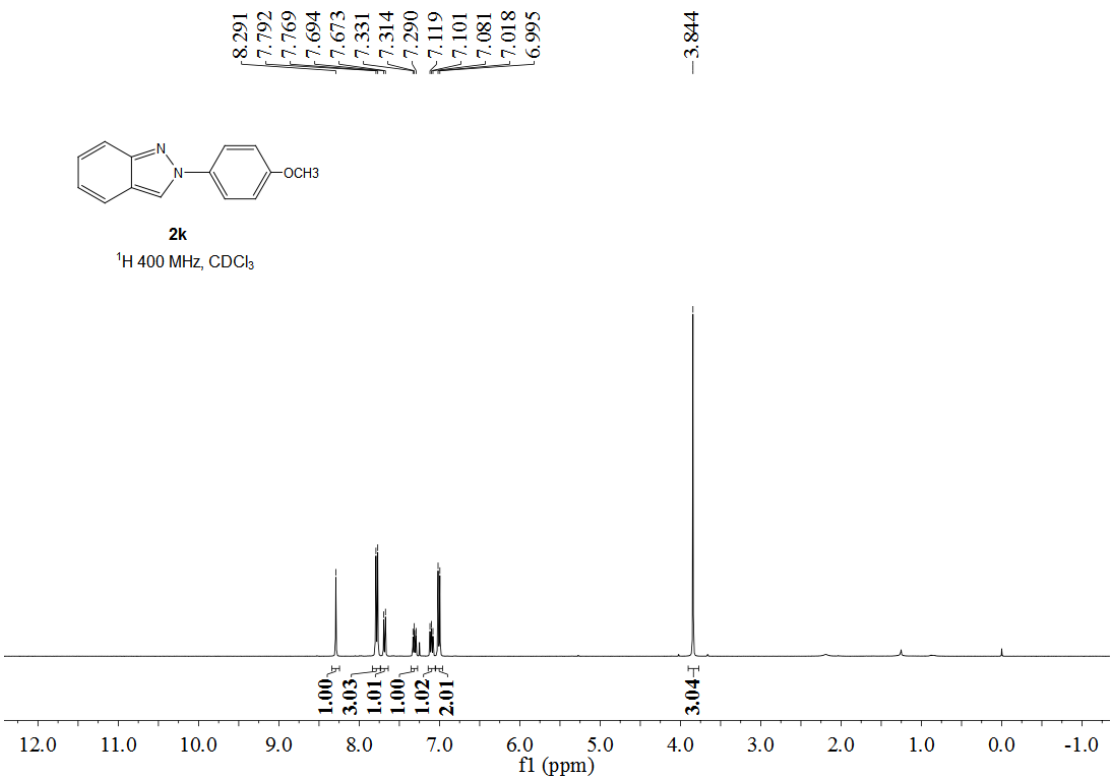
^{13}C 500MHz, $CDCl_3$

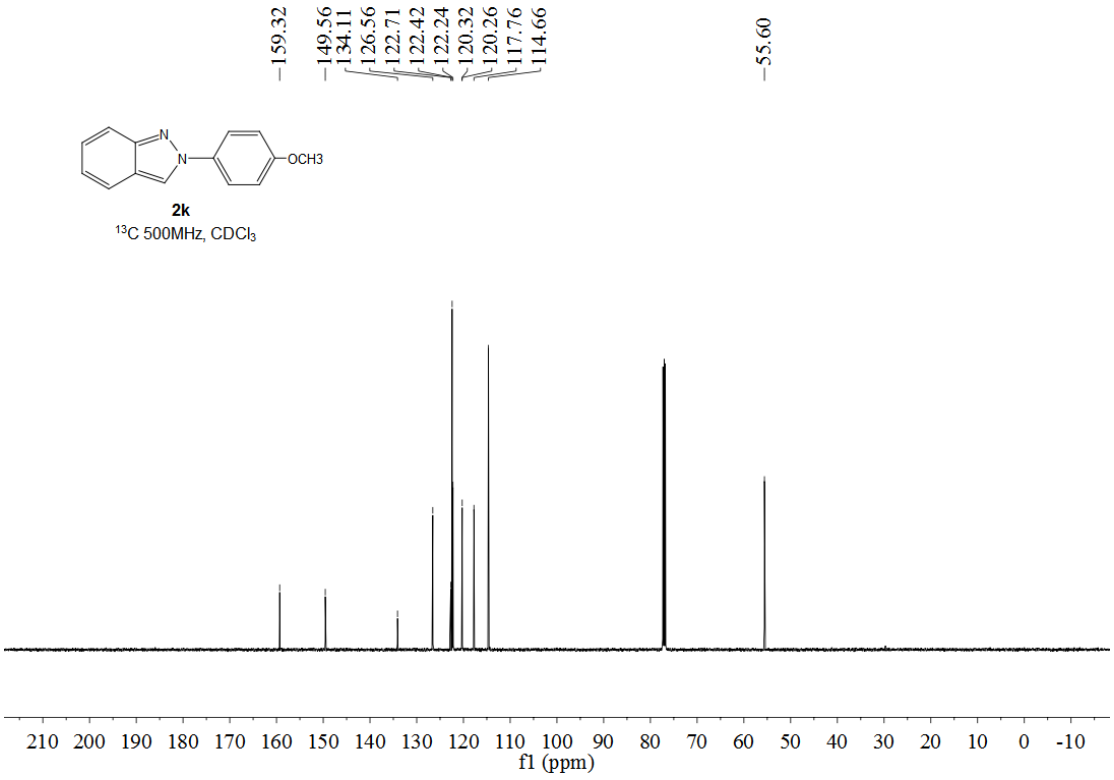


2j

^{1}H 400 MHz, $CDCl_3$

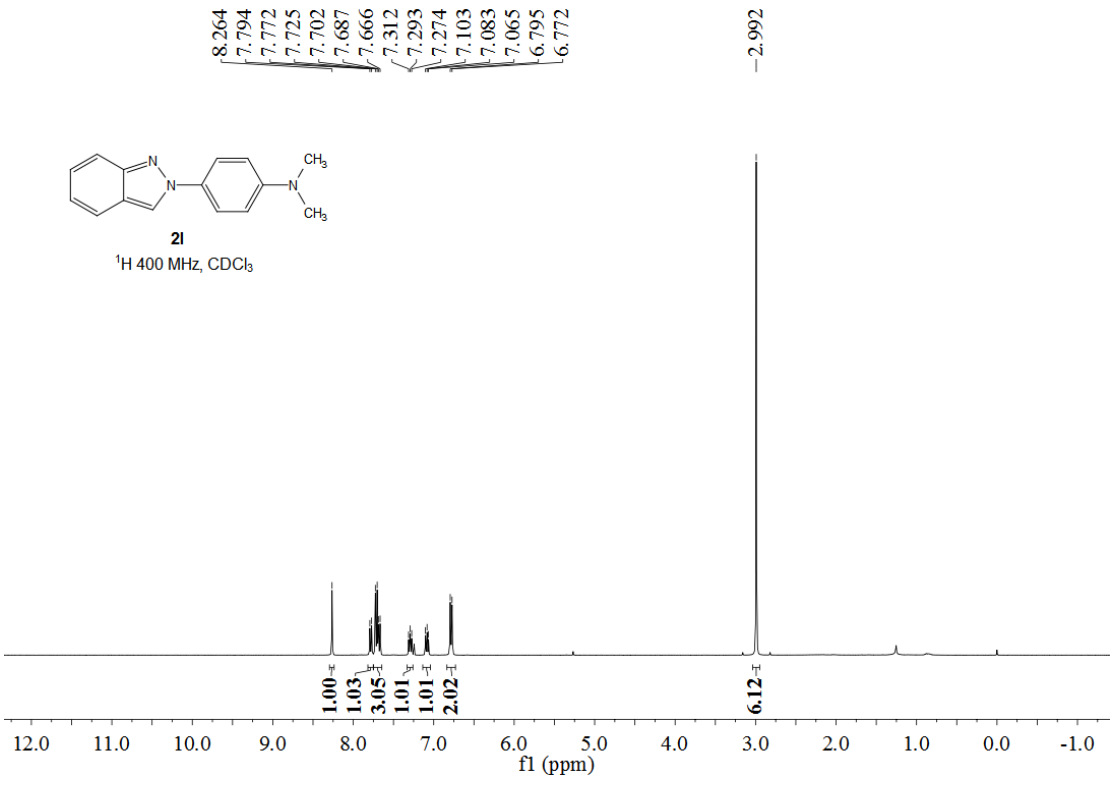

149.25
140.15
136.50
131.07
130.45
129.85
127.15
126.32
124.29
122.08
121.98
120.31
117.93
20.75
17.45
H3C
CH3
2j
13C 500MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.291
7.792
7.769
7.694
7.673
7.331
7.314
7.290
7.119
7.101
7.081
7.018
6.995
3.844
OCH3
2k
1H 400 MHz, CDCl3
1.00
3.03
1.01
1.00
1.02
2.01
3.04
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0
f1 (ppm)



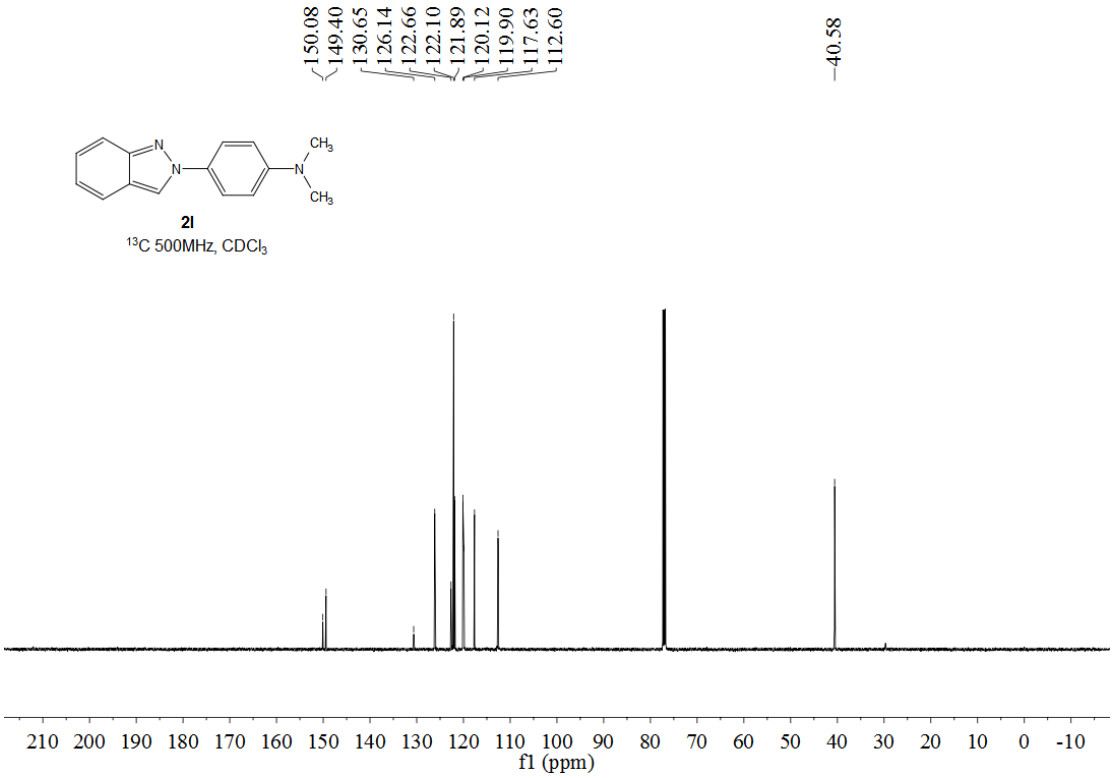
2k

^{13}C 500MHz, $CDCl_3$



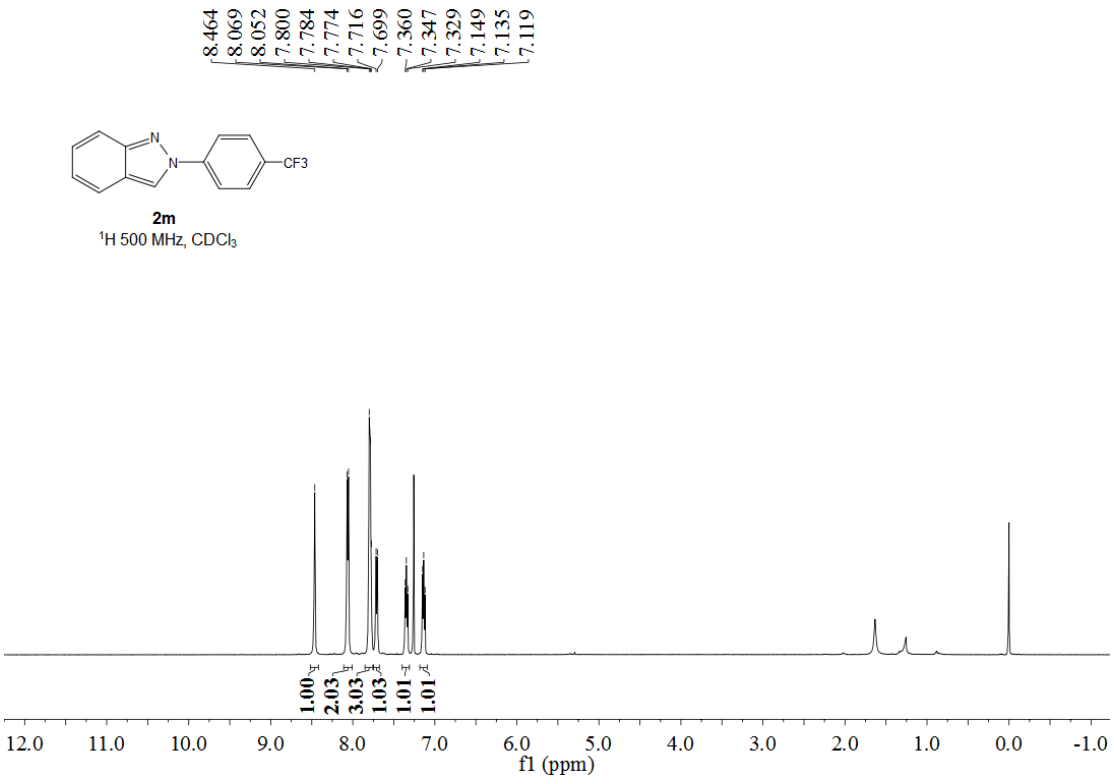
2l

^{1}H 400 MHz, $CDCl_3$



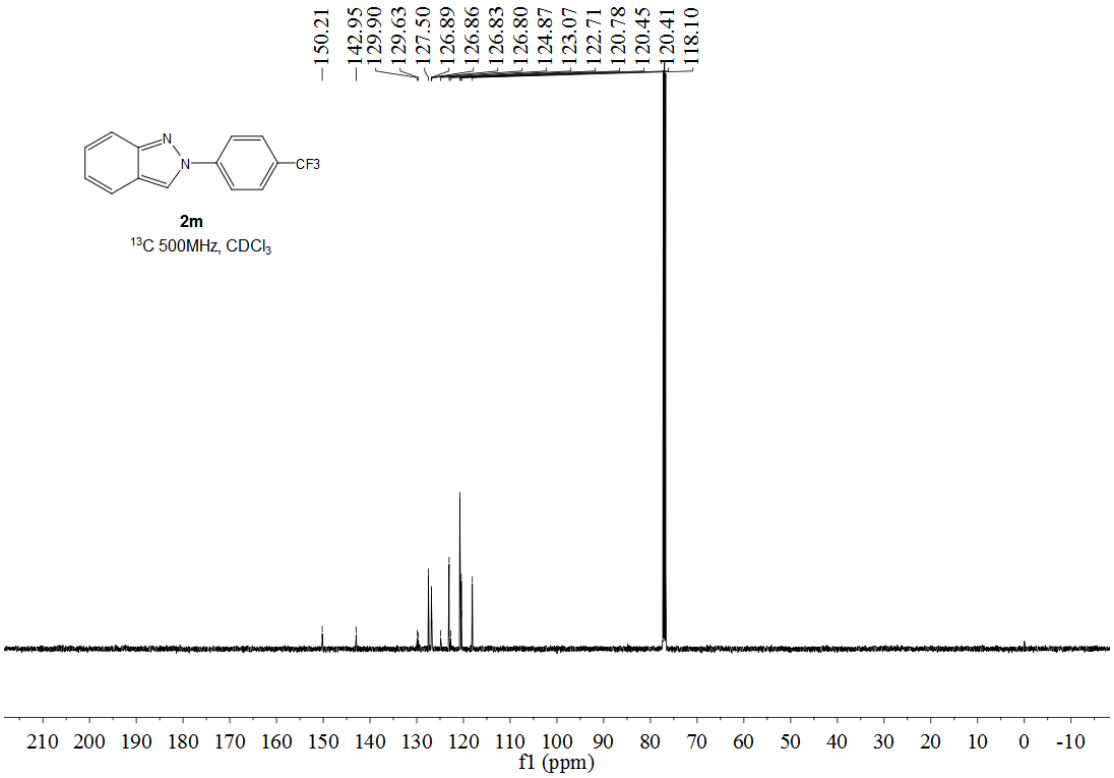
2l

^{13}C 500MHz, $CDCl_3$



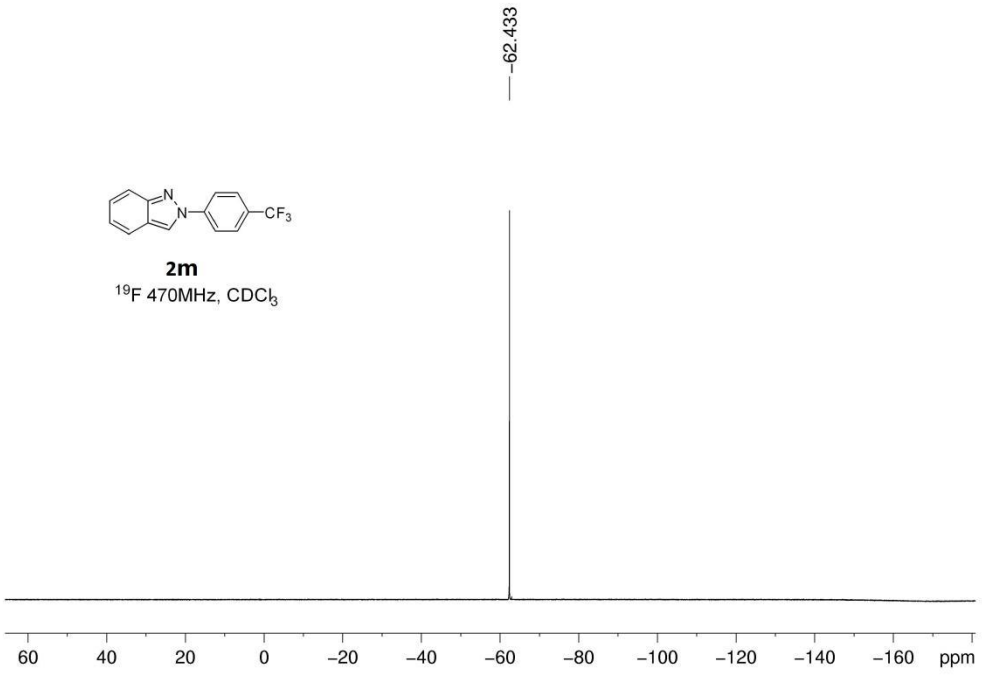
2m

^{1}H 500 MHz, $CDCl_3$



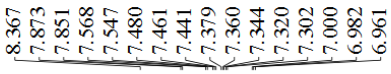
2m

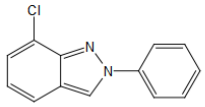
^{13}C 500MHz, $CDCl_3$



2m

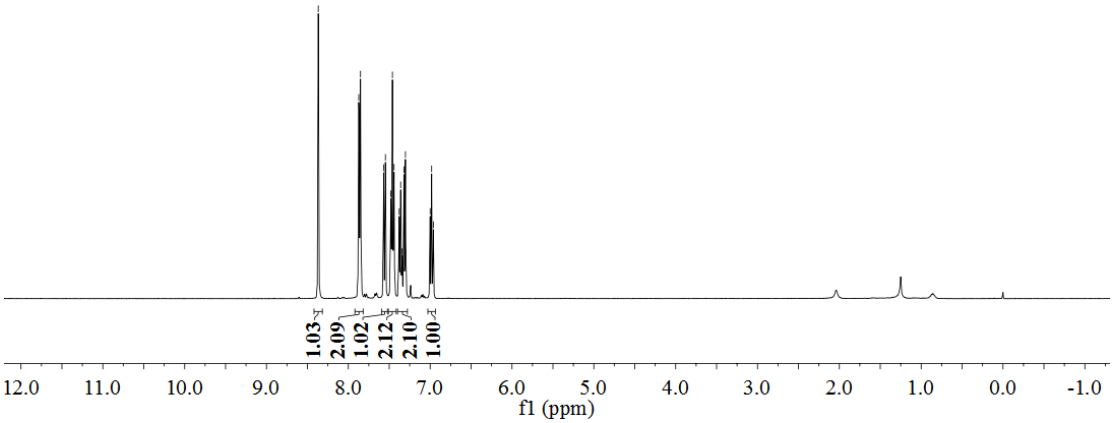
^{19}F 470MHz, $CDCl_3$

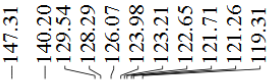


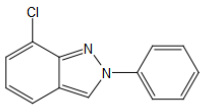


2n

^{1}H 400 MHz, $CDCl_3$

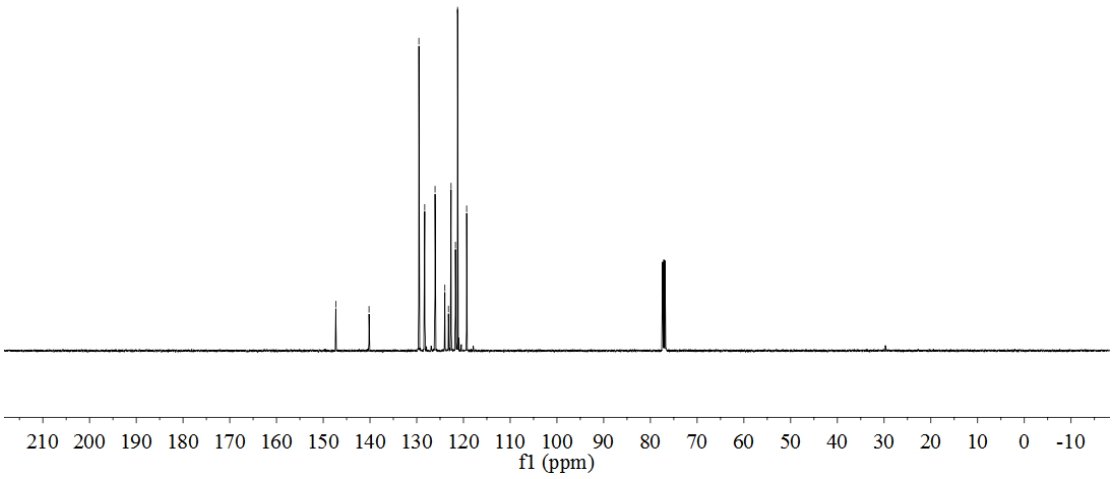


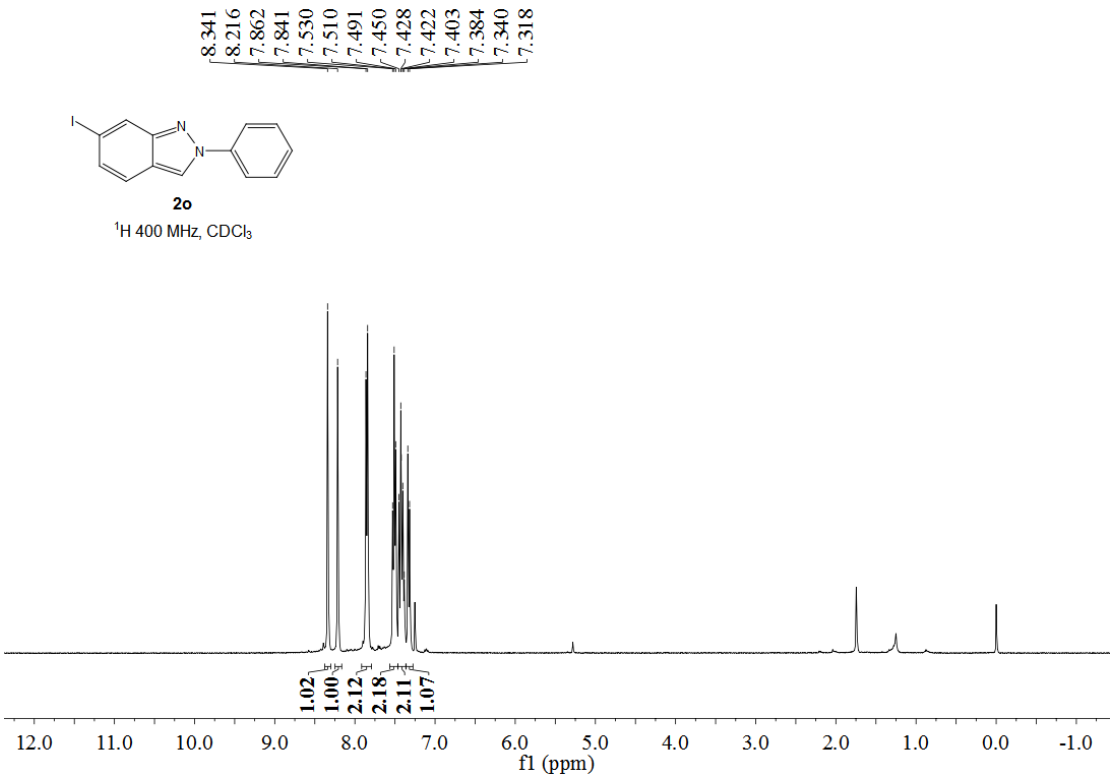


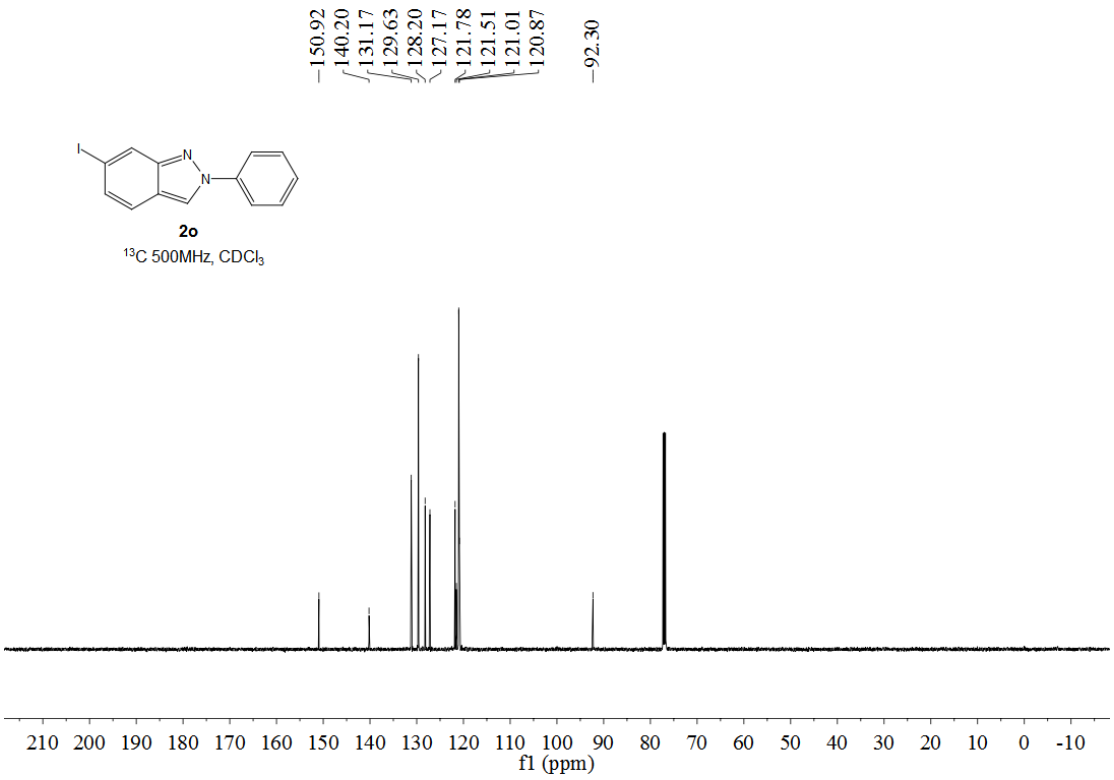


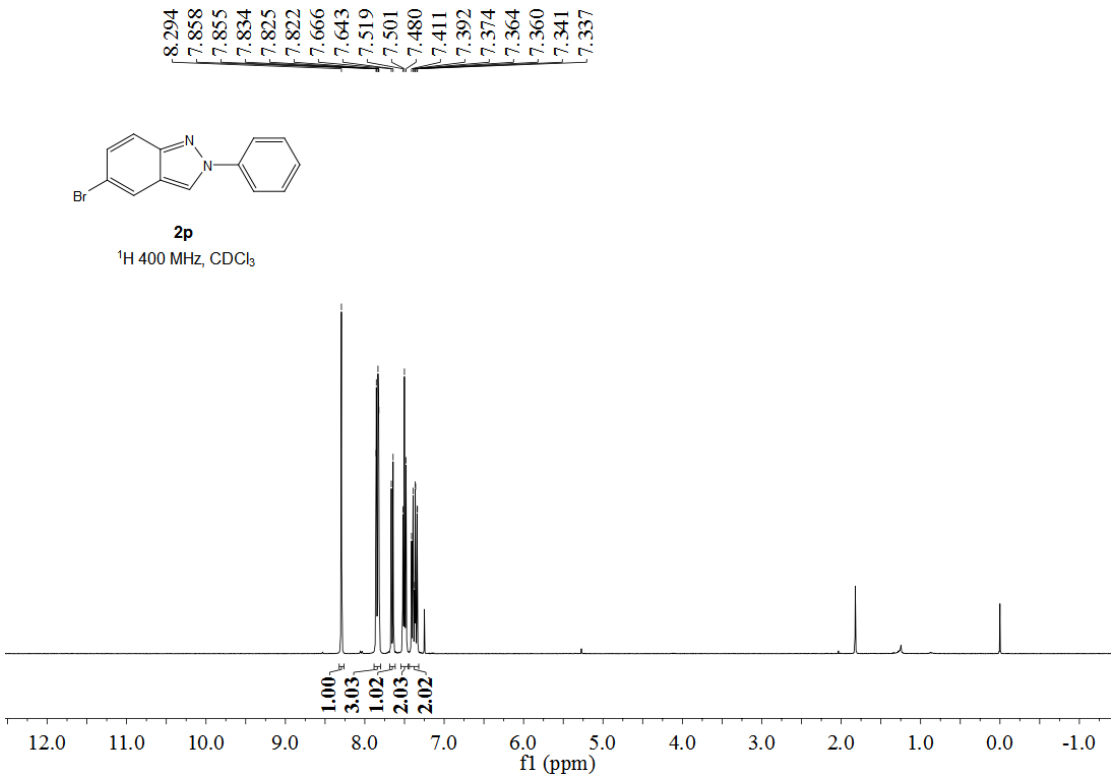
2n

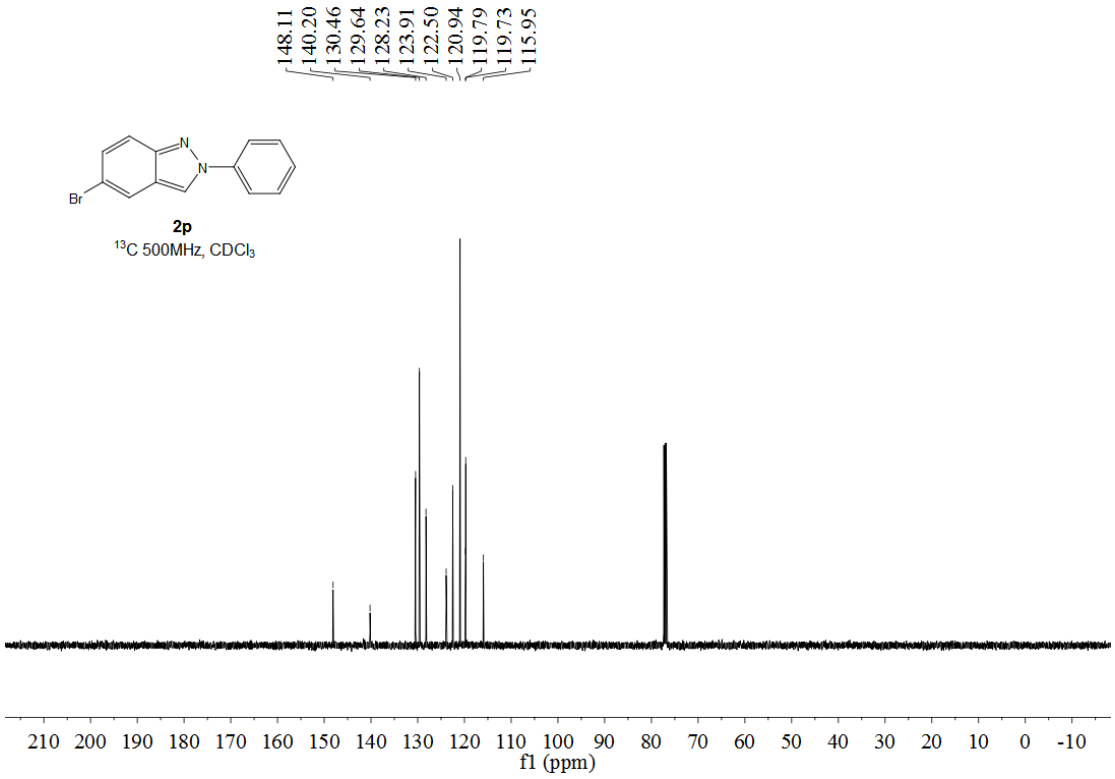
^{13}C 500MHz, $CDCl_3$

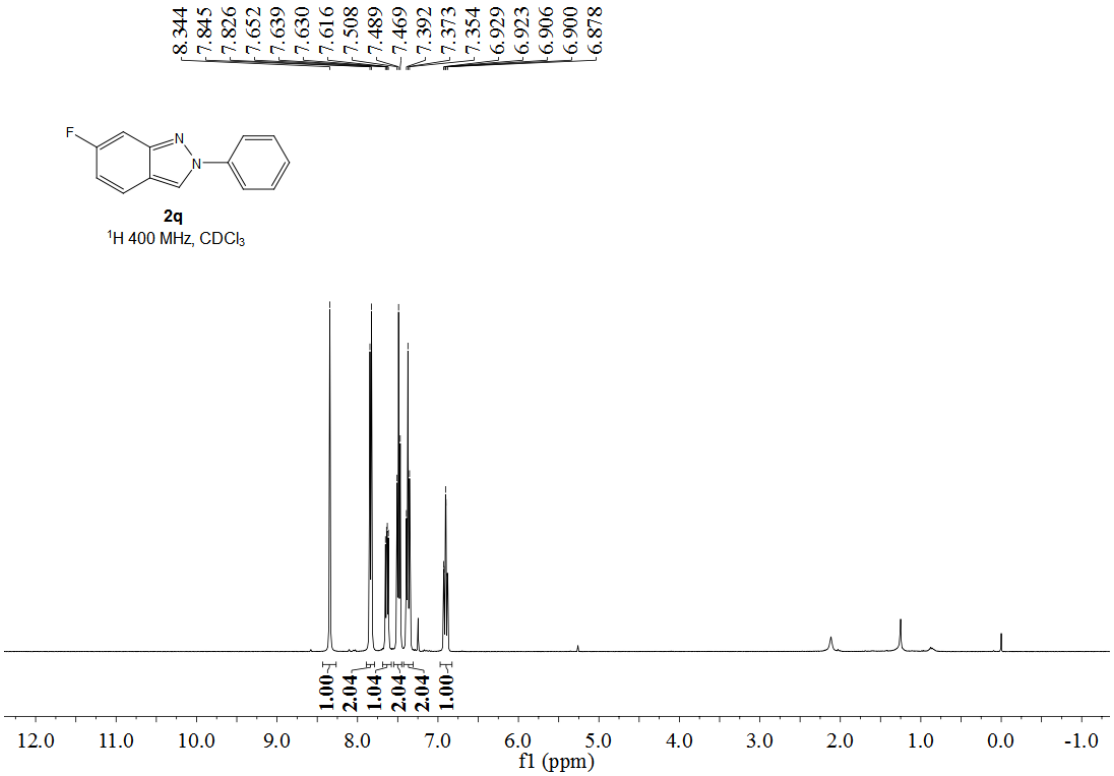


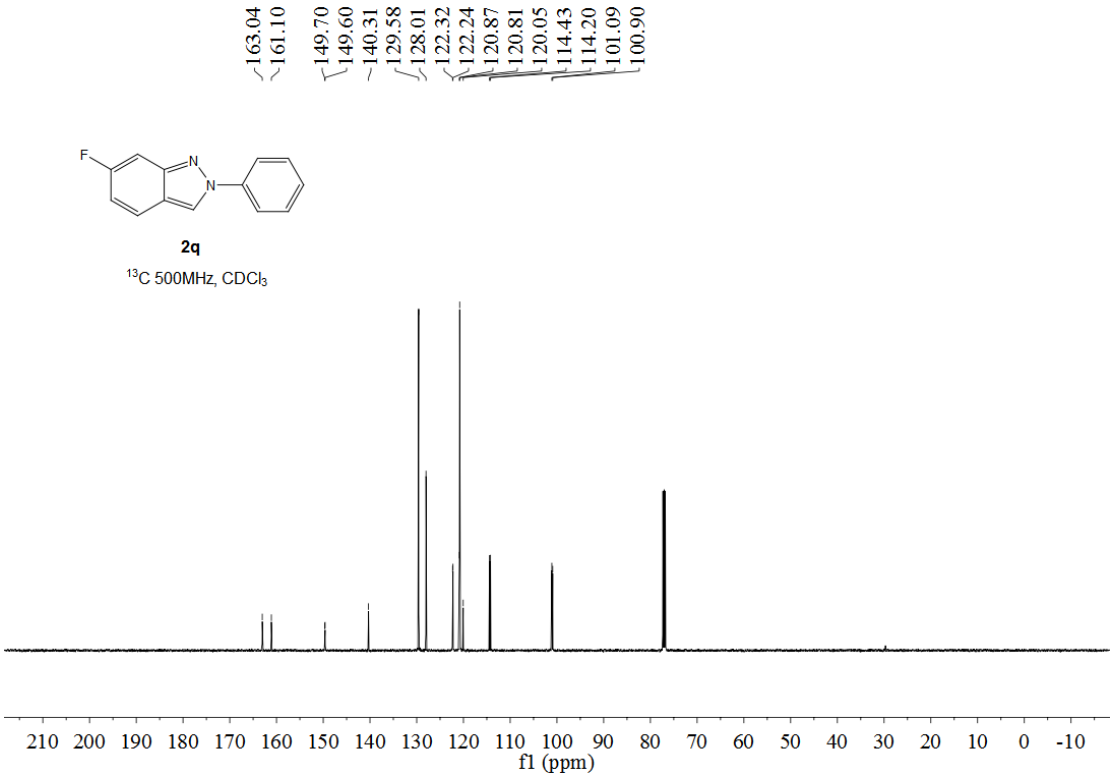

8.341
8.216
7.862
7.841
7.530
7.510
7.491
7.450
7.428
7.422
7.403
7.384
7.340
7.318
I
N
N
2o
1H 400 MHz, CDCl3
1.02
1.00
2.12
2.18
2.11
1.07
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0
f1 (ppm)

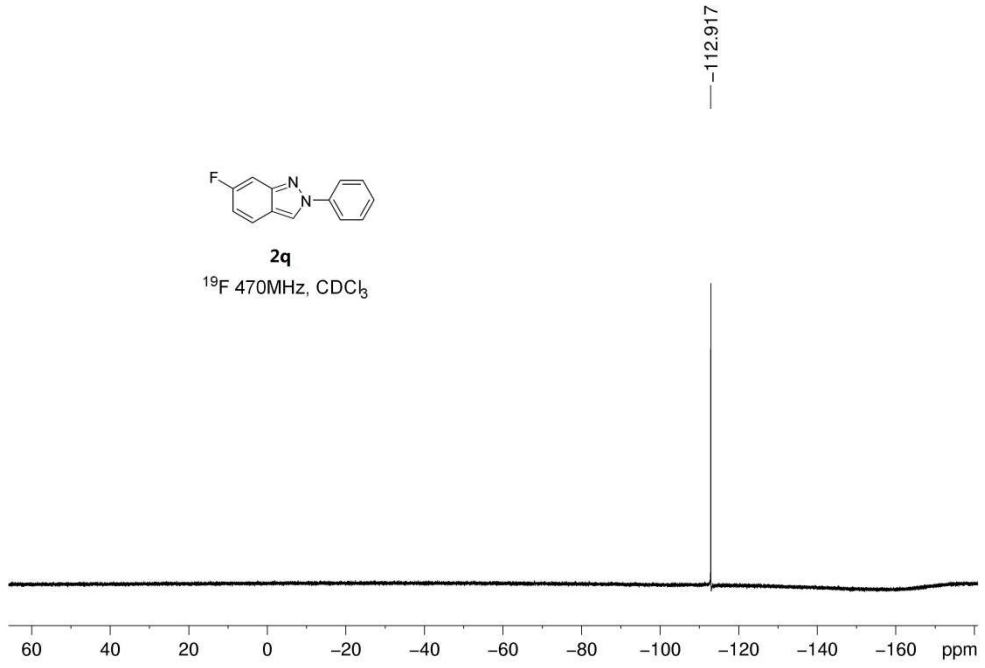

150.92
140.20
131.17
129.63
128.20
127.17
121.78
121.51
121.01
120.87
92.30
I
N
N
2o
13C 500MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.294
7.858
7.855
7.834
7.825
7.822
7.666
7.643
7.519
7.501
7.480
7.411
7.392
7.374
7.364
7.360
7.341
7.337
Br
N
N
2p
1H 400 MHz, CDCl3
1.00
3.03
1.02
2.03
2.02
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)


148.11
140.20
130.46
129.64
128.23
123.91
122.50
120.94
119.79
119.73
115.95
Br
N
N
2p
13C 500MHz, CDCl3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

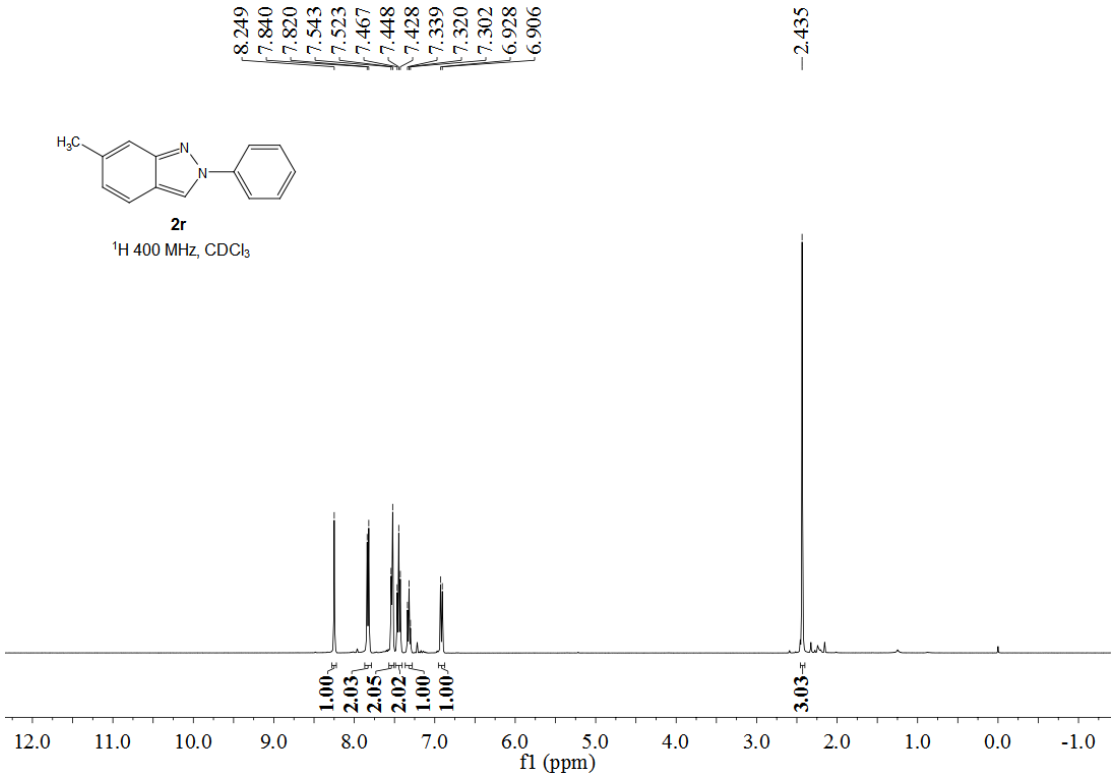

8.344
7.845
7.826
7.652
7.639
7.630
7.616
7.508
7.489
7.469
7.392
7.373
7.354
6.929
6.923
6.906
6.900
6.878
F
N
N
2q
1H 400 MHz, CDCl3
1.00
2.04
1.04
2.04
2.04
1.00
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0
f1 (ppm)


163.04
161.10
149.70
149.60
140.31
129.58
128.01
122.32
122.24
120.87
120.81
120.05
114.43
114.20
101.09
100.90
F
N
N
2q
13C 500MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



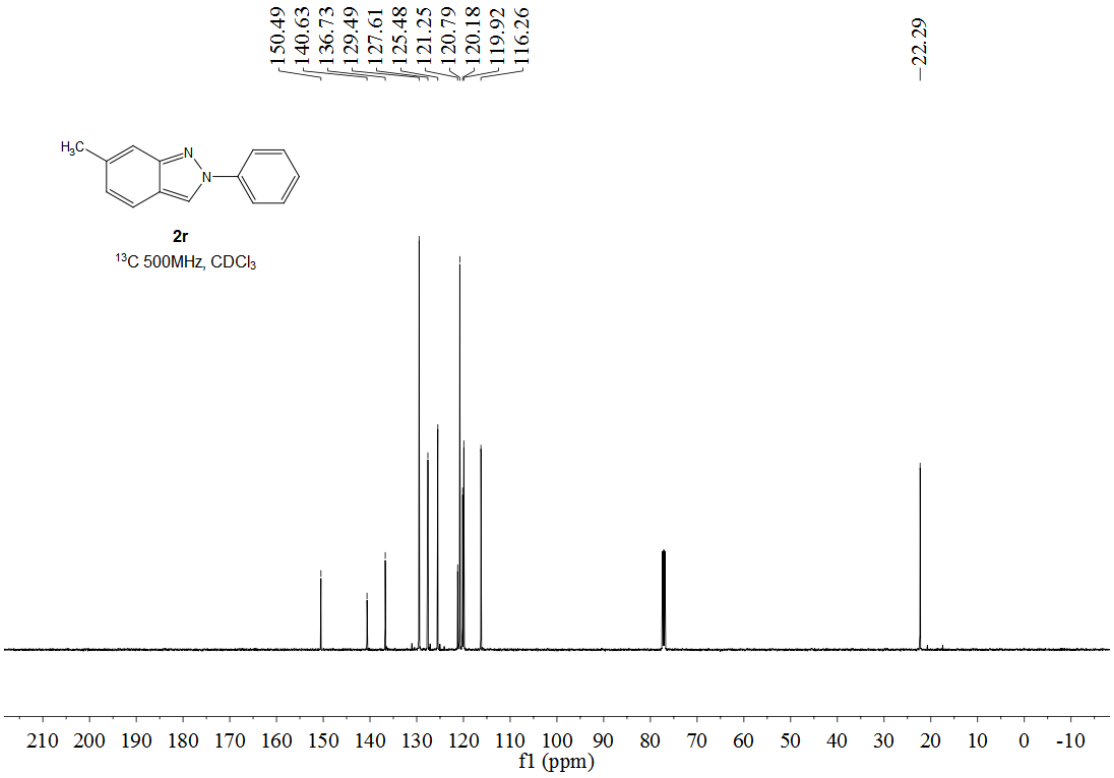
2q

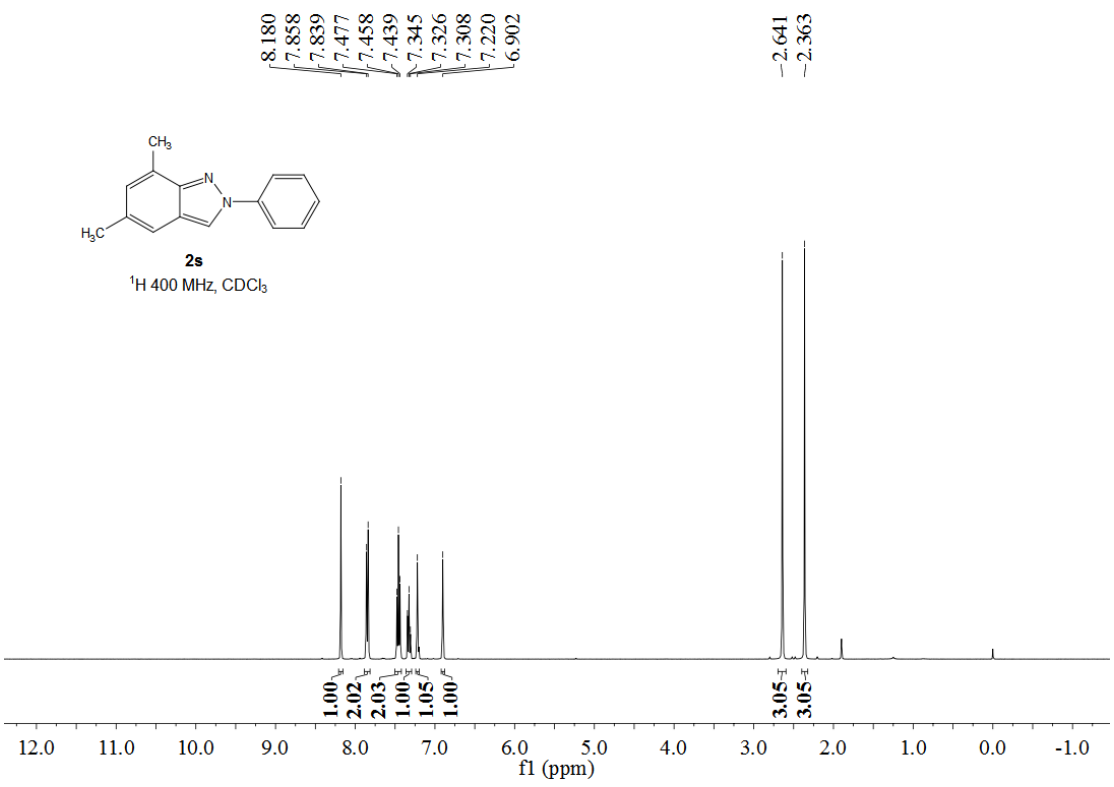
^{19}F 470MHz, $CDCl_3$

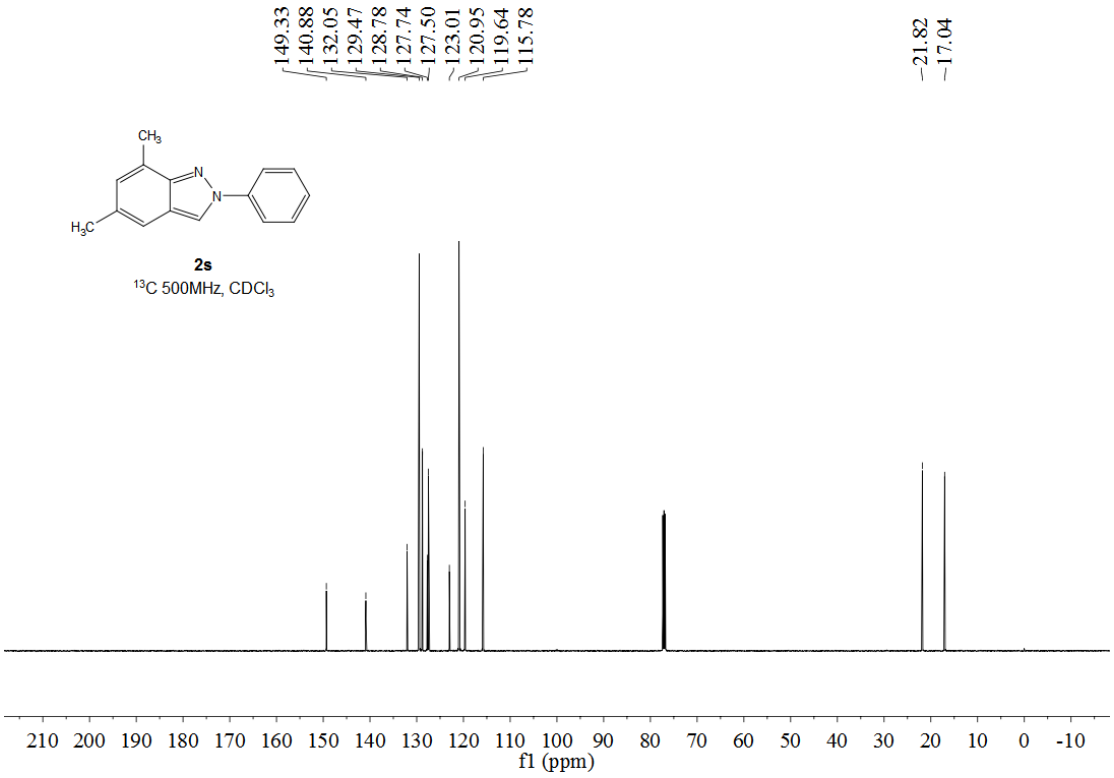


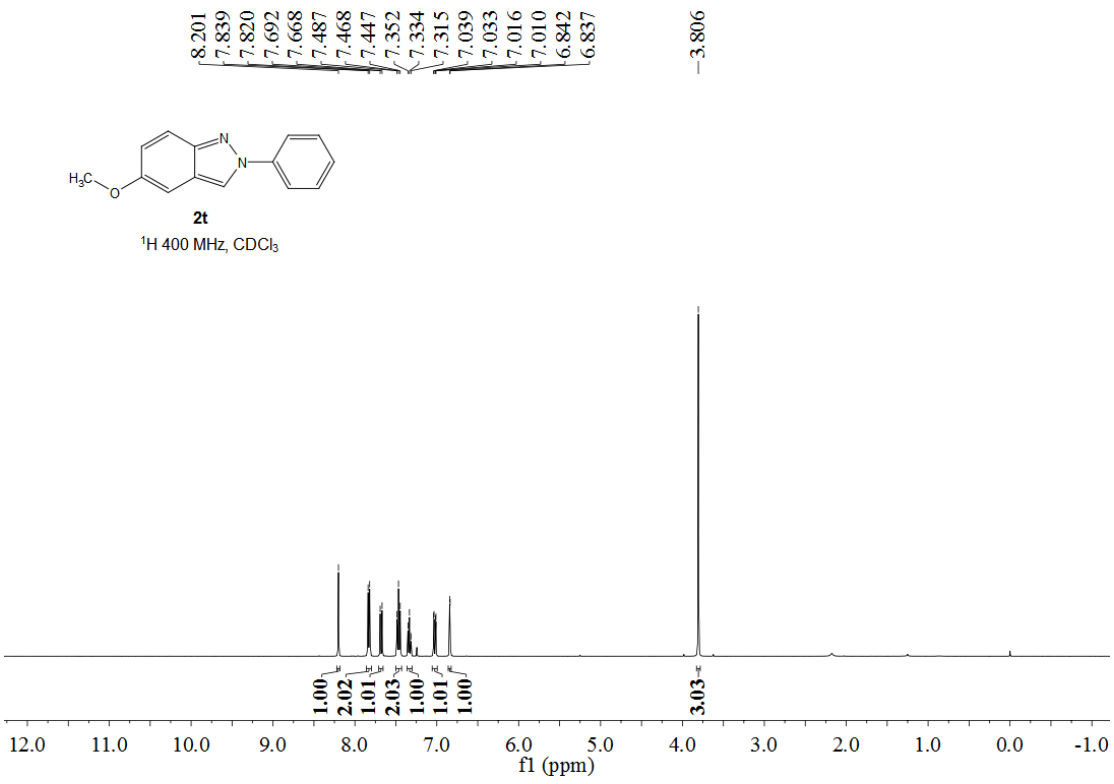
2r

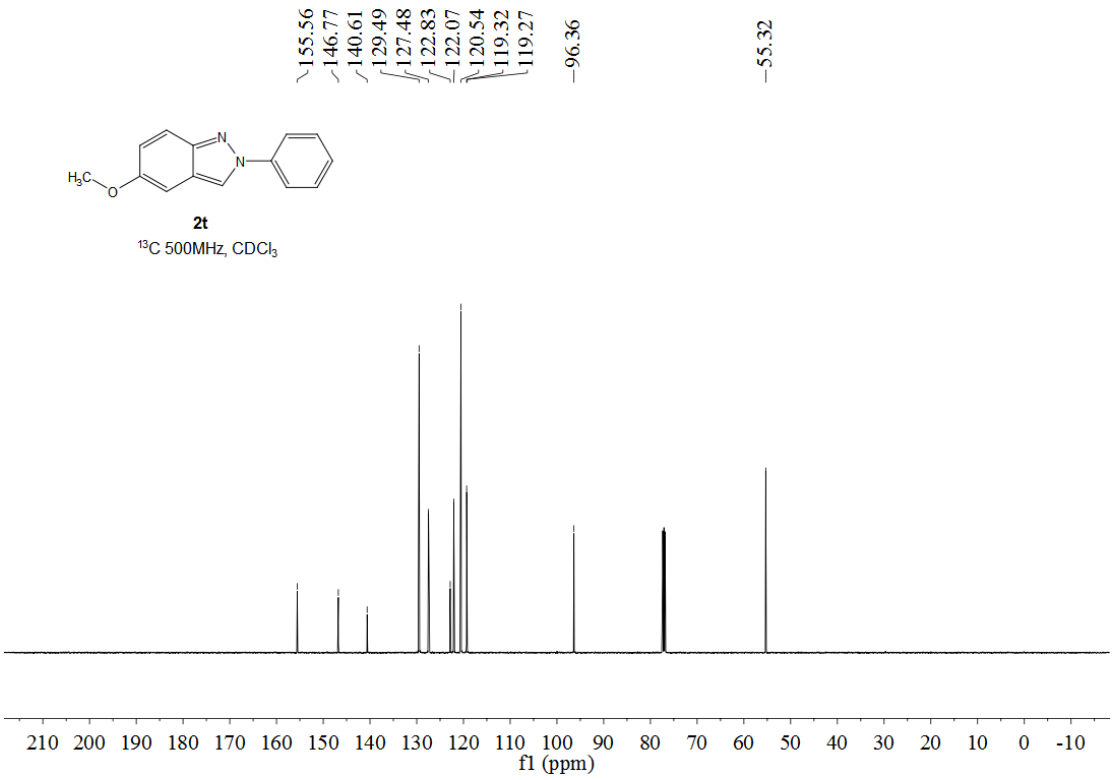
^{1}H 400 MHz, $CDCl_3$

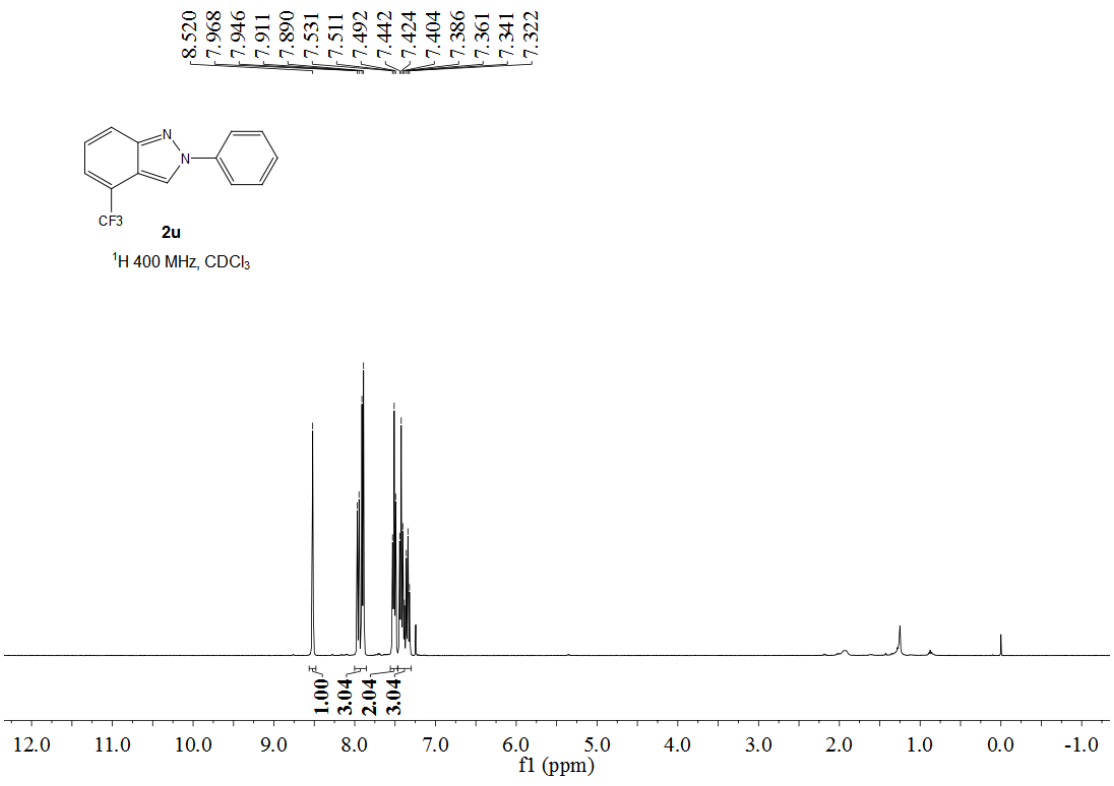

150.49
140.63
136.73
129.49
127.61
125.48
121.25
120.79
120.18
119.92
116.26
22.29
H3C
N
N
2r
13C 500MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

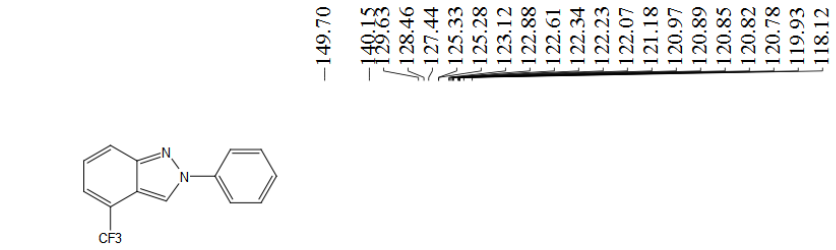

8.180
7.858
7.839
7.477
7.458
7.439
7.345
7.326
7.308
7.220
6.902
2.641
2.363
CH3
N
N
H3C
2s
1H 400 MHz, CDCl3
1.00
2.02
2.03
1.00
1.05
1.00
3.05
3.05
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0
f1 (ppm)


149.33
140.88
132.05
129.47
128.78
127.74
127.50
123.01
120.95
119.64
115.78
21.82
17.04
CH3
H3C
N
N
2s
13C 500MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.201
7.839
7.820
7.692
7.668
7.487
7.468
7.447
7.352
7.334
7.315
7.039
7.033
7.016
7.010
6.842
6.837
3.806
H3C
O
N
N
2t
1H 400 MHz, CDCl3
1.00
2.02
1.01
2.03
1.00
1.01
1.00
3.03
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0
f1 (ppm)

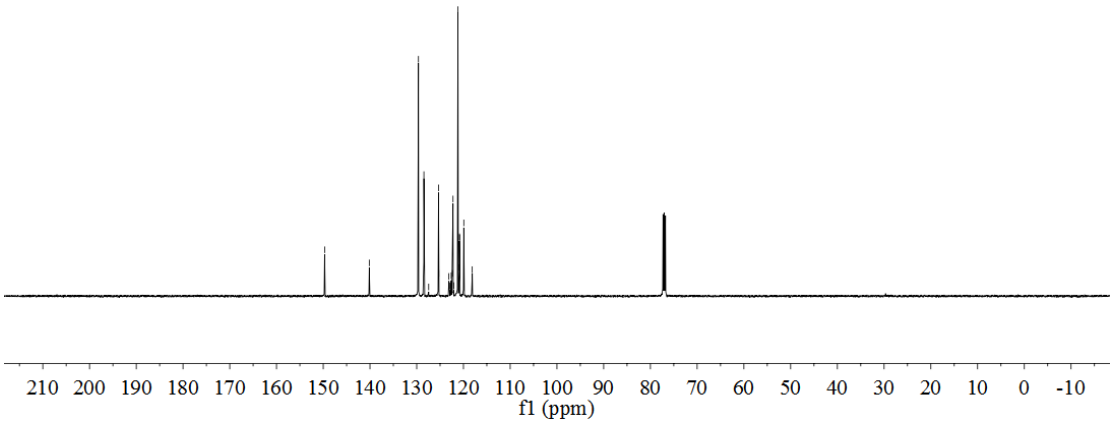

155.56
146.77
140.61
129.49
127.48
122.83
122.07
120.54
119.32
119.27
96.36
55.32
H3C
O
N
N
2t
13C 500MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

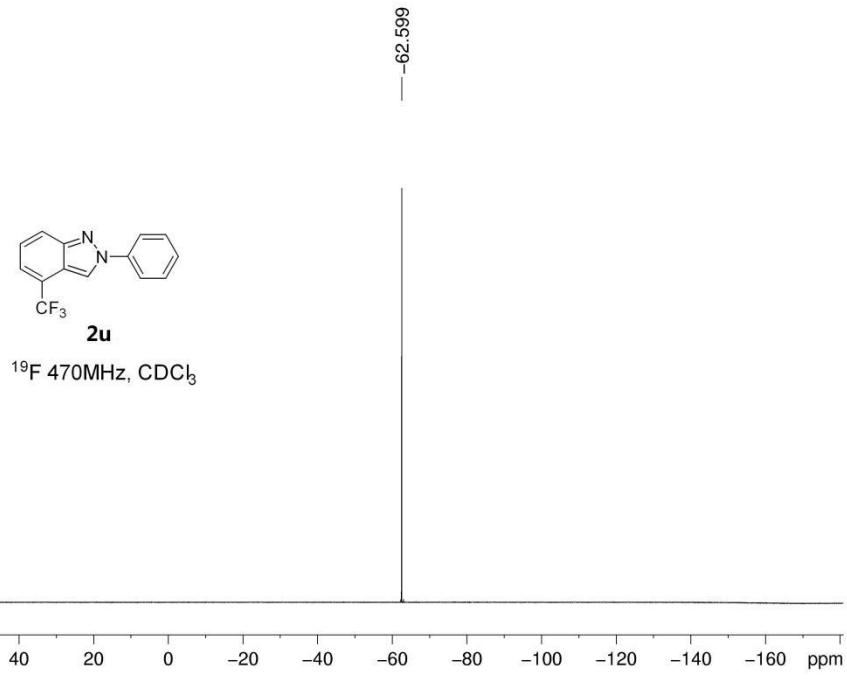

8.520
7.968
7.946
7.911
7.890
7.531
7.511
7.492
7.442
7.424
7.404
7.386
7.361
7.341
7.322
N
N
CF3
2u
1H 400 MHz, CDCl3
1.00
3.04
2.04
3.04
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0
f1 (ppm)



2u

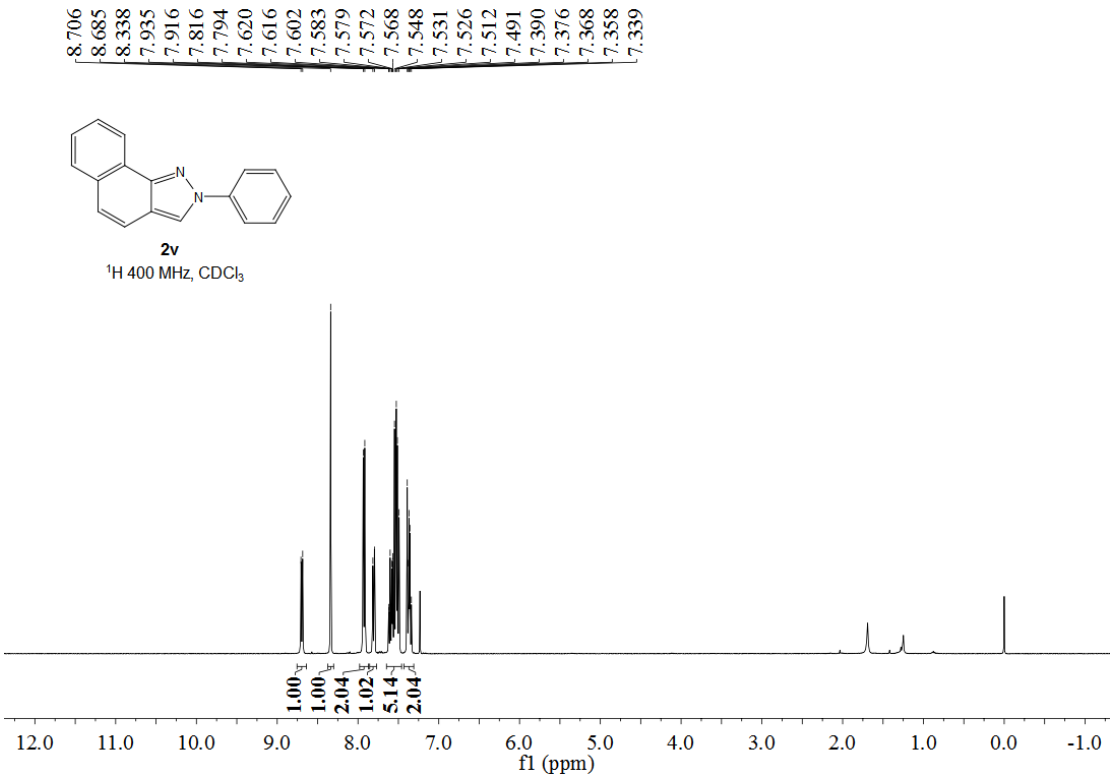
^{13}C 500MHz, $CDCl_3$

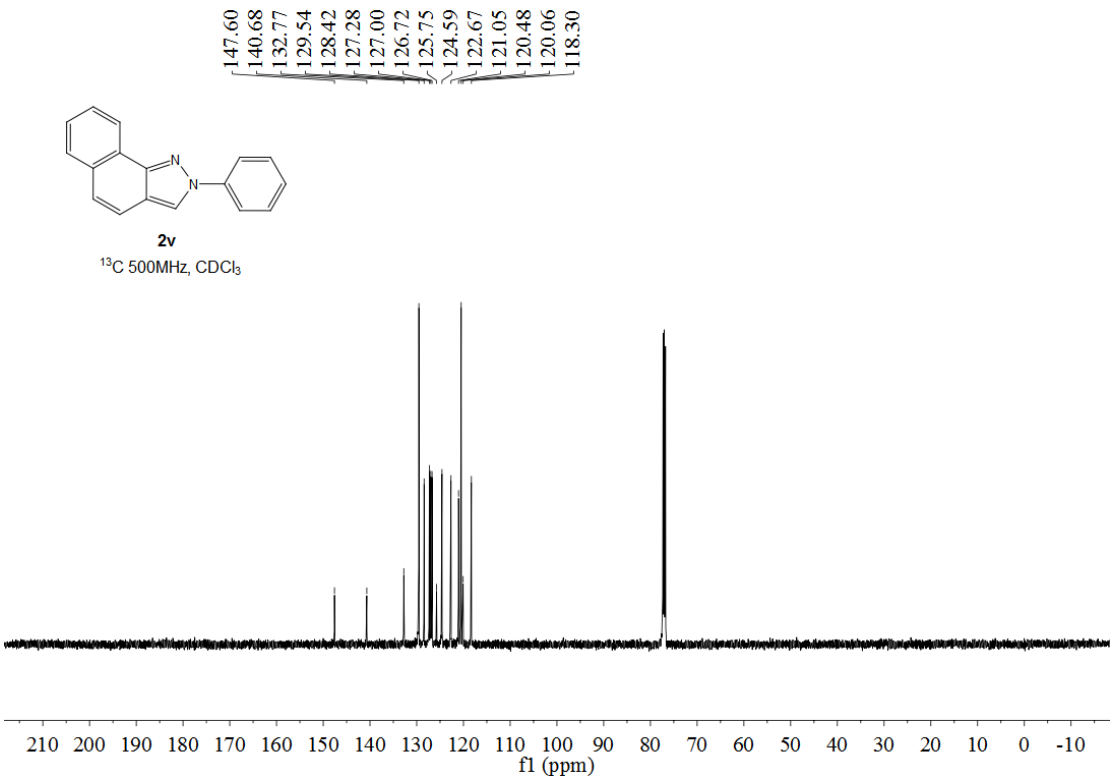


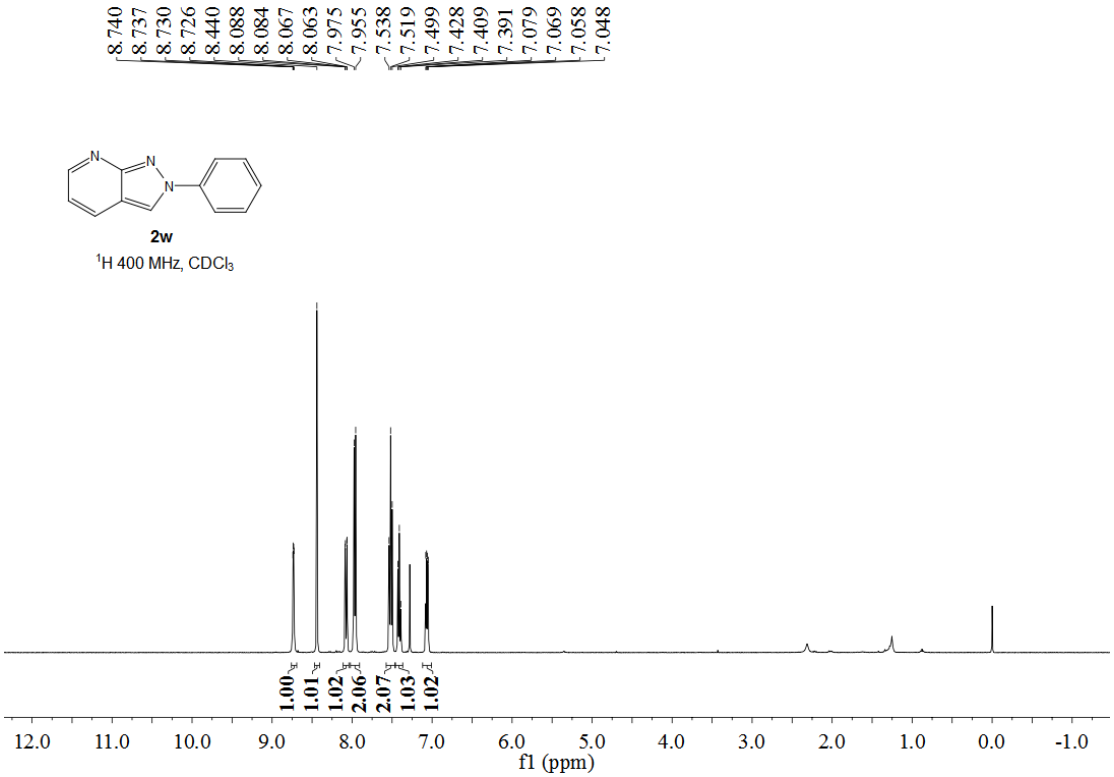


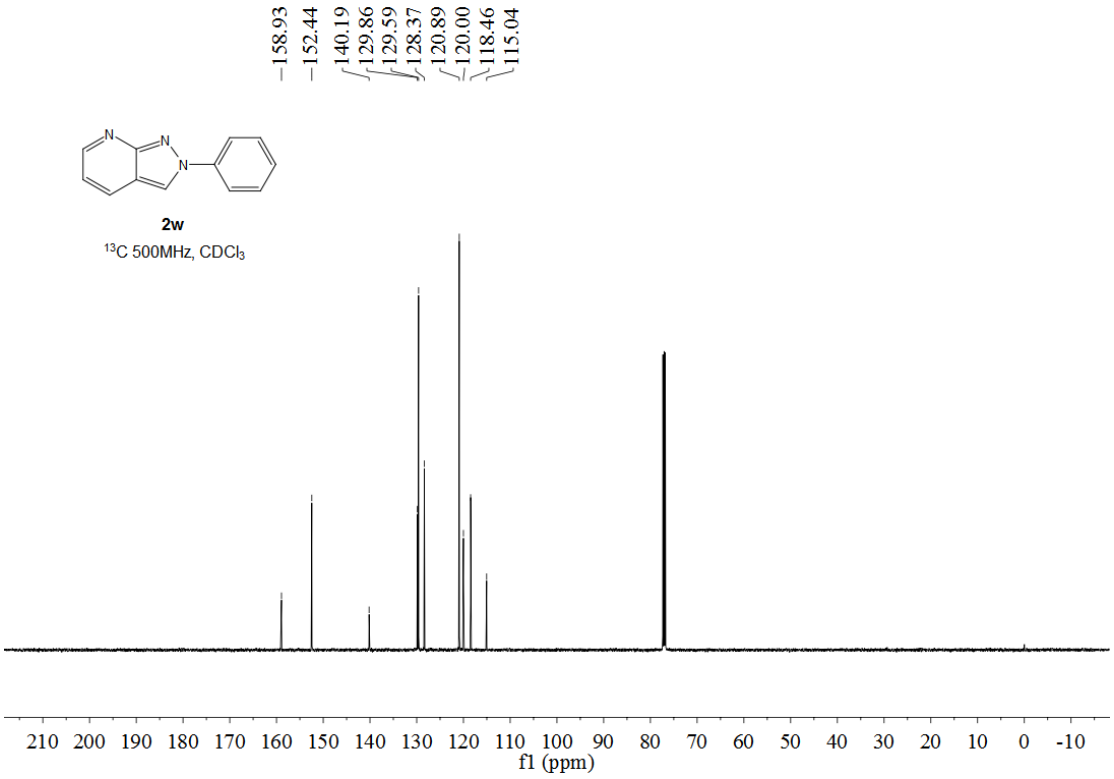
2u

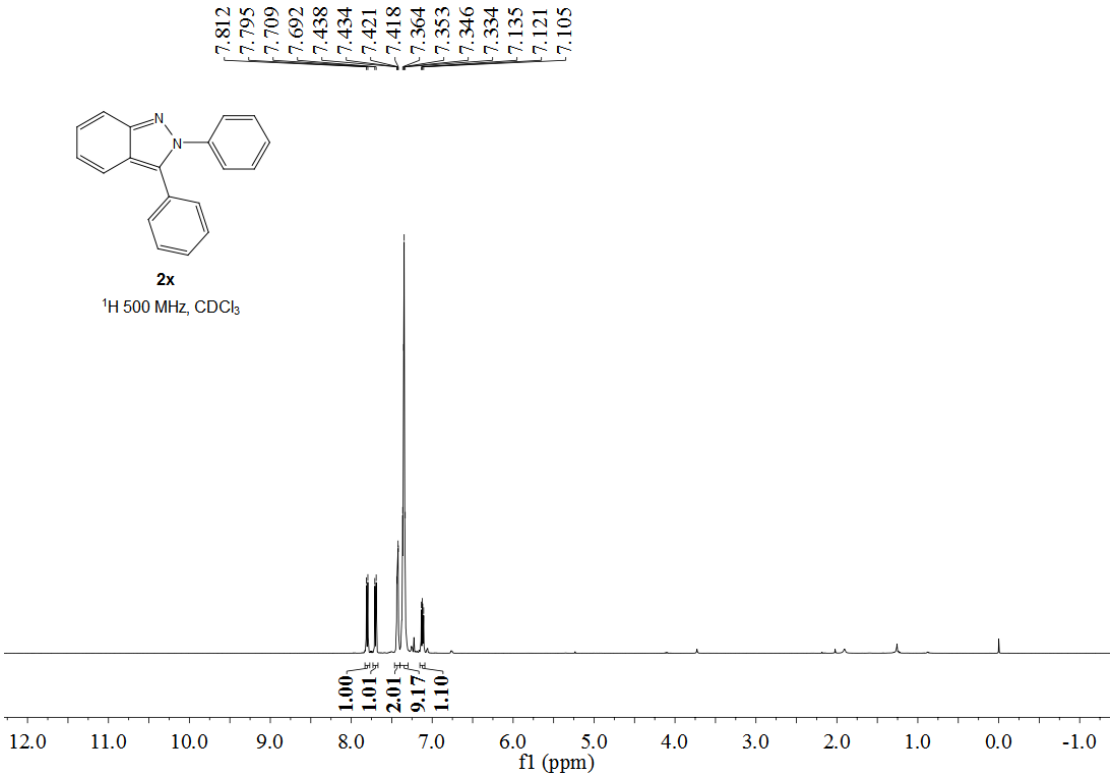
^{19}F 470MHz, $CDCl_3$

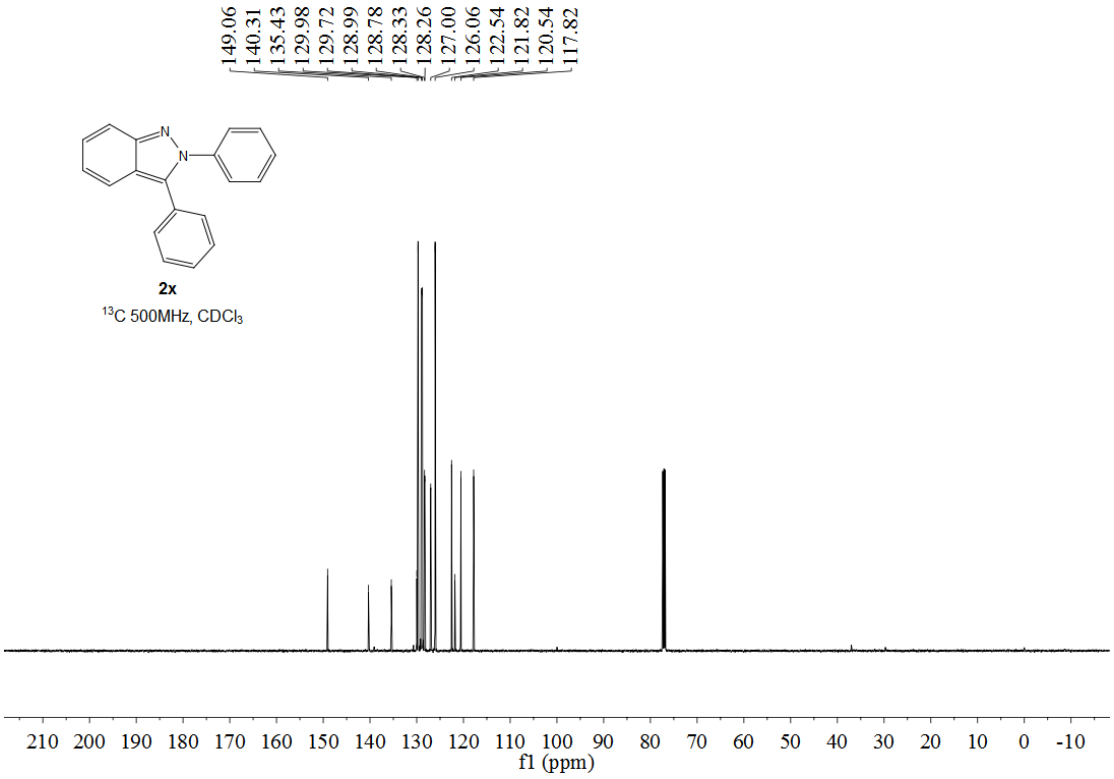

8.706
8.685
8.338
7.935
7.916
7.816
7.794
7.620
7.616
7.602
7.583
7.579
7.572
7.568
7.548
7.531
7.526
7.512
7.491
7.390
7.376
7.368
7.358
7.339
N
N
2v
1H 400 MHz, CDCl3
1.00
1.00
2.04
1.02
5.14
2.04
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)

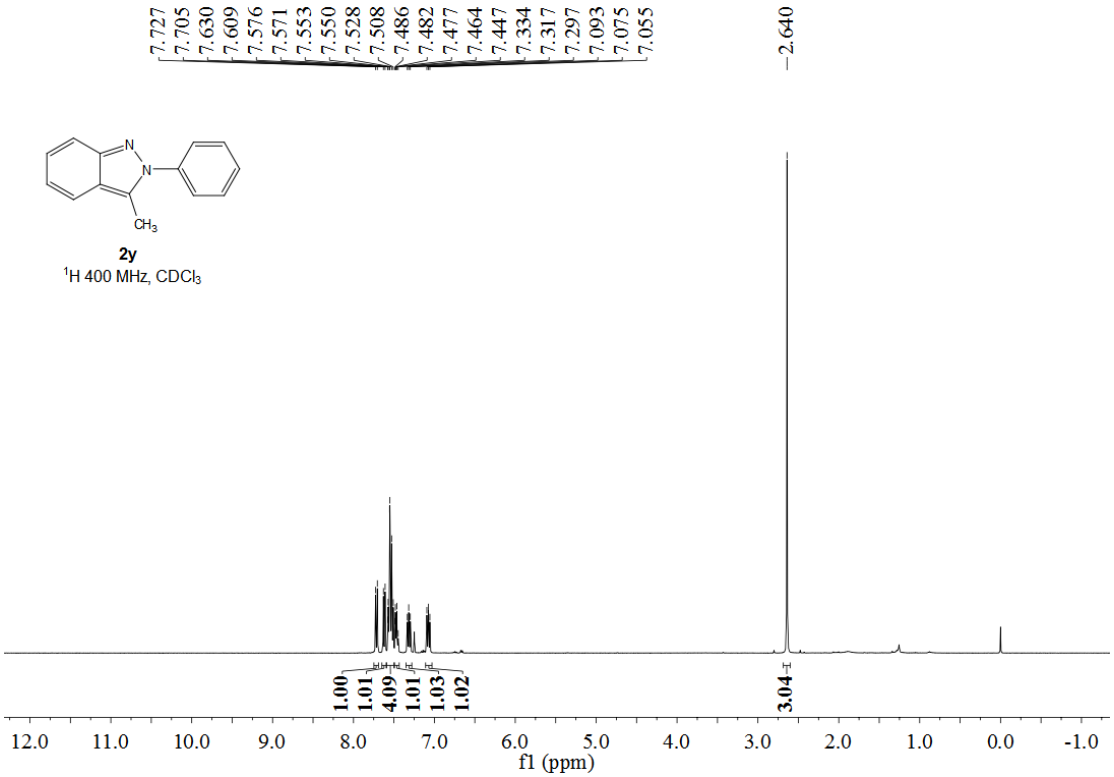

147.60
140.68
132.77
129.54
128.42
127.28
127.00
126.72
125.75
124.59
122.67
121.05
120.48
120.06
118.30
N
N
2v
13C 500MHz, CDCl3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

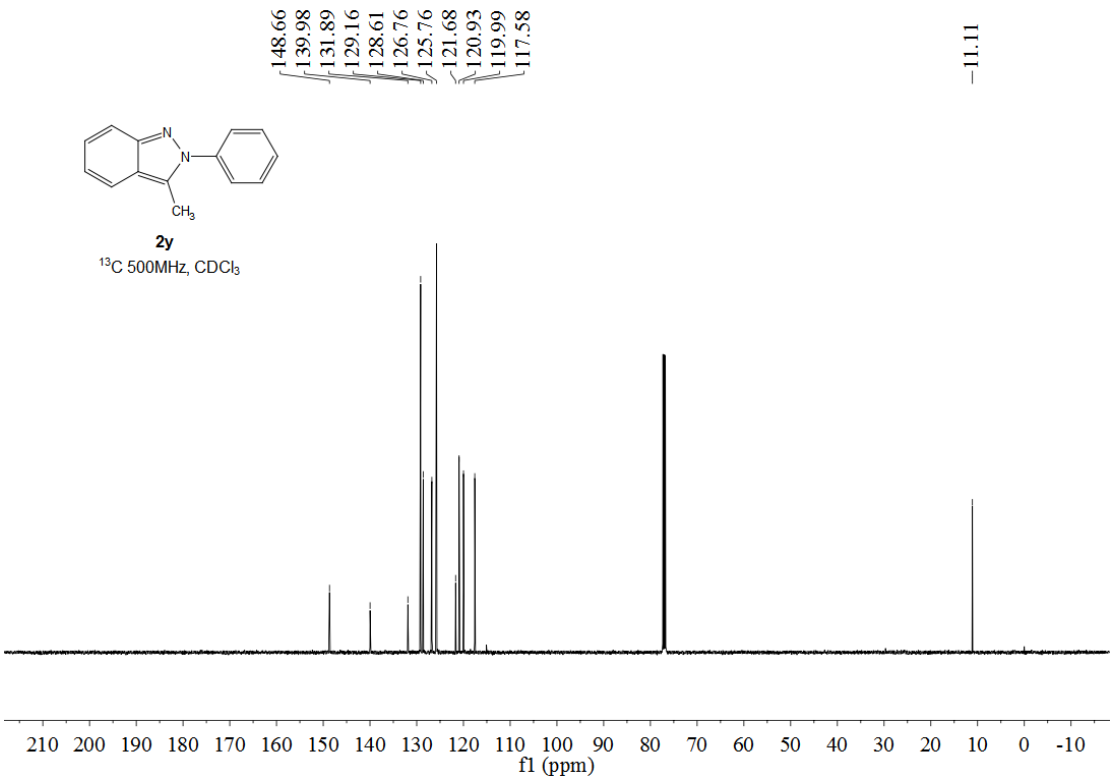

8.740
8.737
8.730
8.726
8.440
8.088
8.084
8.067
8.063
7.975
7.955
7.538
7.519
7.499
7.428
7.409
7.391
7.079
7.069
7.058
7.048
2w
1H 400 MHz, CDCl3
1.00
1.01
1.02
2.06
2.07
1.03
1.02
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0
f1 (ppm)

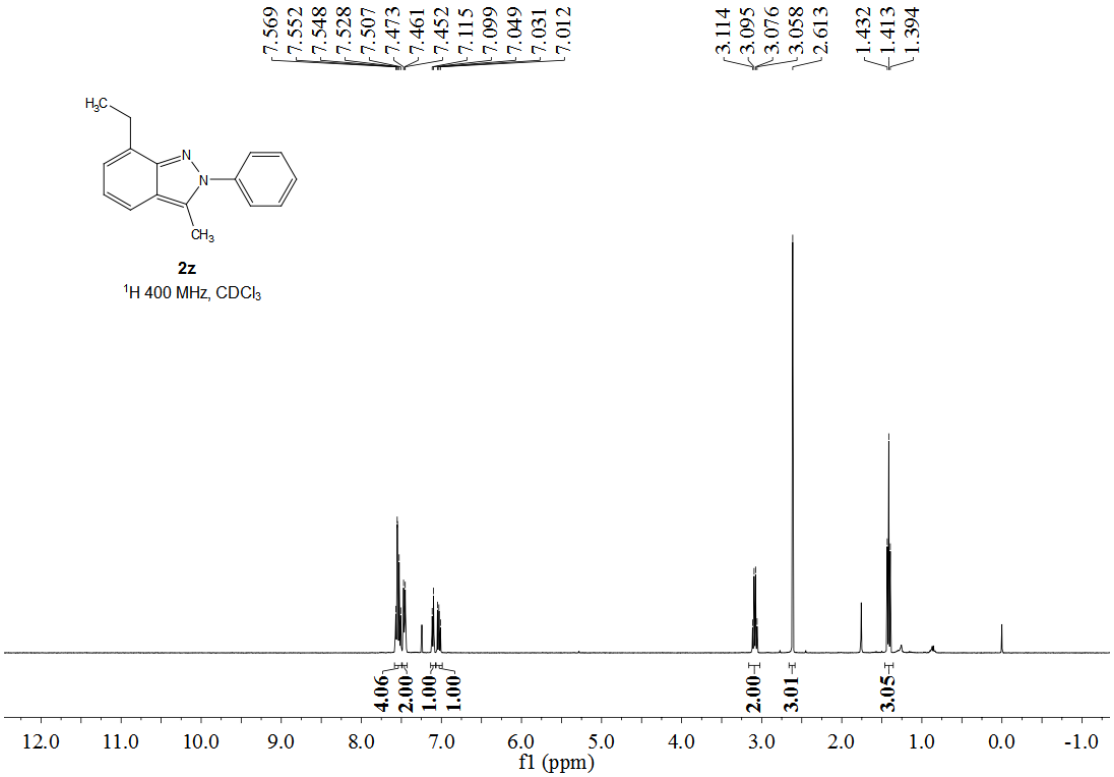

158.93
152.44
140.19
129.86
129.59
128.37
120.89
120.00
118.46
115.04
2w
13C 500MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.812
7.795
7.709
7.692
7.438
7.434
7.421
7.418
7.364
7.353
7.346
7.334
7.135
7.121
7.105
2x
1H 500 MHz, CDCl3
1.00
1.01
2.01
9.17
1.10
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0
f1 (ppm)


149.06
140.31
135.43
129.98
129.72
128.99
128.78
128.33
128.26
127.00
126.06
122.54
121.82
120.54
117.82
2x
13C 500MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

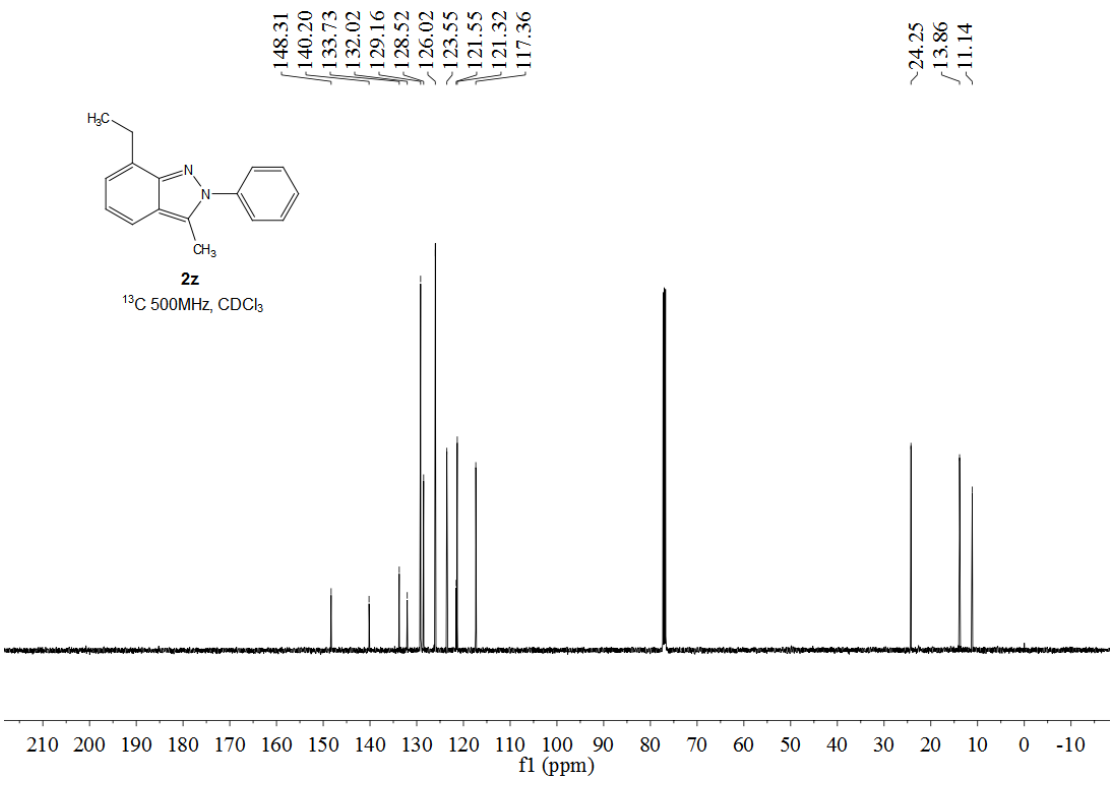

7.727
7.705
7.630
7.609
7.576
7.571
7.553
7.550
7.528
7.508
7.486
7.482
7.477
7.464
7.447
7.334
7.317
7.297
7.093
7.075
7.055
2.640
N
N
CH3
2y
1H 400 MHz, CDCl3
1.00
1.01
4.09
1.01
1.03
1.02
3.04
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)


148.66
139.98
131.89
129.16
128.61
126.76
125.76
121.68
120.93
119.99
117.58
11.11
N
N
CH3
2y
13C 500MHz, CDCl3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



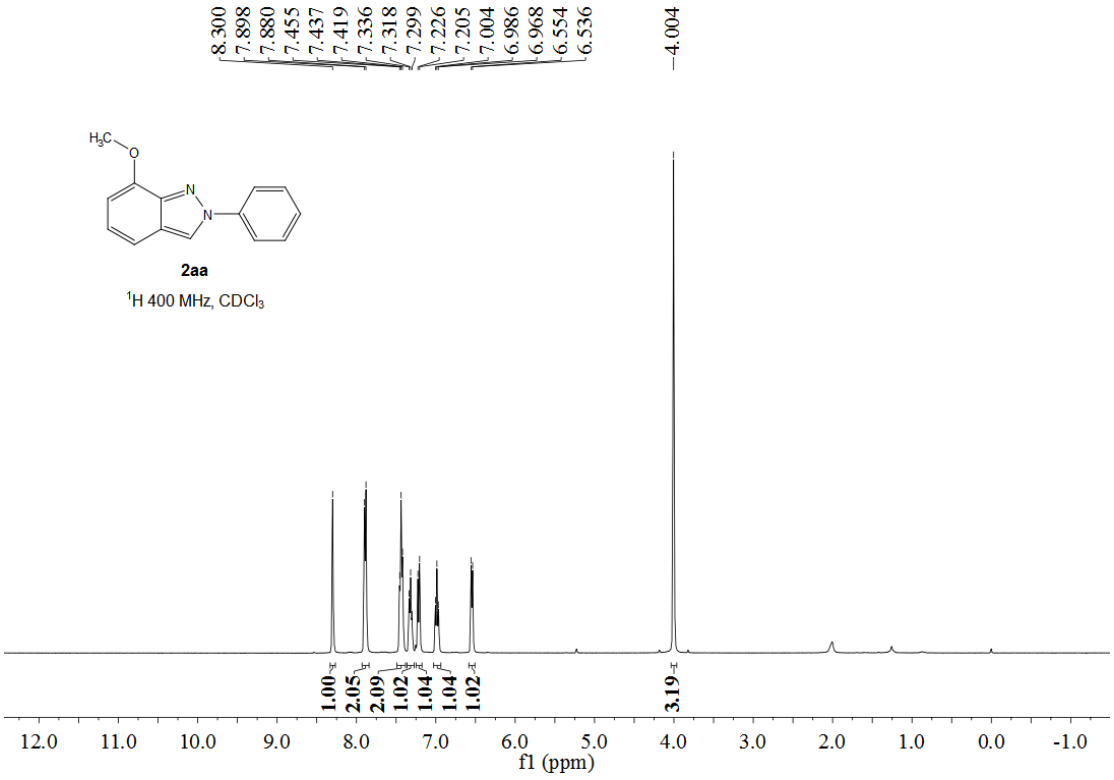
2z

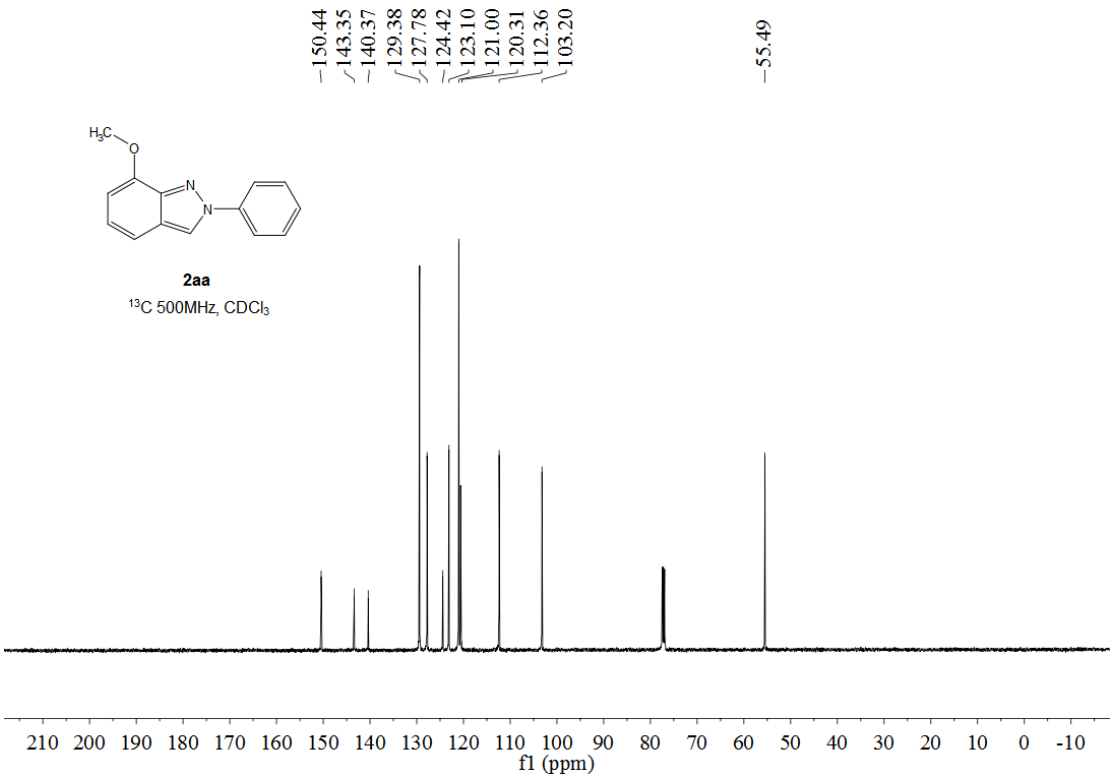
^{1}H 400 MHz, $CDCl_3$

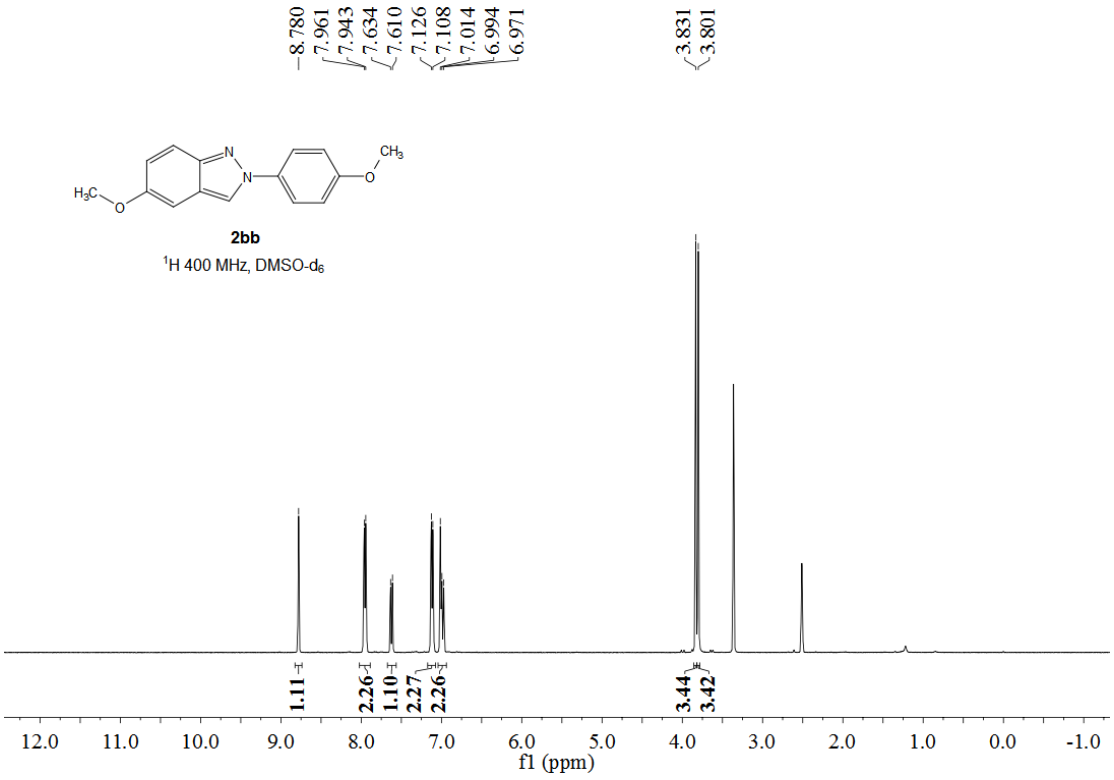


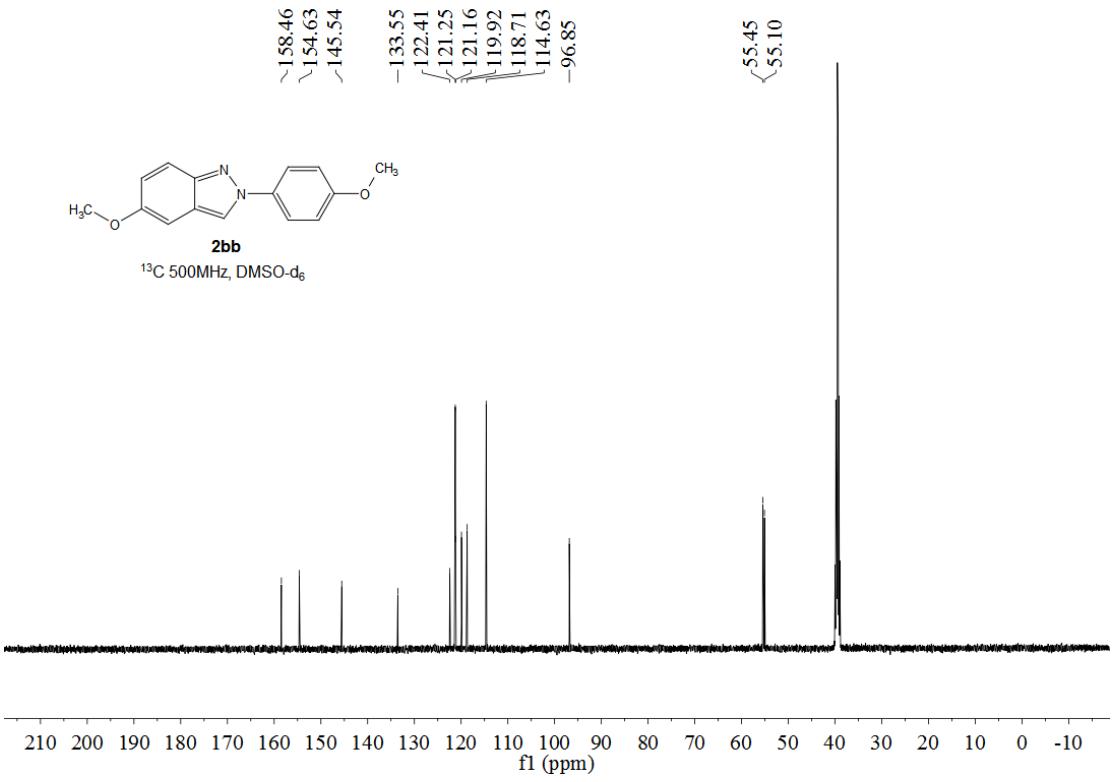
2z

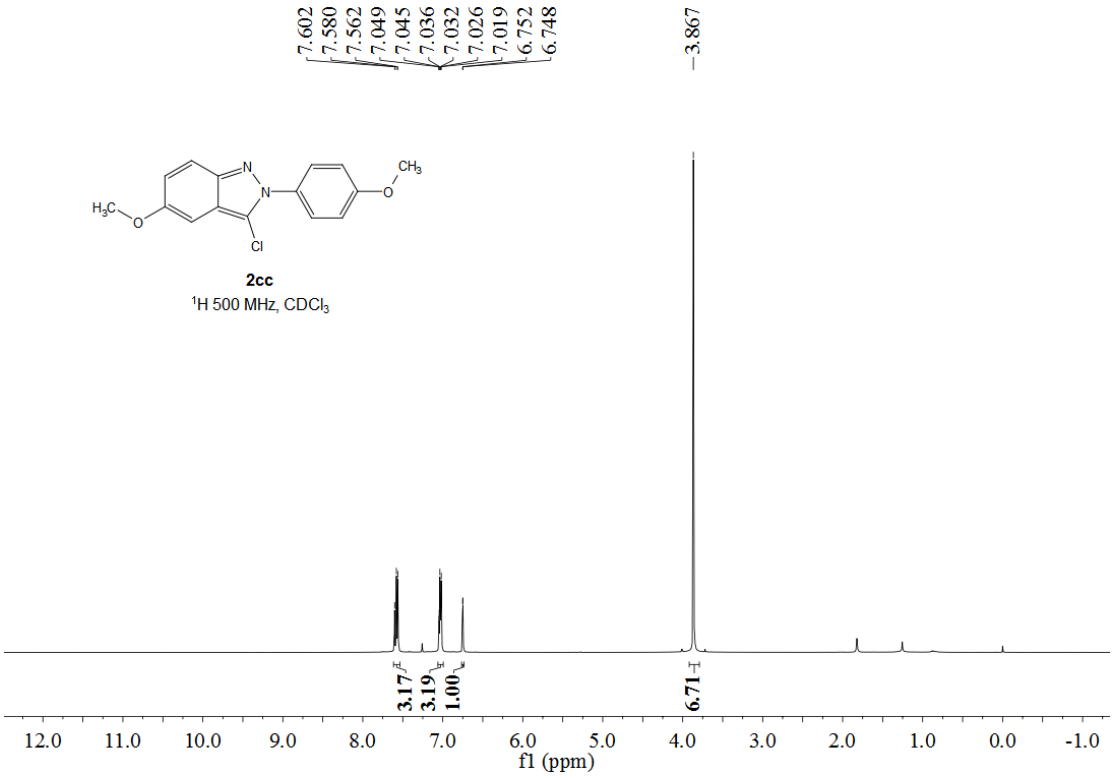
^{13}C 500MHz, $CDCl_3$


8.300
7.898
7.880
7.455
7.437
7.419
7.336
7.318
7.299
7.226
7.205
7.004
6.986
6.968
6.554
6.536
4.004
H3C
O
N
N
2aa
1H 400 MHz, CDCl3
1.00
2.05
2.09
1.02
1.04
1.04
1.02
3.19
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)


150.44
143.35
140.37
129.38
127.78
124.42
123.10
121.00
120.31
112.36
103.20
55.49
H3C
O
N
N
2aa
13C 500MHz, CDCl3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

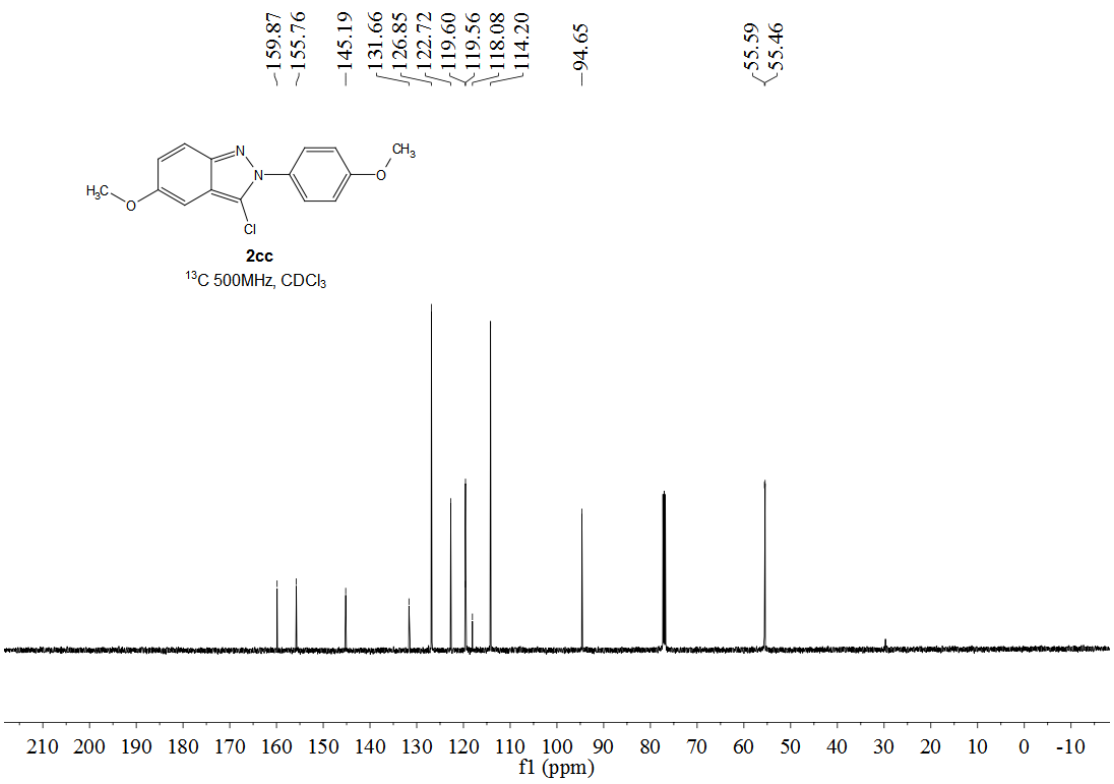

8.780
7.961
7.943
7.634
7.610
7.126
7.108
7.014
6.994
6.971
3.831
3.801
2bb
1H 400 MHz, DMSO-d6
1.11
2.26
1.10
2.27
2.26
3.44
3.42
f1 (ppm)


158.46
154.63
145.54
133.55
122.41
121.25
121.16
119.92
118.71
114.63
96.85
55.45
55.10
2bb
13C 500MHz, DMSO-d6
f1 (ppm)



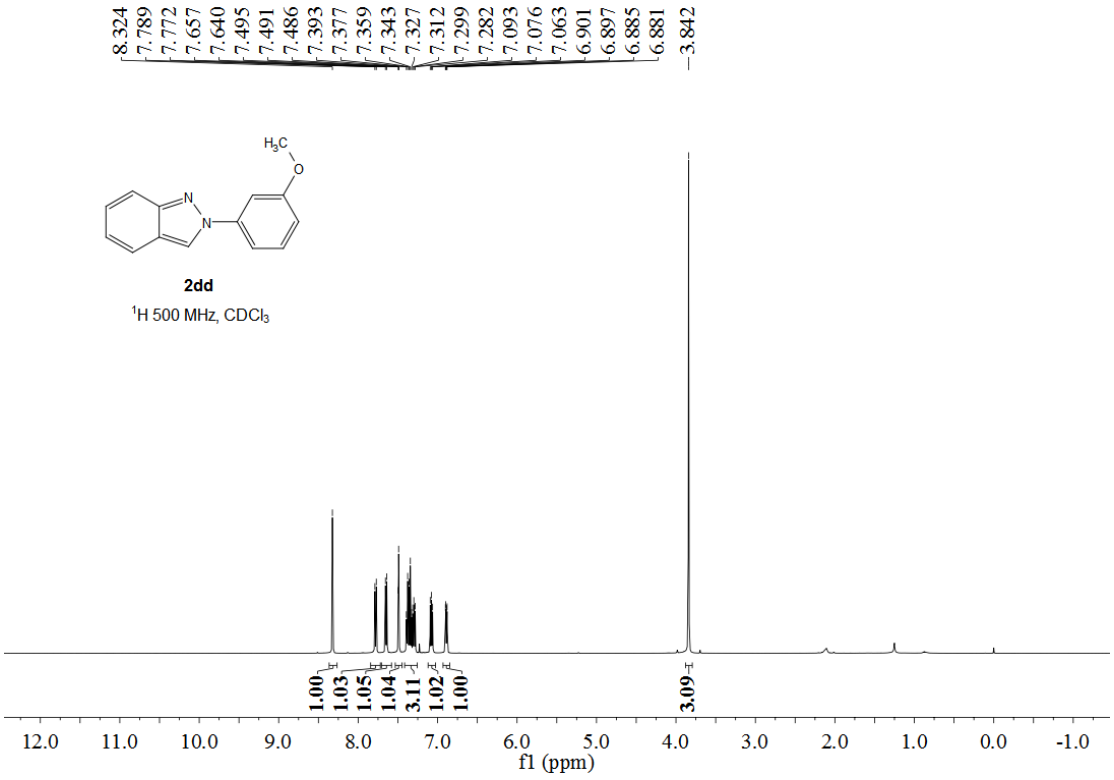
2cc

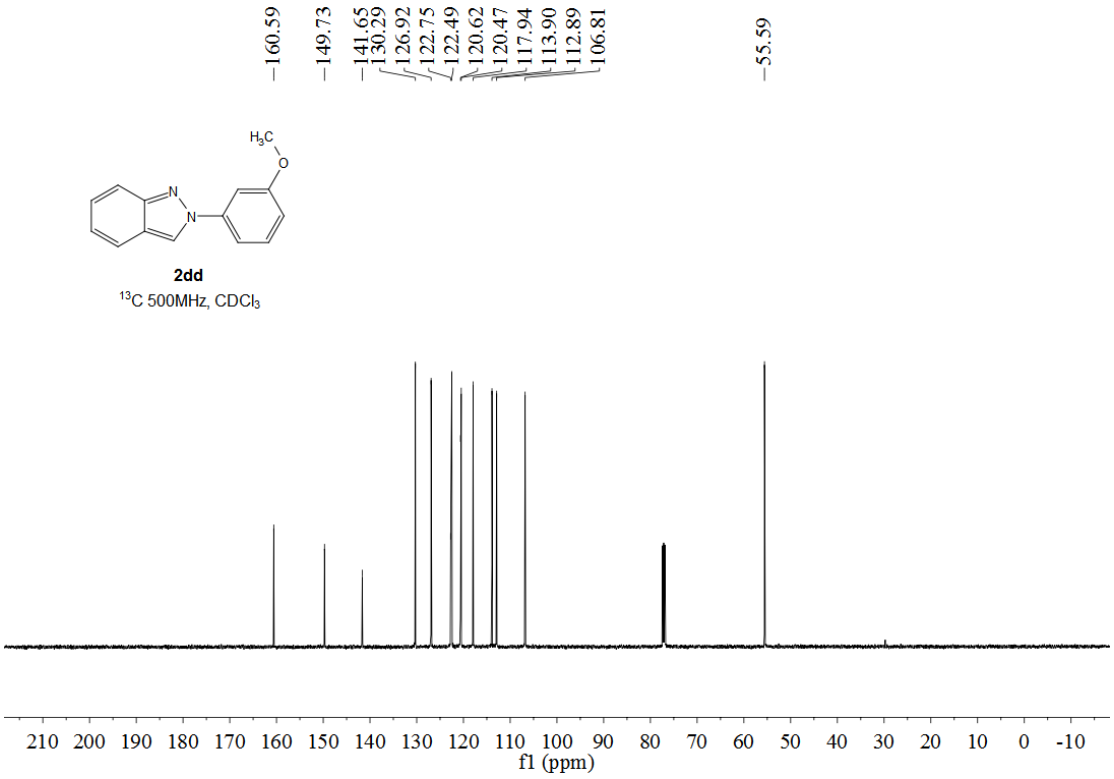
^{1}H 500 MHz, $CDCl_3$

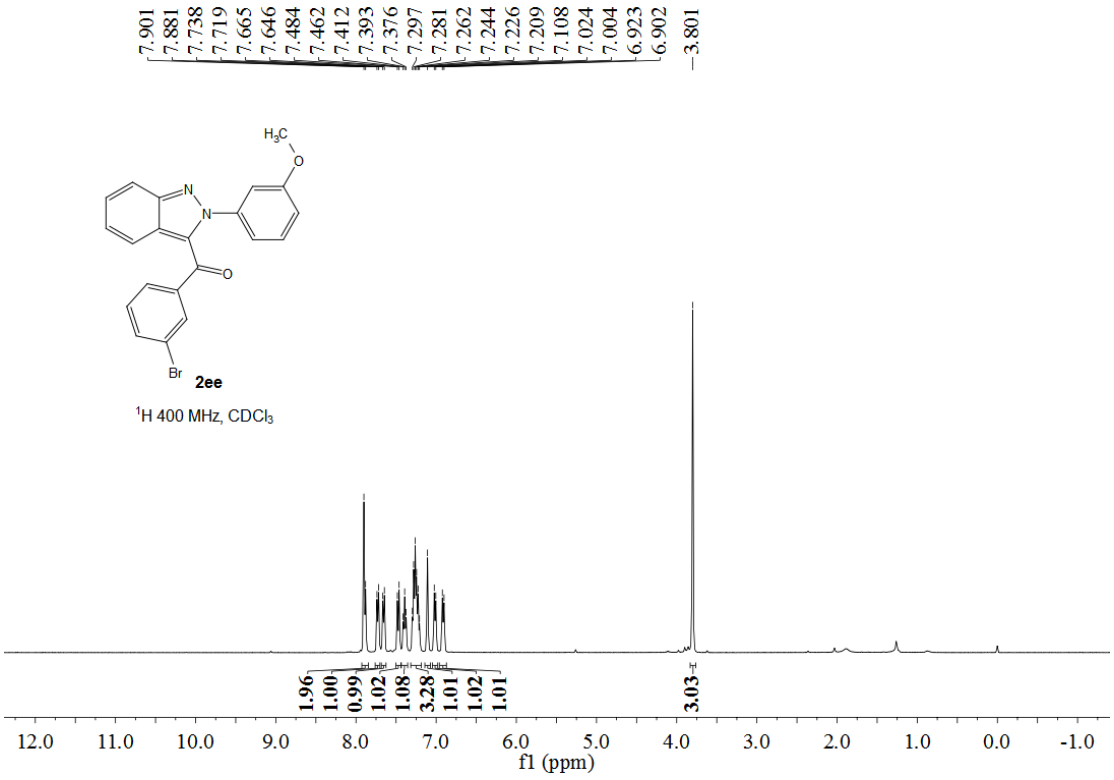


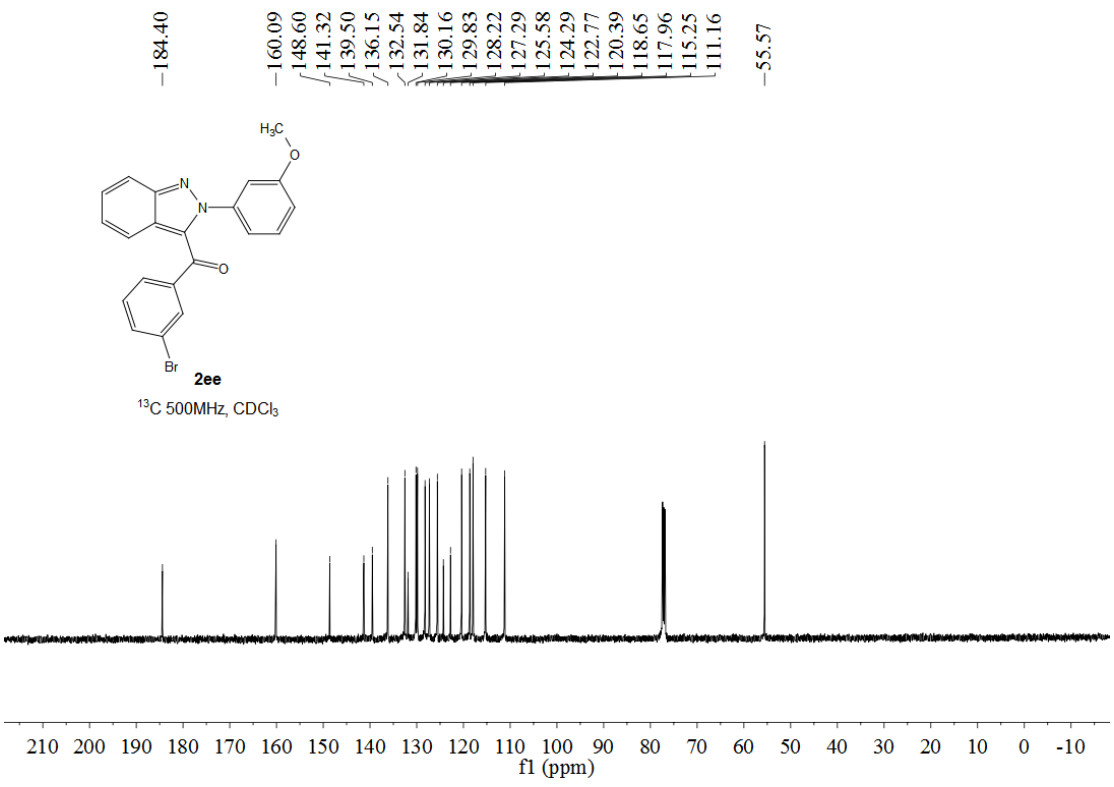
2cc

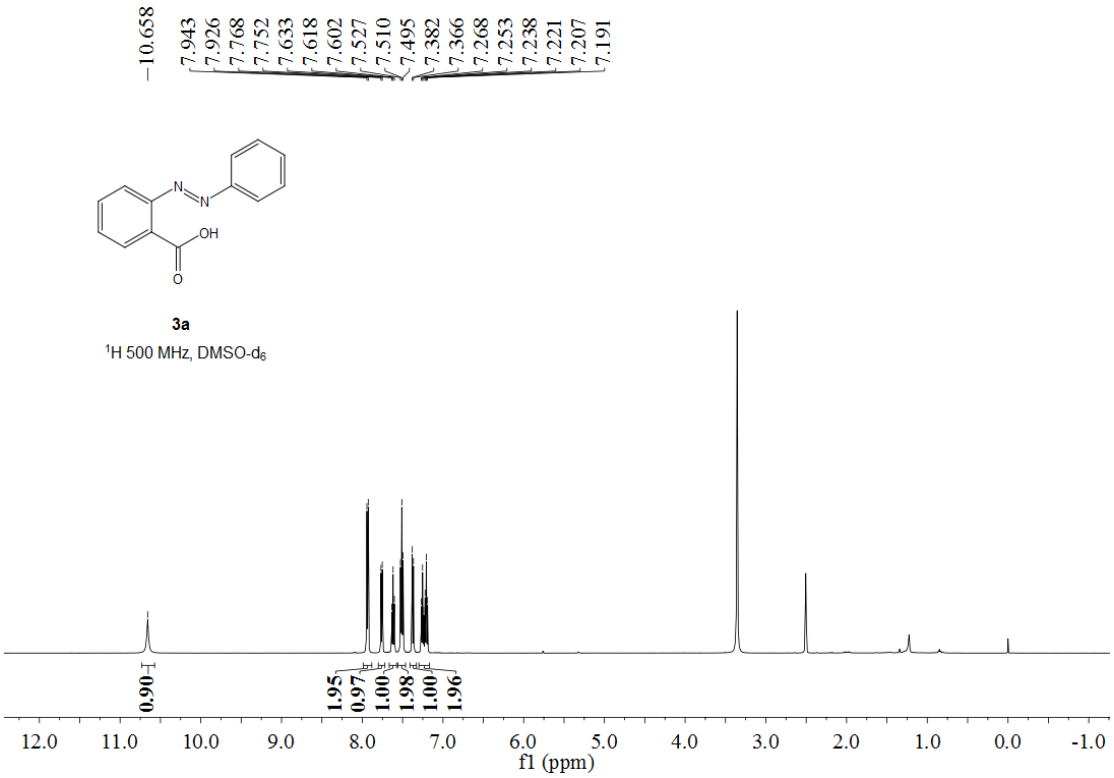
^{13}C 500MHz, $CDCl_3$


8.324
7.789
7.772
7.657
7.640
7.495
7.491
7.486
7.393
7.377
7.359
7.343
7.327
7.312
7.299
7.282
7.093
7.076
7.063
6.901
6.897
6.885
6.881
3.842
H3C
O
N
N
2dd
1H 500 MHz, CDCl3
1.00
1.03
1.05
1.04
3.11
1.02
1.00
3.09
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)


160.59
149.73
141.65
130.29
126.92
122.75
122.49
120.62
120.47
117.94
113.90
112.89
106.81
55.59
H3C
O
N
N
2dd
13C 500MHz, CDCl3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

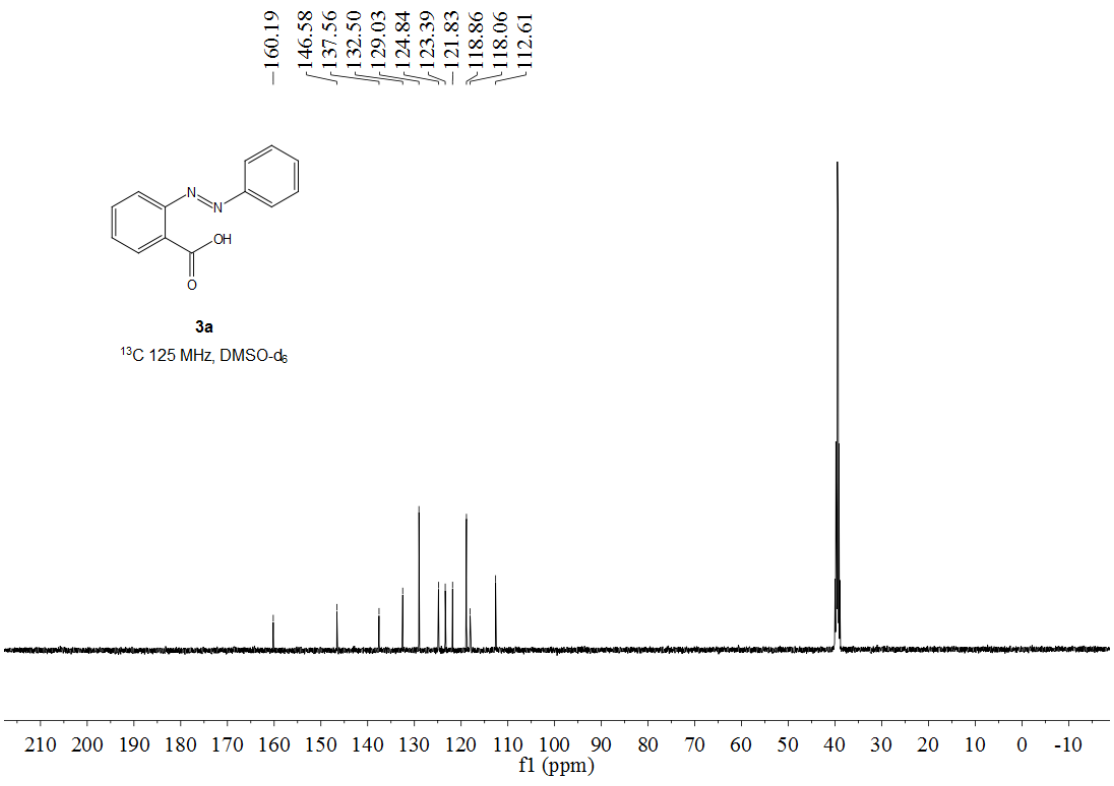

7.901
7.881
7.738
7.719
7.665
7.646
7.484
7.462
7.412
7.393
7.376
7.297
7.281
7.262
7.244
7.226
7.209
7.108
7.024
7.004
6.923
6.902
3.801
H3C
O
N
N
O
Br
2ee
1H 400 MHz, CDCl3
1.96
1.00
0.99
1.02
1.08
3.28
1.01
1.02
1.01
3.03
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)


184.40
160.09
148.60
141.32
139.50
136.15
132.54
131.84
130.16
129.83
128.22
127.29
125.58
124.29
122.77
120.39
118.65
117.96
115.25
111.16
55.57
H3C
O
N
N
O
Br
2ee
13C 500MHz, CDCl3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



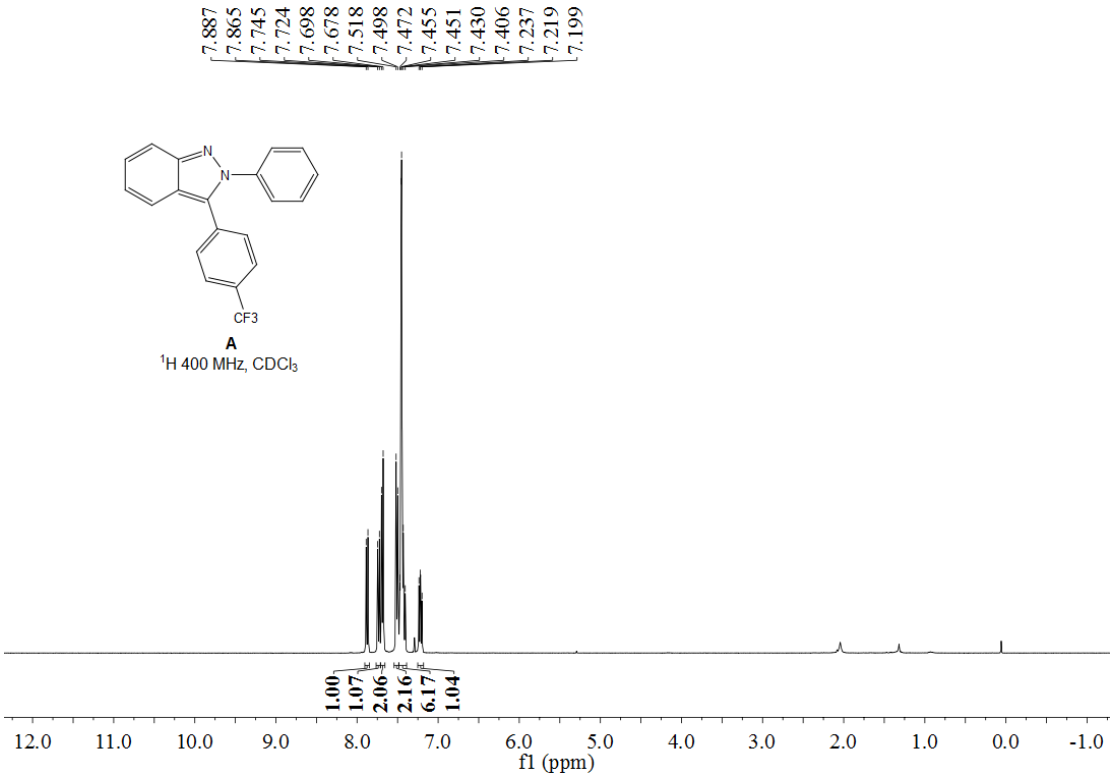
3a

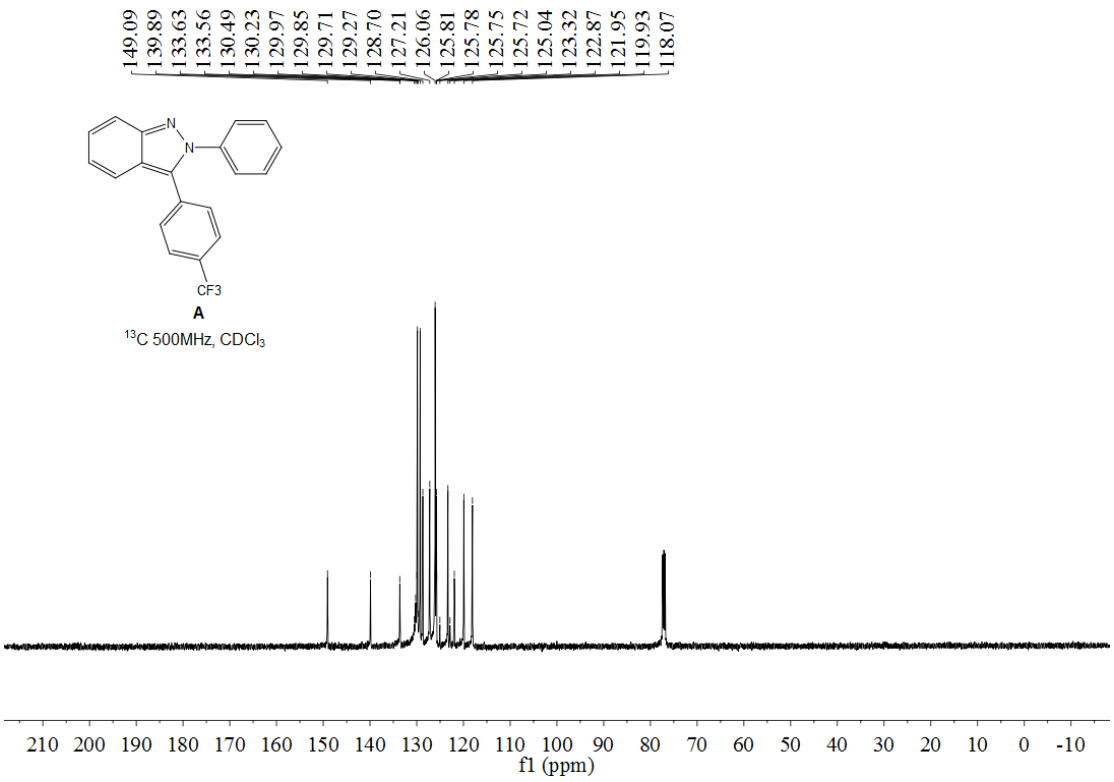
^{1}H 500 MHz, DMSO-d_6

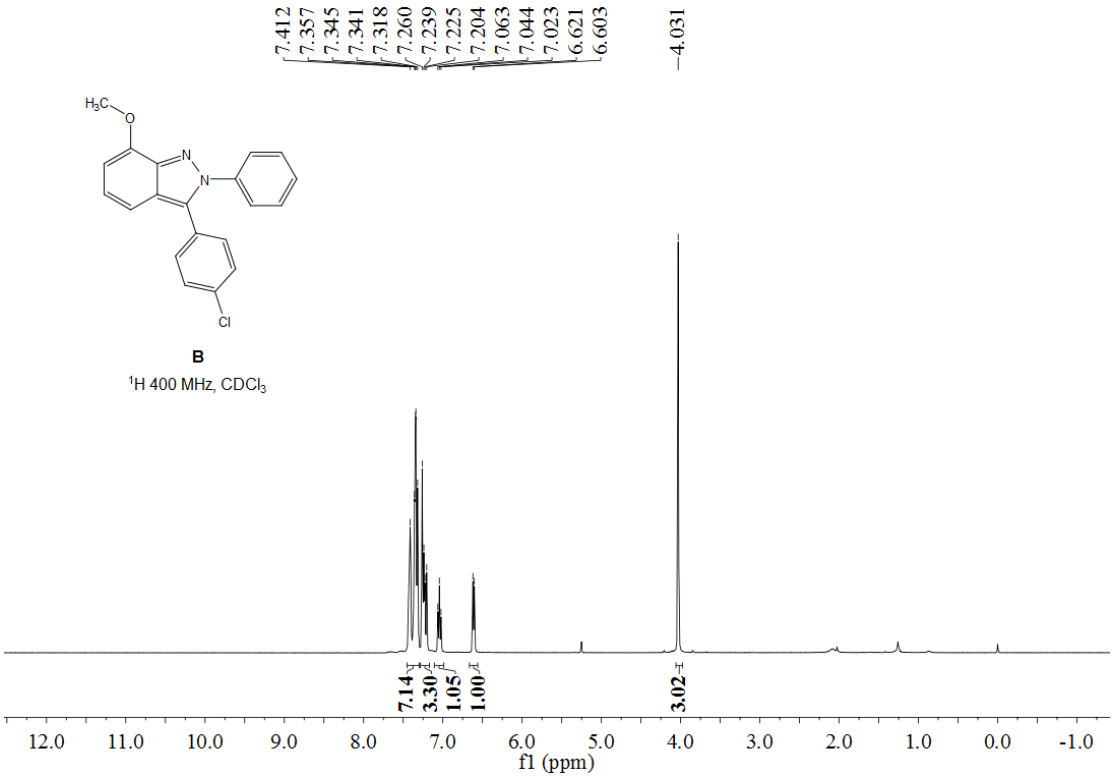


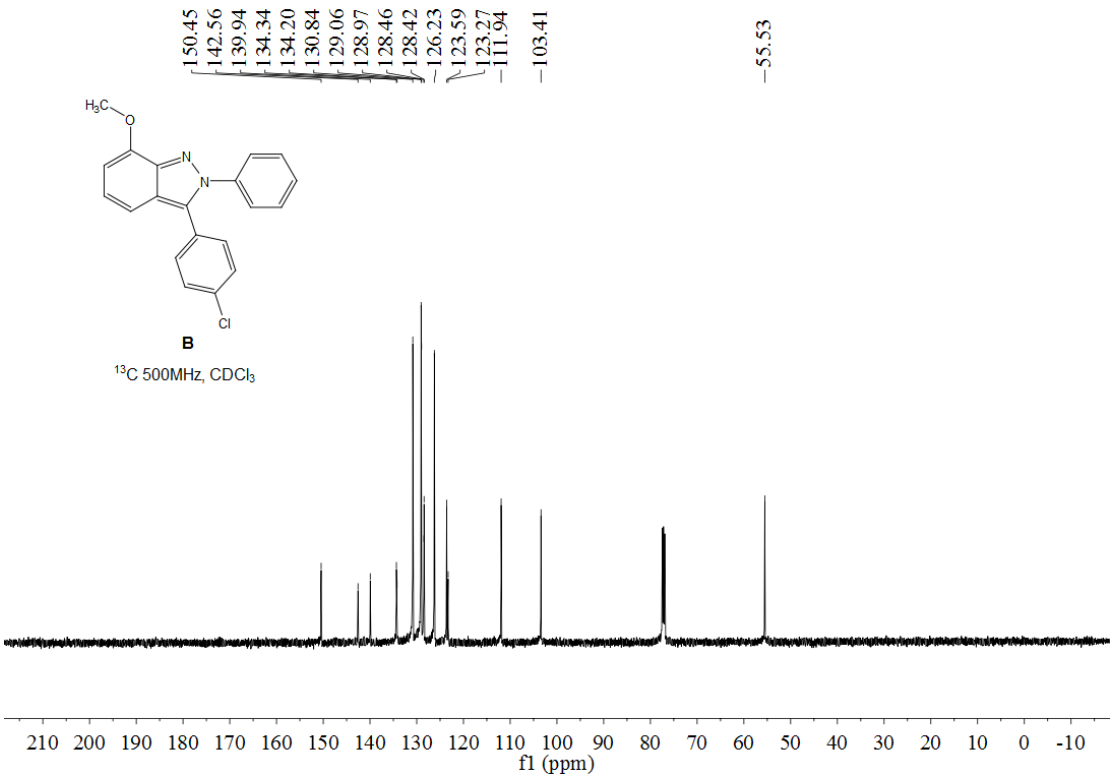
3a

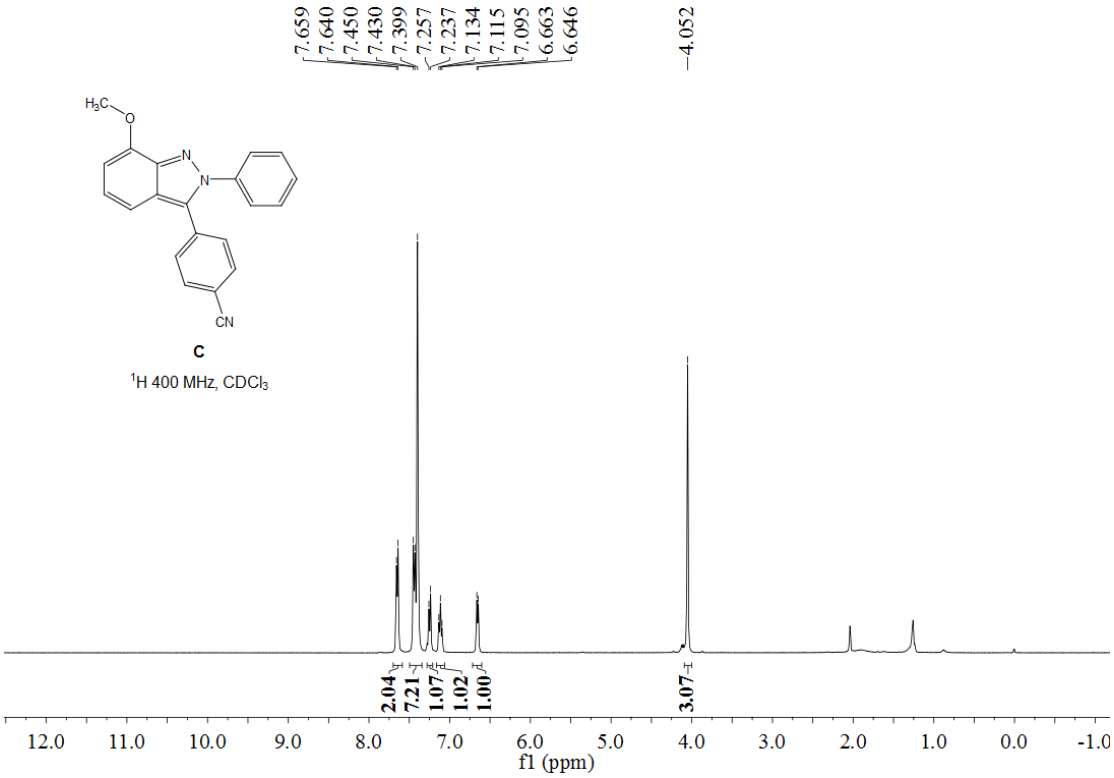
^{13}C 125 MHz, DMSO-d_6


7.887
7.865
7.745
7.724
7.698
7.678
7.518
7.498
7.472
7.455
7.451
7.430
7.406
7.237
7.219
7.199
CF3
A
1H 400 MHz, CDCl3
1.00
1.07
2.06
2.16
6.17
1.04
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0
f1 (ppm)


149.09
139.89
133.63
133.56
130.49
130.23
129.97
129.85
129.71
129.27
128.70
127.21
126.06
125.81
125.78
125.75
125.72
125.04
123.32
122.87
121.95
119.93
118.07
CF3
A
13C 500MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

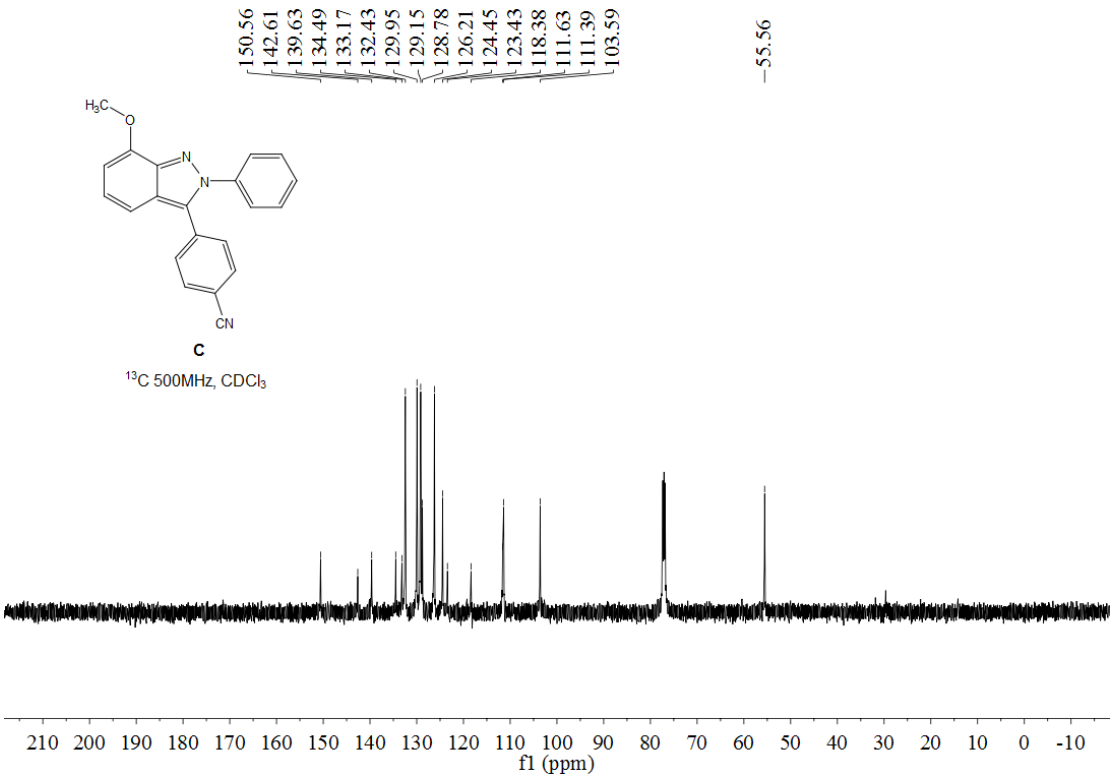

7.412
7.357
7.345
7.341
7.318
7.260
7.239
7.225
7.204
7.063
7.044
7.023
6.621
6.603
4.031
H3C
O
N
N
Cl
B
1H 400 MHz, CDCl3
7.14
3.30
1.05
1.00
3.02
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0
f1 (ppm)


150.45
142.56
139.94
134.34
134.20
130.84
129.06
128.97
128.46
128.42
126.23
123.59
123.27
111.94
103.41
55.53
H3C
O
N
N
Cl
B
13C 500MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



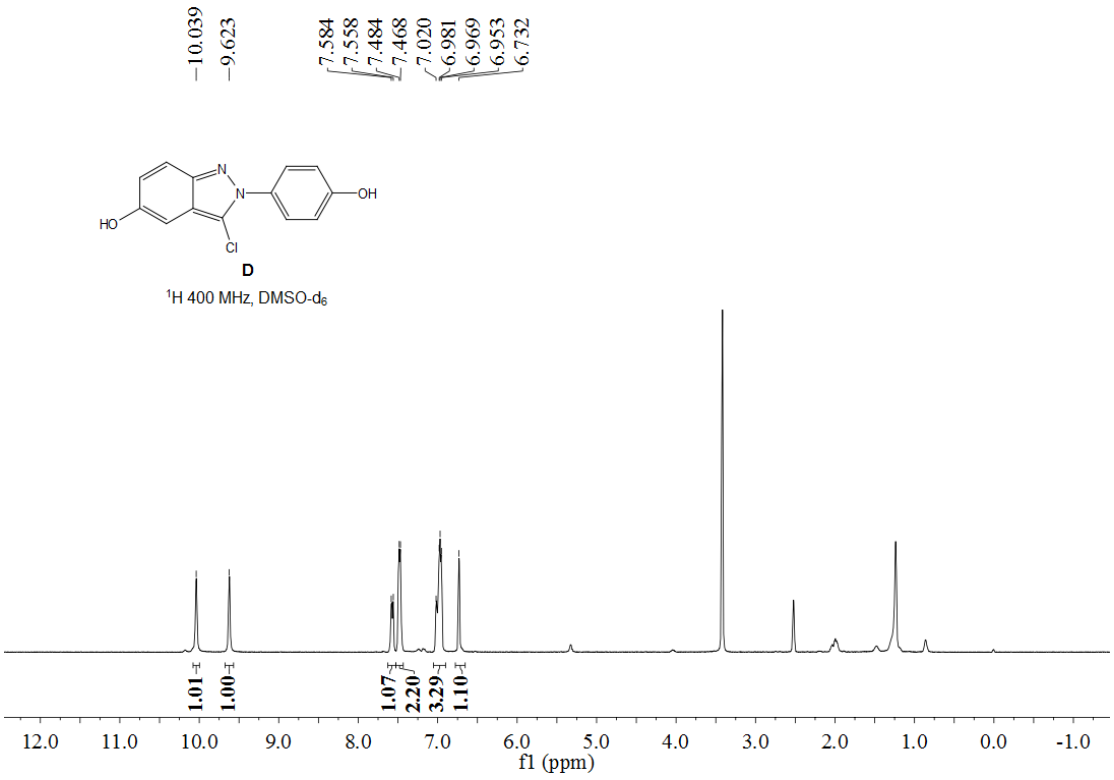
C

^{1}H 400 MHz, $CDCl_3$



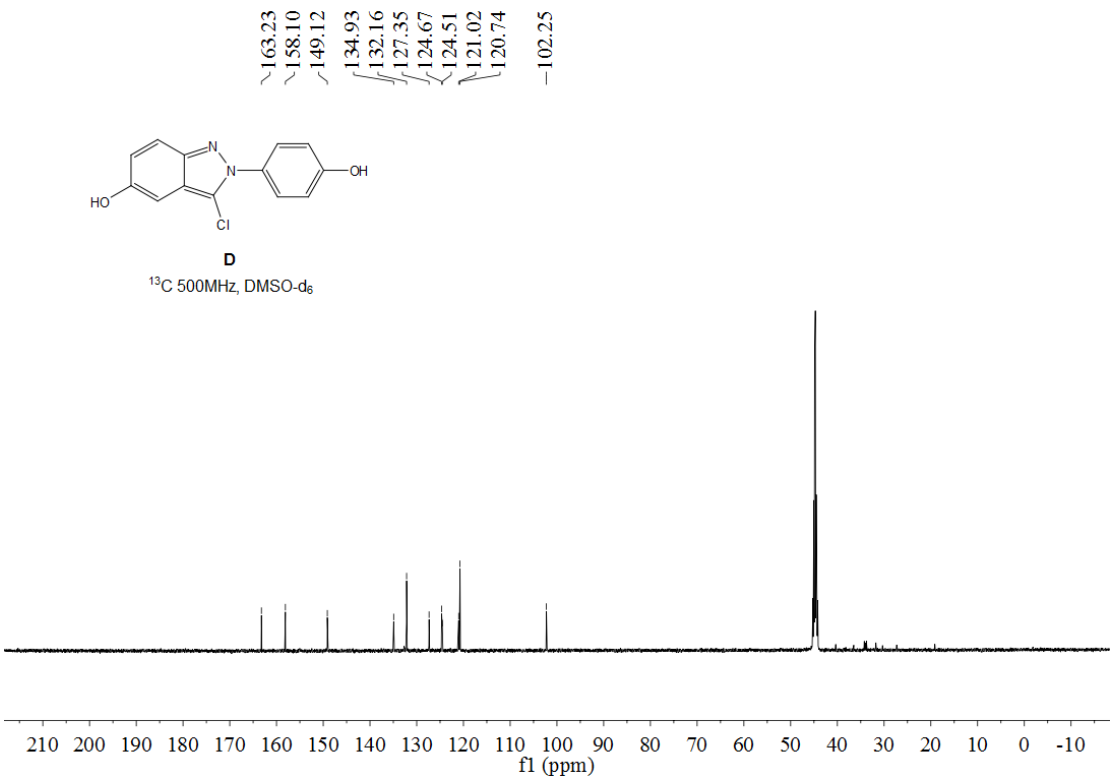
C

^{13}C 500MHz, $CDCl_3$



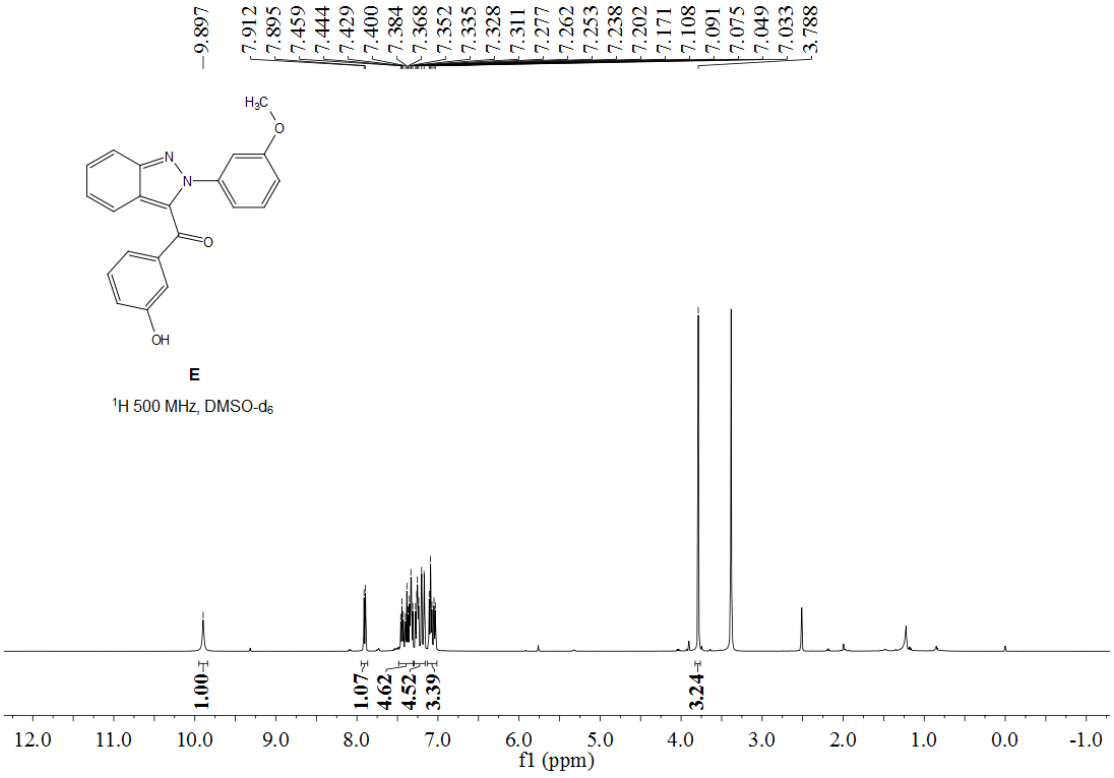
D

^{1}H 400 MHz, DMSO-d_6



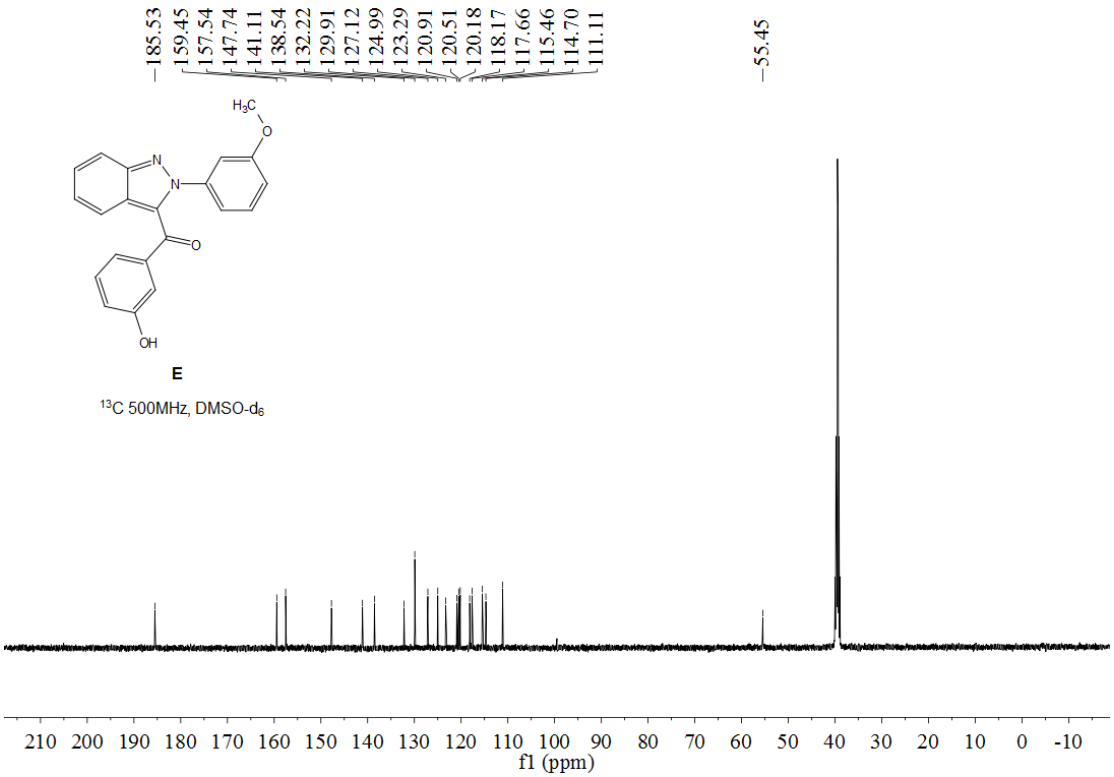
D

^{13}C 500MHz, DMSO-d_6



E

^{1}H 500 MHz, DMSO-d_6



E

^{13}C 500MHz, DMSO-d_6