Supporting Information

for

TfOH-Catalyzed Regioselective *N*^{2}-Alkylation of Indazoles with Diazo Compounds

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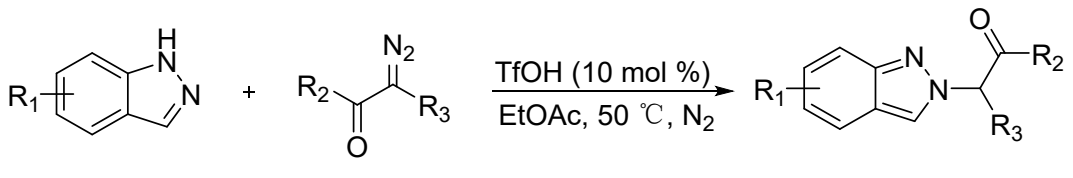
1. General Information and Materials

All ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) and ^{19}F NMR (376 MHz) spectra were recorded on Brucker spectrometers in $CDCl_3$ or DMSO-d_6. Chemical shifts (δ) for NMR were quoted in ppm relative to the solvent peak (7.26 ppm for ^{1}H and 77.16 ppm for ^{13}C in $CDCl_3$; 2.50 ppm for ^{1}H and 40.00 ppm for ^{13}C in DMSO-d_6). Chemical shifts are reported in parts per million as follows: chemical shift, multiplicity (s =singlet, d = doublet, t = triplet, q = quartet, m = multiplet). Coupling constants *J* are recorded in Hz. High-resolution mass spectra (HRMS) were reported from the Thermo Orbitrap Elite or Bruker Daltonics APEXII 47e FT-ICR instrument with an ESI source. Melting points (m.p.) were uncorrected. Single crystal X-ray diffraction data (**3m**) was recorded on Bruker-AXS SMART APEX II single crystal X-ray diffractometer.

Unless otherwise noted, all reactions were carried out under nitrogen in a flamedried or oven-dried flask containing magnetic stir bar. All indazoles (**1a–y**) were purchased from Bidepharm.com and were used directly without further purification. Diazo compounds **2a–w** were prepared according to literature reported procedure [1-5]. The other materials obtained from commercial suppliers were used directly without further purification. Reactions were monitored by thin layer chromatography (TLC) using pre-coated silica gel plates (GF254). Flash column chromatography was performed on silica gel (particle size 200-300 mesh ASTM) and eluted with petroleum ether/ethylacetate. Solvents for the column chromatography were distilled before used.

2. General Experimental Procedures



1 **2** **3**

Indazole **1** (0.50 mmol), diazo keone **2** (0.70 mmol) and EtOAc (1 mL) were added

into a 10 mL glass tube. Then a solution of CF_3SO_3H (7.5 mg, 0.05 mmol, 10 mol%) dissolved in EtOAc (1 mL) was introduced into the reaction mixture. The resulting mixture was continually stirred under nitrogen atmosphere at 50 °C for 2 hours. The reaction solution was quenched with saturated aq. NH_4Cl and extracted with CH_2Cl_2 (5 mL×3). The combined organic phase was dried over anhydrous Na_2SO_4, filtrated and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford the pure product **3**.

3. References

[1] Zhang, J.; Chen, W.; Huang, D.; Zeng, X.; Wang, X.; Hu, Y. *J. Org. Chem*. **2017**, *82*, 9171-9174.

[2] Sthalam, V. K.; Singh, A. K.; Pabbaraja, S. *Org. Process Res. Dev*. **2019**, *23*, 1892-1899.

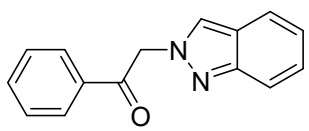
[3] Kale, B. S.; Lee, H. -F.; Liu, R. -S. *Adv. Synth. Catal*. **2017**, *359*, 402-409.

[4] Xia, Z.; Hu, J.; Y Gao, Q.; Yao, Q.; Xie, W. *Chem. Commun*. **2017**, *53*, 7485-7488.

[5] Hauptmann, S.; Wilde, H. *J. Prakt. Chem*, **1969**, *311*, 604-613.

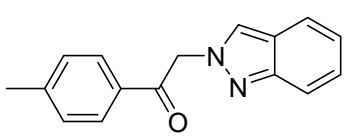
4. Characterization Data of Compounds

2-(2*H*-indazol-2-yl)-1-phenylethan-1-one (3a)



Yellow solid, m.p.: 120-122 °C, yield: 85%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.40 (s, 1H), 8.12 – 8.07 (m, 2H), 7.74 (dd, J = 14.9, 7.9 Hz, 2H), 7.61 (t, J = 7.6 Hz, 3H), 7.28 – 7.22 (m, 1H), 7.10 – 7.03 (m, 1H), 6.20 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 193.3, 148.6, 134.9, 134.6, 129.5, 128.6, 126.1, 126.0, 122.2, 121.5, 121.2, 117.4, 59.7; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{15}H_{13}N_2O^+$: 237.1022; found: 237.1030.

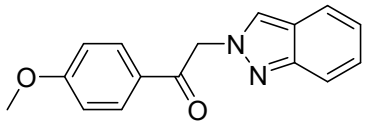
2-(2*H*-indazol-2-yl)-1-(*p*-tolyl)ethan-1-one (3b)



Yellow solid, m.p.: 187-188 °C, yield: 81%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.38 (s, 1H), 7.99 (d, J = 8.2 Hz, 2H), 7.75 (d, J = 8.4 Hz, 1H), 7.59 (d, J = 8.7

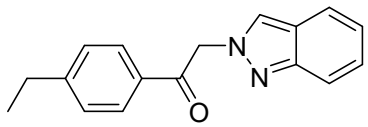
Hz, 1H), 7.41 (d, J = 8.0 Hz, 2H), 7.27 – 7.21 (m, 1H), 7.08 – 7.02 (m, 1H), 6.14 (s, 2H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 192.8, 148.6, 145.1, 132.5, 130.0, 128.7, 126.1, 125.9, 122.1, 121.4, 121.2, 117.4, 59.6, 21.7; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{16}H_{15}N_2O^+$: 251.1179; found: 251.1184.

2-(2*H*-indazol-2-yl)-1-(4-methoxyphenyl)ethan-1-one (3c)



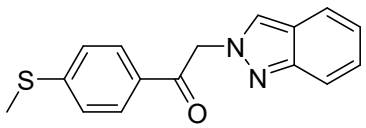
Yellow solid, m.p.: 147-148 °C, yield: 73%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.38 (s, 1H), 8.07 (d, J = 8.9 Hz, 2H), 7.75 (d, J = 8.4 Hz, 1H), 7.60 (d, J = 8.7 Hz, 1H), 7.26 – 7.22 (m, 1H), 7.12 (d, J = 8.9 Hz, 2H), 7.07 – 7.03 (m, 1H), 6.12 (s, 2H), 3.88 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 191.6, 164.3, 148.6, 131.0, 127.8, 126.1, 125.9, 122.1, 121.4, 121.2, 117.4, 114.7, 59.3, 56.1; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{16}H_{15}N_2O_2^+$: 267.1128; found: 267.1106.

1-(4-ethylphenyl)-2-(2*H*-indazol-2-yl)ethan-1-one(3d)



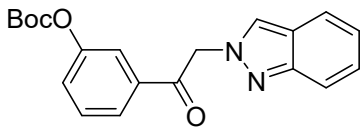
White solid, m.p.: 170-172 °C, yield: 70%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.38 (s, 1H), 8.02 (d, J = 8.2 Hz, 2H), 7.75 (d, J = 8.4 Hz, 1H), 7.60 (dd, J = 8.7, 0.7 Hz, 1H), 7.44 (d, J = 8.0 Hz, 2H), 7.27 – 7.23 (m, 1H), 7.07 – 7.04 (m, 1H), 6.16 (s, 2H), 2.71 (q, J = 7.6 Hz, 2H), 1.22 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 192.8, 151.1, 148.6, 132.7, 128.8, 126.1, 126.0, 122.1, 121.5, 121.2, 117.4, 59.6, 28.7, 15.7; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{17}H_{17}N_2O^+$: 265.1335; found: 265.1345.

2-(2*H*-indazol-2-yl)-1-(4-(methylthio)phenyl)ethan-1-one (3e)



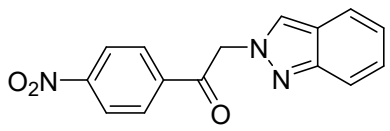
White solid, m.p.: 186-187 °C, yield: 91%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.38 (s, 1H), 8.00 (d, J = 8.4 Hz, 2H), 7.75 (d, J = 8.4 Hz, 1H), 7.59 (d, J = 8.7 Hz, 1H), 7.43 (d, J = 8.4 Hz, 2H), 7.26 – 7.23 (m, 1H), 7.07 – 7.03 (m, 1H), 6.13 (s, 2H), 2.57 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 192.2, 148.6, 147.2, 131.0, 129.1, 126.1, 126.0, 125.5, 122.1, 121.5, 121.2, 117.4, 59.5, 14.4; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{16}H_{15}N_2OS^+$: 283.0900; found: 283.0908.

3-(2-(2*H*-indazol-2-yl)acetyl)phenyl tert-butyl carbonate (3f)



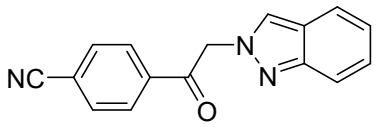
Yellow solid, m.p.: 104-105 °C, yield: 78%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.39 (d, J = 0.7 Hz, 1H), 8.04 – 7.95 (m, 1H), 7.93 – 7.86 (m, 1H), 7.75 (d, J = 8.4 Hz, 1H), 7.71 – 7.53 (m, 3H), 7.25 (m, 1H), 7.06 (m, 1H), 6.20 (s, 2H), 1.51 (s, 9H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 192.7, 151.5, 151.4, 148.6, 136.3, 130.8, 127.8, 126.2, 126.1, 126.0, 122.1, 121.5, 121.2, 117.4, 84.2, 59.8, 27.7; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{20}H_{21}N_2O_4^+$: 353.1496; found: 353.1498.

2-(2*H*-indazol-2-yl)-1-(4-nitrophenyl)ethan-1-one (3g)



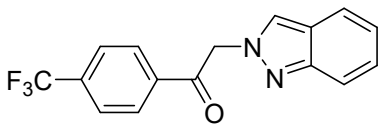
Yellow solid, m.p.: 125-126 °C, yield: 93%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.42 – 8.40 (m, 3H), 8.31 (d, J = 8.8 Hz, 2H), 7.76 (d, J = 8.4 Hz, 1H), 7.61 (d, J = 8.7 Hz, 1H), 7.27 – 7.23 (m, 1H), 7.09 – 7.04 (m, 1H), 6.28 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 192.8, 150.8, 148.7, 139.5, 130.10, 126.1, 126.1, 124.5, 122.2, 121.6, 121.2, 117.4, 60.1; HRMS (ESI): *m/z* [M+H]$^+$ calcd for $C_{15}H_{12}N_3O_3^+$: 282.0873; found: 282.0878.

4-(2-(2*H*-indazol-2-yl)acetyl)benzonitrile (3h)



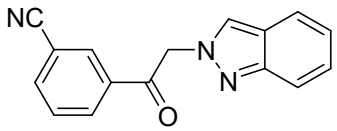
Yellow solid, m.p.: 191-192 °C, yield: 75%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.39 (s, 1H), 8.23 (d, J = 8.3 Hz, 2H), 8.10 (d, J = 8.2 Hz, 2H), 7.76 (d, J = 8.4 Hz, 1H), 7.60 (d, J = 8.7 Hz, 1H), 7.32 – 7.21 (m, 1H), 7.13 – 7.02 (m, 1H), 6.25 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 193.0, 148.7, 138.1, 133.4, 129.3, 126.1, 126.1, 122.2, 121.6, 121.2, 118.5, 117.4, 116.4, 59.9; HRMS (ESI): *m/z* [M+H]$^+$ calcd for $C_{16}H_{15}N_3O^+$: 262.0975; found: 262.0977.

2-(2*H*-indazol-2-yl)-1-(4-(trifluoromethyl)phenyl)ethan-1-one (3i)



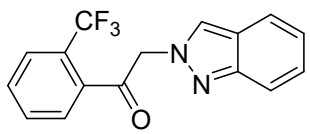
Yellow solid, m.p.: 162-164 °C, yield: 73%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.39 (s, 1H), 8.28 (d, J = 8.1 Hz, 2H), 7.99 (d, J = 8.2 Hz, 2H), 7.76 (d, J = 8.4 Hz, 1H), 7.60 (d, J = 8.7 Hz, 1H), 7.32 – 7.20 (m, 1H), 7.16 – 6.98 (m, 1H), 6.26 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 193.0, 148.7, 138.1, 133.9, 133.5, 129.5, 126.4, 126.4, 126.1, 126.1, 122.2, 121.6, 121.2, 117.4, 59.9; ^{19}F NMR (376 MHz, DMSO-d_6): δ = -61.6; HRMS (ESI): *m/z* [M+H]$^+$ calcd for $C_{16}H_{12}F_3N_2O^+$: 305.0896; found: 305.0903.

3-(2-(2*H*-indazol-2-yl)acetyl)benzonitrile (3j)



Yellow solid, m.p.: 134-136 °C, yield: 81%
^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.29 (s, 1H), 8.22 (d, J = 8.0 Hz, 1H), 8.03 (s, 1H), 7.89 (d, J = 7.8 Hz, 1H), 7.71 – 7.63 (m, 3H), 7.33 – 7.28 (m, 1H), 7.11 (dd, J = 8.5, 6.9 Hz, 1H), 5.84 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 190.0, 149.4, 137.1, 135.3, 132.2, 132.0, 130.2, 126.7, 124.8, 122.6, 122.4, 120.4, 117.6, 113.9, 59.1; HRMS (ESI): *m/z* [M+H]$^+$ calcd for $C_{16}H_{12}N_3O^+$: 262.0975; found: 262.0976.

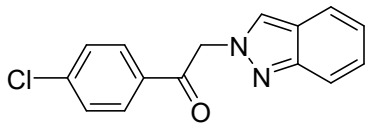
2-(2*H*-indazol-2-yl)-1-(2-(trifluoromethyl)phenyl)ethan-1-one (3k)



Yellow solid, m.p.: 126-128 °C, yield: 85%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.40 (s, 1H), 8.10 (d, J = 7.6 Hz, 1H), 7.93 – 7.85 (m, 2H), 7.78 (dd, J = 17.1, 8.1 Hz, 2H), 7.62 (d, J = 8.7 Hz, 1H), 7.28 – 7.22 (m, 1H), 7.09 – 7.03 (m, 1H), 6.07 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 196.8, 148.8, 136.5,

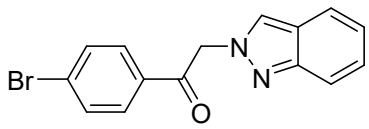
133.1, 132.3, 128.8, 127.6, 127.6, 126.9, 126.5, 126.2, 126.0, 125.3, 122.2, 121.7, 121.2, 117.5, 61.7; ^{19}F NMR (376 MHz, DMSO-d_6): δ = -56.9; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{16}H_{12}F_3N_2O^+$: 305.0896; found: 305.0903.

1-(4-chlorophenyl)-2-(2*H*-indazol-2-yl)ethan-1-one (3l)



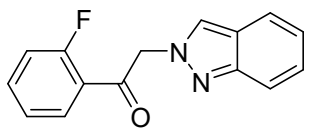
Yellow solid, m.p.: 150-151 °C, yield: 87%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.40 (s, 1H), 8.10 – 8.04 (m, 3H), 7.73 (t, *J* = 7.4 Hz, 1H), 7.63 – 7.59 (m, 3H), 7.34 (dd, *J* = 9.1, 1.9 Hz, 1H), 6.22 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 193.1, 146.9, 134.8, 134.6, 129.5, 129.2, 128.6, 126.2, 123.4, 123.4, 119.8, 114.1, 59.9; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{15}H_{12}ClN_2O^+$: 271.0633; found: 271.0638.

1-(4-bromophenyl)-2-(2*H*-indazol-2-yl)ethan-1-one (3m)



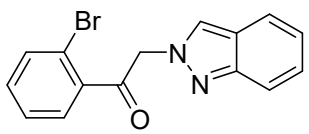
Yellow solid, m.p.: 132-133 °C, yield: 80%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.38 (s, 1H), 8.02 (d, *J* = 8.5 Hz, 2H), 7.82 (d, *J* = 8.5 Hz, 2H), 7.75 (d, *J* = 8.4 Hz, 1H), 7.60 (d, *J* = 8.7 Hz, 1H), 7.27 – 7.23 (m, 1H), 7.08 – 7.04 (m, 1H), 6.18 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 192.7, 148.6, 134.0, 132.5, 130.6, 128.7, 126.1, 126.0, 122.2, 121.5, 121.2, 117.4, 59.7; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{15}H_{12}BrN_2O^+$: 315.0128; found: 315.0132.

1-(2-fluorophenyl)-2-(2*H*-indazol-2-yl)ethan-1-one (3n)



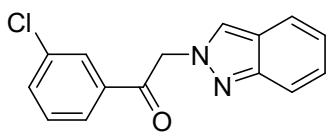
Yellow solid, m.p.: 93-95 °C, yield: 82%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.39 (s, 1H), 7.96 (td, *J* = 7.6, 1.6 Hz, 1H), 7.79 – 7.73 (m, 2H), 7.61 (d, *J* = 8.7 Hz, 1H), 7.48 – 7.38 (m, 2H), 7.26 (dd, *J* = 8.1, 7.2 Hz, 1H), 7.09 – 7.03 (m, 1H), 6.04 (d, *J* = 2.7 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 191.3, 163.2, 160.7, 148.6, 136.6, 130.8, 126.1, 126.0, 125.6, 123.4, 123.3, 122.1, 121.5, 121.2, 117.5, 62.5, 62.4; ^{19}F NMR (376 MHz, DMSO-d_6): δ = -108.64; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{15}H_{12}FN_2O^+$: 255.0928; found: 255.0931.

1-(2-bromophenyl)-2-(2*H*-indazol-2-yl)ethan-1-one (3o)



Yellow solid, m.p.: 95-96 °C, yield: 81%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.40 (s, 1H), 7.92 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.79 – 7.73 (m, 2H), 7.58 (ddd, *J* = 11.1, 8.5, 4.7 Hz, 2H), 7.50 (td, *J* = 7.7, 1.7 Hz, 1H), 7.28 – 7.22 (m, 1H), 7.08 – 7.04 (m, 1H), 6.03 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 196.0, 148.7, 137.8, 134.5, 133.6, 130.1, 128.3, 126.1, 126.0, 122.1, 121.6, 121.2, 119.2, 117.5, 61.5; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{15}H_{12}BrN_2O^+$: 315.0128; found: 315.0131.

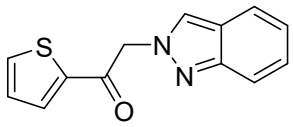
1-(3-chlorophenyl)-2-(2*H*-indazol-2-yl)ethan-1-one (3p)



Yellow solid, m.p.: 134-136 °C, yield: 82%

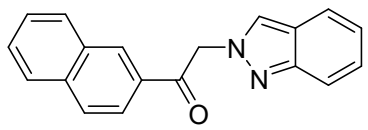
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.38 (s, 1H), 8.11 (t, J = 1.7 Hz, 1H), 8.04 (d, J = 7.8 Hz, 1H), 7.81 – 7.74 (m, 2H), 7.66 – 7.59 (m, 2H), 7.27 – 7.23 (m, 1H), 7.08 – 7.04 (m, 1H), 6.21 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 192.6, 148.6, 136.8, 134.4, 134.2, 131.4, 128.3, 127.3, 126.1, 126.0, 122.2, 121.5, 121.2, 117.4, 59.8; HRMS (ESI): *m/z* [M+H]$^+$ calcd for $C_{15}H_{12}ClN_2O^+$: 271.0633; found: 271.0635.

2-(2*H*-indazol-2-yl)-1-(thiophen-2-yl)ethan-1-one (3q)



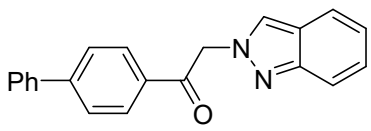
Yellow solid, m.p.: 123-125 °C, yield: 87%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.42 (s, 1H), 8.23 – 8.18 (m, 1H), 8.14 (dd, J = 4.9, 0.7 Hz, 1H), 7.75 (d, J = 8.4 Hz, 1H), 7.60 (d, J = 8.7 Hz, 1H), 7.35 (dd, J = 4.8, 4.0 Hz, 1H), 7.25 (dd, J = 11.5, 3.8 Hz, 1H), 7.09 – 7.03 (m, 1H), 6.10 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 186.4, 148.7, 141.3, 136.6, 134.9, 129.6, 126.3, 126.2, 122.1, 121.6, 121.2, 117.4, 59.3; HRMS (ESI): *m/z* [M+H]$^+$ calcd for $C_{13}H_{11}N_2OS^+$: 243.0587; found: 243.0593.

2-(2*H*-indazol-2-yl)-1-(naphthalen-2-yl)ethan-1-one (3r)



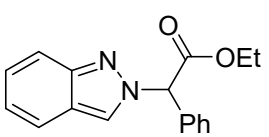
Yellow solid, m.p.: 193-195 °C, yield: 74%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.88 (s, 1H), 8.44 (s, 1H), 8.18 (d, J = 7.9 Hz, 1H), 8.07 (dd, J = 20.1, 8.5 Hz, 3H), 7.78 – 7.67 (m, 3H), 7.62 (d, J = 8.6 Hz, 1H), 7.29 – 7.22 (m, 1H), 7.10 – 7.04 (m, 1H), 6.33 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 193.3, 148.6, 135.9, 132.6, 132.2, 130.9, 130.1, 129.6, 129.1, 128.3, 127.7, 126.2, 126.0, 123.8, 122.2, 121.5, 121.2, 117.4, 59.7; HRMS (ESI): *m/z* [M+H]$^+$ calcd for $C_{19}H_{15}N_2O^+$: 287.1179; found: 287.1188.

1-([1,1'-biphenyl]-4-yl)-2-(2*H*-indazol-2-yl)ethan-1-one (3s)



White solid, m.p.: 224-226 °C, yield: 76%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.41 (d, J = 0.7 Hz, 1H), 8.18 (d, J = 8.5 Hz, 2H), 7.91 (d, J = 8.5 Hz, 2H), 7.81 – 7.74 (m, 3H), 7.61 (dd, J = 8.7, 0.8 Hz, 1H), 7.53 (dd, J = 10.2, 4.7 Hz, 2H), 7.48 – 7.43 (m, 1H), 7.26 (ddd, J = 8.7, 6.6, 1.0 Hz, 1H), 7.06 (ddd, J = 8.2, 6.6, 0.7 Hz, 1H), 6.22 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 192.9, 148.6, 145.8, 139.2, 133.7, 129.6, 129.4, 129.1, 127.6, 127.6, 126.1, 126.0, 122.2, 121.5, 121.2, 117.4, 59.7; HRMS (ESI): *m/z* [M+H]$^+$ calcd for $C_{21}H_{17}N_2O^+$: 313.1335; found: 313.1346.

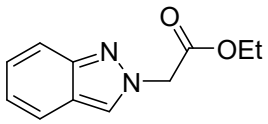
ethyl 2-(2*H*-indazol-2-yl)-2-phenylacetate (3t)



Yellow oil, yield: 88%
^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.91 (s, 1H), 7.71 (d, J = 8.8 Hz, 1H), 7.60 (d, J = 8.5 Hz, 1H), 7.49 – 7.43 (m, 5H), 7.29 (dd, J = 6.7, 0.8 Hz, 1H), 7.05 (dd, J = 8.0, 7.0 Hz, 1H), 6.51 (s, 1H), 4.36 – 4.26 (m, 2H), 1.29 (t, J = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 168.6, 148.5, 134.7, 129.5, 129.4, 129.3, 126.4, 124.5, 121.8, 121.6, 121.3, 117.7, 68.4,

62.2, 14.3; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{17}H_{17}N_2O_2^+$: 281.1285; found: 281.1285.

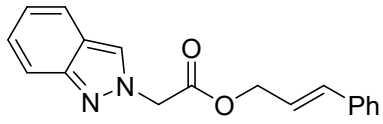
ethyl 2-(2*H*-indazol-2-yl)acetate (3u)



White oil, yield: 78%

^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.39 (s, 1H), 7.73 (d, J = 8.4 Hz, 1H), 7.59 (d, J = 8.7 Hz, 1H), 7.27 – 7.22 (m, 1H), 7.08 – 7.02 (m, 1H), 5.40 (s, 2H), 4.18 (q, J = 7.1 Hz, 2H), 1.22 (t, J = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 168.2, 148.7, 126.2, 125.9, 122.0, 121.6, 121.2, 117.4, 61.7, 54.4, 14.4; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{11}H_{13}N_2O_2^+$: 205.0972; found: 205.0970.

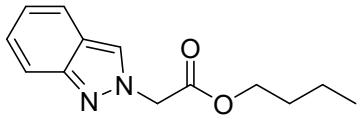
cinnamyl 2-(2*H*-indazol-2-yl)acetate (3v)



Yellow oil, yield: 82%

^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.43 (s, 1H), 7.74 (d, J = 8.4 Hz, 1H), 7.61 (d, J = 8.7 Hz, 1H), 7.43 (d, J = 7.3 Hz, 2H), 7.35 (t, J = 7.4 Hz, 2H), 7.27 (dd, J = 14.3, 7.4 Hz, 2H), 7.09 – 7.03 (m, 1H), 6.65 (d, J = 16.0 Hz, 1H), 6.37 (dt, J = 16.0, 6.0 Hz, 1H), 5.49 (s, 2H), 4.83 (d, J = 5.8 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 168.0, 148.7, 136.3, 133.9, 129.1, 128.6, 127.0, 126.3, 126.0, 123.5, 122.0, 121.7, 121.3, 117.5, 65.9, 54.5; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{18}H_{17}N_2O_2^+$: 293.1285; found: 293.1283.

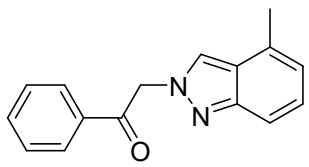
butyl 2-(2*H*-indazol-2-yl)acetate (3w)



Yellow oil, yield: 90%

^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.39 (s, 1H), 7.73 (d, J = 8.4 Hz, 1H), 7.60 (d, J = 8.7 Hz, 1H), 7.25 (dd, J = 8.0, 7.3 Hz, 1H), 7.09 – 7.03 (m, 1H), 5.42 (s, 2H), 4.13 (t, J = 6.5 Hz, 2H), 1.57 (dd, J = 14.1, 7.3 Hz, 2H), 1.31 (dd, J = 14.9, 7.4 Hz, 2H), 0.87 (t, J = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 168.2, 148.7, 126.2, 125.9, 122.0, 121.6, 121.2, 117.4, 65.3, 54.4, 30.5, 18.9, 13.9; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{13}H_{17}N_2O_2^+$: 233.1285; found: 233.1285.

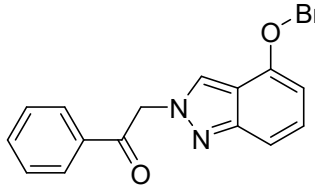
2-(4-methyl-2*H*-indazol-2-yl)-1-phenylethan-1-one (3ab)



Yellow solid, m.p.: 146-147 °C, yield: 80%

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.04 – 7.98 (m, 3H), 7.63 (t, J = 7.4 Hz, 1H), 7.52 (dd, J = 17.1, 9.1 Hz, 3H), 7.20 (dd, J = 8.7, 6.8 Hz, 1H), 6.85 (d, J = 6.7 Hz, 1H), 5.84 (s, 2H), 2.53 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 193.4, 148.7, 135.0, 134.6, 130.7, 129.5, 128.6, 126.3, 125.3, 123.5, 120.6, 114.8, 59.7, 19.4; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{16}H_{15}N_2O^+$: 251.1179; found: 251.1187.

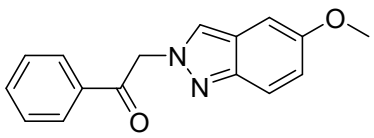
2-(4-(benzyloxy)-2*H*-indazol-2-yl)-1-phenylethan-1-one (3ac)



Yellow solid, m.p.: 75-76 °C, yield: 71%

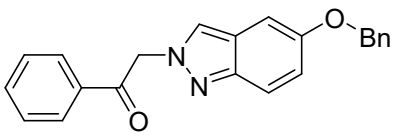
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.45 (s, 1H), 8.09 (d, J = 7.7 Hz, 2H), 7.73 (t, J = 7.3 Hz, 1H), 7.60 (t, J = 7.6 Hz, 2H), 7.53 (d, J = 7.4 Hz, 2H), 7.42 (t, J = 7.4 Hz, 2H), 7.35 (t, J = 7.2 Hz, 1H), 7.19 – 7.13 (m, 2H), 6.53 (dd, J = 5.9, 1.6 Hz, 1H), 6.13 (s, 2H), 5.25 (s, 2H).; ^{13}C NMR (100 MHz, DMSO-d_6): δ = 193.3, 152.5, 150.3, 134.5, 129.4, 128.9, 128.6, 128.3, 128.1, 126.9, 124.5, 110.1, 100.1, 69.6, 59.5; HRMS (ESI): *m/z* [M+H]$^+$ calcd for $C_{22}H_{19}N_2O_2^+$: 343.1441; found: 343.1444.

2-(5-methoxy-2*H*-indazol-2-yl)-1-phenylethan-1-one (3ad)



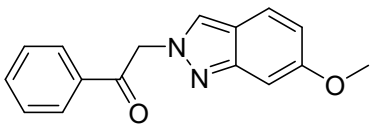
Yellow solid, m.p.: 169-170 °C, yield: 88%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.22 (s, 1H), 8.08 (d, J = 7.2 Hz, 2H), 7.71 (d, J = 6.6 Hz, 1H), 7.61 (d, J = 7.0 Hz, 2H), 7.52 (d, J = 9.1 Hz, 1H), 7.05 (s, 1H), 6.93 (d, J = 9.1 Hz, 1H), 6.12 (s, 2H), 3.78 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 193.5, 154.6, 145.4, 135.0, 134.5, 129.4, 128.6, 125.1, 122.0, 120.5, 118.8, 97.7, 59.6, 55.6; HRMS (ESI): *m/z* [M+H]$^+$ calcd for $C_{16}H_{15}N_2O_2^+$: 267.1128; found: 267.1137.

2-(5-(benzyloxy)-2*H*-indazol-2-yl)-1-phenylethan-1-one (3ae)



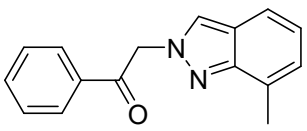
White solid, m.p.: 195-196 °C, yield: 93%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.22 (s, 1H), 8.08 (d, J = 7.6 Hz, 2H), 7.72 (t, J = 7.3 Hz, 1H), 7.64 – 7.48 (m, 5H), 7.37 (dt, J = 27.8, 7.2 Hz, 3H), 7.16 (s, 1H), 7.02 (dd, J = 9.2, 1.9 Hz, 1H), 6.13 (s, 2H), 5.11 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 193.5, 153.6, 145.4, 137.7, 135.0, 134.5, 129.4, 128.9, 128.6, 128.2, 128.2, 125.2, 122.0, 120.8, 118.9, 99.3, 69.8, 59.6; HRMS (ESI): *m/z* [M+H]$^+$ calcd for $C_{22}H_{19}N_2O_2^+$: 343.1441; found: 343.1450.

2-(6-methoxy-2*H*-indazol-2-yl)-1-phenylethan-1-one (3af)



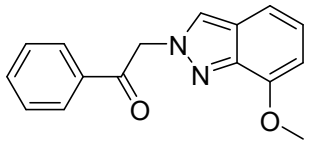
Yellow solid, m.p.: 137-139 °C, yield: 73%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.26 (s, 1H), 8.08 (d, J = 7.6 Hz, 2H), 7.72 (t, J = 7.3 Hz, 1H), 7.64 – 7.57 (m, 3H), 6.91 (s, 1H), 6.72 (dd, J = 9.0, 1.8 Hz, 1H), 6.09 (s, 2H), 3.79 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 193.5, 158.4, 149.6, 135.0, 134.5, 129.4, 128.6, 126.2, 122.0, 117.7, 116.1, 94.9, 59.4, 55.5; HRMS (ESI): *m/z* [M+H]$^+$ calcd for $C_{16}H_{15}N_2O_2^+$: 267.1128; found: 267.1132.

2-(7-methyl-2*H*-indazol-2-yl)-1-phenylethan-1-one (3ag)



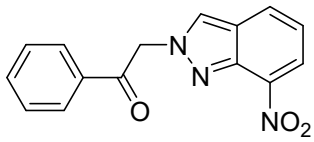
Yellow solid, m.p.: 107-108 °C, yield: 97%
^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.98 (d, J = 8.3 Hz, 3H), 7.60 (t, J = 7.2 Hz, 1H), 7.48 (t, J = 7.6 Hz, 3H), 7.14 (t, J = 7.6 Hz, 1H), 6.79 (d, J = 6.4 Hz, 1H), 5.84 (s, 2H), 2.49 (s, 3H).; ^{13}C NMR (100 MHz, DMSO-d_6): δ = 193.5, 149.0, 134.9, 134.6, 129.5, 128.6, 126.9, 126.4, 124.9, 121.9, 121.7, 118.6, 59.7, 17.5; HRMS (ESI): *m/z* [M+H]$^+$ calcd for $C_{16}H_{15}N_2O^+$: 251.1179; found: 251.1186.

2-(7-methoxy-2*H*-indazol-2-yl)-1-phenylethan-1-one (3ah)



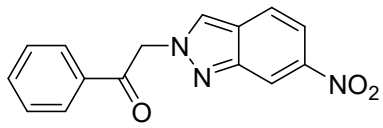
Yellow solid, m.p.: 132-133 °C, yield: 70%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.26 (s, 1H), 8.08 (d, J = 7.6 Hz, 2H), 7.72 (t, J = 7.3 Hz, 1H), 7.65 – 7.57 (m, 3H), 6.91 (s, 1H), 6.72 (dd, J = 9.0, 1.8 Hz, 1H), 6.09 (s, 2H), 3.79 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 193.5, 158.4, 149.6, 135.0, 134.5, 129.4, 128.6, 126.2, 122.0, 117.7, 116.1, 94.9, 59.4, 55.5; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{16}H_{15}N_2O_2^+$: 267.1128; found: 267.1135.

2-(7-nitro-2*H*-indazol-2-yl)-1-phenylethan-1-one (3ai)



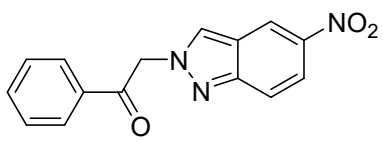
Yellow solid, m.p.: 197-199 °C, yield: 85%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.80 (s, 1H), 8.35 (d, J = 7.9 Hz, 2H), 8.12 (d, J = 7.4 Hz, 2H), 7.76 (t, J = 7.4 Hz, 1H), 7.63 (t, J = 7.7 Hz, 2H), 7.30 (t, J = 7.9 Hz, 1H), 6.40 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 192.8, 140.1, 137.1, 134.8, 134.7, 130.8, 129.7, 129.5, 128.7, 125.9, 125.6, 120.4, 60.4; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{15}H_{12}N_3O_3^+$: 282.0873; found: 282.0877.

2-(6-nitro-2*H*-indazol-2-yl)-1-phenylethan-1-one (3aj)



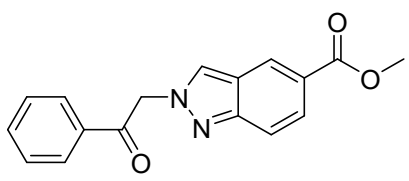
Yellow solid, m.p.: 219-220 °C, yield: 77%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.65 (s, 2H), 8.13 – 8.08 (m, 2H), 8.05 (d, J = 9.1 Hz, 1H), 7.87 – 7.82 (m, 1H), 7.75 (t, J = 7.4 Hz, 1H), 7.63 (t, J = 7.7 Hz, 2H), 6.36 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 192.7, 146.4, 134.8, 134.7, 129.5, 128.7, 128.1, 124.6, 123.3, 115.3, 115.2, 60.6; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{15}H_{12}N_3O_3^+$: 282.0873; found: 282.0878.

2-(5-nitro-2*H*-indazol-2-yl)-1-phenylethan-1-one (3ak)



Yellow solid, m.p.: 167-168 °C, yield: 74%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.97 (d, J = 1.8 Hz, 1H), 8.84 (s, 1H), 8.10 (d, J = 7.5 Hz, 2H), 8.03 (dd, J = 9.4, 2.1 Hz, 1H), 7.82 – 7.73 (m, 2H), 7.62 (t, J = 7.7 Hz, 2H), 6.34 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 192.7, 149.5, 142.5, 134.8, 134.7, 131.8, 129.5, 128.7, 121.2, 120.5, 120.1, 118.6, 60.3; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{15}H_{12}N_3O_3^+$: 282.0873; found: 282.0879.

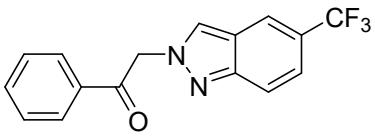
methyl 2-(2-oxo-2-phenylethyl)-2*H*-indazole-5-carboxylate (3al)



Yellow solid, m.p.: 154-156 °C, yield: 82%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.65 (s, 1H), 8.59 (s, 1H), 8.10 (d, J = 7.4 Hz, 2H), 7.74 (ddd, J = 25.3, 13.5, 8.4 Hz, 3H), 7.61 (t, J = 7.7 Hz, 2H), 6.27 (s, 2H), 3.87 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 193.0, 167.1, 149.7, 134.8, 134.7, 129.5, 129.4, 128.6, 125.9, 125.4, 122.9, 121.5, 117.6, 60.0, 52.4; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{17}H_{15}N_2O_3^+$: 295.1077;

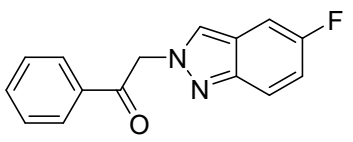
found: 295.1079.

1-phenyl-2-(5-(trifluoromethyl)-2*H*-indazol-2-yl)ethan-1-one (3am)



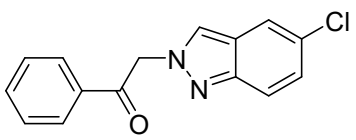
White solid, m.p.: 191-192 °C, yield: 76%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.66 (s, 1H), 8.31 (s, 1H), 8.12 – 8.07 (m, 2H), 7.85 – 7.80 (m, 1H), 7.76 – 7.71 (m, 1H), 7.61 (t, J = 7.7 Hz, 2H), 7.47 (dd, J = 9.1, 1.7 Hz, 1H), 6.30 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 193.0, 148.9, 134.8, 134.7, 129.5, 129.0, 128.6, 126.8, 124.1, 122.3, 122.0, 121.6, 120.8, 120.7, 119.0, 60.1; ^{19}F NMR (376 MHz, DMSO-d_6): δ = -59.98; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{16}H_{12}F_3N_2O^+$: 305.0896; found: 305.0901.

2-(5-fluoro-2*H*-indazol-2-yl)-1-phenylethan-1-one (3an)



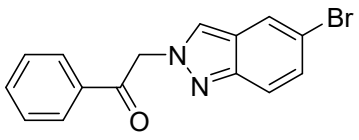
White solid, m.p.: 146-147 °C, yield: 65%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.39 (s, 1H), 8.09 (d, J = 7.5 Hz, 2H), 7.78 – 7.66 (m, 2H), 7.60 (t, J = 7.5 Hz, 2H), 7.53 – 7.46 (m, 1H), 7.22 – 7.13 (m, 1H), 6.21 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 193.2, 159.0, 156.7, 146.1, 134.9, 134.6, 129.5, 128.6, 126.6, 119.9, 119.8, 103.8, 103.6, 59.9; ^{19}F NMR (376 MHz, DMSO-d_6): δ = -121.08; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{15}H_{12}FN_2^+$: 255.0928; found: 255.0935.

2-(5-chloro-2*H*-indazol-2-yl)-1-phenylethan-1-one (3ao)



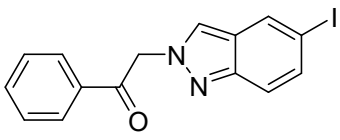
White solid, m.p.: 195-196 °C, yield: 78%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.40 (s, 1H), 8.10 – 8.08 (m, 2H), 7.87 (d, J = 1.8 Hz, 1H), 7.73 (t, J = 7.4 Hz, 1H), 7.68 – 7.59 (m, 3H), 7.24 (dd, J = 9.1, 2.0 Hz, 1H), 6.22 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 193.1, 146.9, 134.8, 134.6, 129.5, 128.6, 126.9, 126.4, 126.0, 122.5, 120.1, 119.6, 59.9; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{15}H_{12}ClN_2^+$: 271.0633; found: 271.0636.

2-(5-bromo-2*H*-indazol-2-yl)-1-phenylethan-1-one (3ap)



White solid, m.p.: 201-202 °C, yield: 79%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.40 (s, 1H), 8.10 – 8.04 (m, 3H), 7.73 (t, J = 7.4 Hz, 1H), 7.63 – 7.59 (m, 3H), 7.34 (dd, J = 9.1, 1.9 Hz, 1H), 6.22 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 193.1, 147.0, 134.8, 134.6, 129.5, 129.2, 128.6, 126.2, 123.4, 123.4, 119.8, 114.1, 59.9; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{15}H_{12}BrN_2^+$: 315.0128; found: 315.0131.

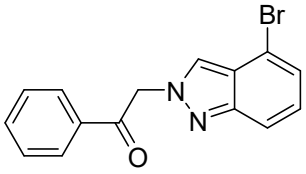
2-(5-iodo-2*H*-indazol-2-yl)-1-phenylethan-1-one (3aq)



Yellow solid, m.p.: 202-203 °C, yield: 72%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.37 (s, 1H), 8.23 (s, 1H), 8.09 – 8.07 (m, 2H), 7.73 (t, J = 7.4 Hz, 1H), 7.61 (t,

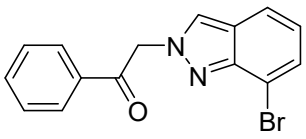
J = 7.7 Hz, 2H), 7.47 (s, 2H), 6.21 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 193.1, 147.1, 134.8, 134.6, 134.1, 130.0, 129.5, 128.6, 125.7, 124.6, 119.8, 85.8, 59.8; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{15}H_{12}IN_2^+$: 362.9989; found: 362.9993.

2-(4-bromo-2*H*-indazol-2-yl)-1-phenylethan-1-one (3ar)



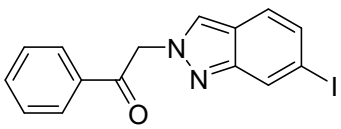
Yellow solid, m.p.: 150-151 °C, yield: 71%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.45 (d, J = 0.6 Hz, 1H), 8.10 – 8.08 (m, 2H), 7.74 (t, J = 7.4 Hz, 1H), 7.63 (dd, J = 15.8, 8.0 Hz, 3H), 7.32 (d, J = 7.0 Hz, 1H), 7.20 (dd, J = 8.6, 7.2 Hz, 1H), 6.23 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 193.0, 148.6, 134.8, 134.7, 129.5, 128.6, 127.1, 127.1, 124.2, 123.7, 117.1, 112.9, 60.0; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{15}H_{12}BrN_2^+$: 315.0128; found: 315.0132.

2-(7-bromo-2*H*-indazol-2-yl)-1-phenylethan-1-one (3as)



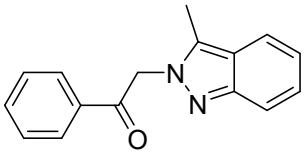
Yellow solid, m.p.: 140-142 °C, yield: 96%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.57 (s, 1H), 8.12 – 8.10 (m, 2H), 7.82 – 7.72 (m, 2H), 7.62 (t, J = 7.7 Hz, 2H), 7.55 (d, J = 7.0 Hz, 1H), 6.99 (dd, J = 8.2, 7.3 Hz, 1H), 6.30 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 193.1, 147.0, 134.8, 134.7, 129.5, 128.9, 128.6, 128.2, 123.1, 122.5, 121.2, 110.5, 60.1; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{15}H_{12}BrN_2^+$: 315.0128; found: 315.0132.

2-(6-iodo-2*H*-indazol-2-yl)-1-phenylethan-1-one (3at)



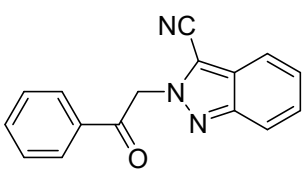
Yellow solid, m.p.: 202-203 °C, yield: 82%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.37 (s, 1H), 8.23 (s, 1H), 8.10 – 8.07 (m, 2H), 7.73 (t, J = 7.4 Hz, 1H), 7.61 (t, J = 7.7 Hz, 2H), 7.47 (s, 2H), 6.21 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 193.1, 147.1, 134.8, 134.6, 134.1, 130.0, 129.5, 128.6, 125.7, 124.6, 119.8, 85.9, 59.8; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{15}H_{12}IN_2^+$: 362.9989; found: 362.9992.

2-(3-methyl-2*H*-indazol-2-yl)-1-phenylethan-1-one (3au)



Yellow solid, m.p.: 132-133 °C, yield: 66%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.12 (d, J = 7.3 Hz, 2H), 7.76 – 7.68 (m, 2H), 7.62 (t, J = 7.7 Hz, 2H), 7.50 (d, J = 8.7 Hz, 1H), 7.25 – 7.20 (m, 1H), 7.03 – 6.97 (m, 1H), 6.17 (s, 2H), 2.53 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 193.2, 147.8, 134.9, 134.6, 133.5, 129.4, 128.8, 126.2, 121.2, 120.8, 120.2, 117.1, 57.4, 9.9; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{16}H_{15}N_2O^+$: 251.1179; found: 251.1180.

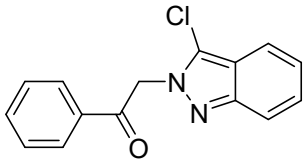
2-(2-oxo-2-phenylethyl)-2*H*-indazole-3-carbonitrile (3av)



White oil, yield: 65%
^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.14 (d, J = 7.6 Hz, 2H), 7.91 (t, J = 8.1 Hz, 2H), 7.79 (t, J = 7.4 Hz, 1H), 7.65 (t, J =

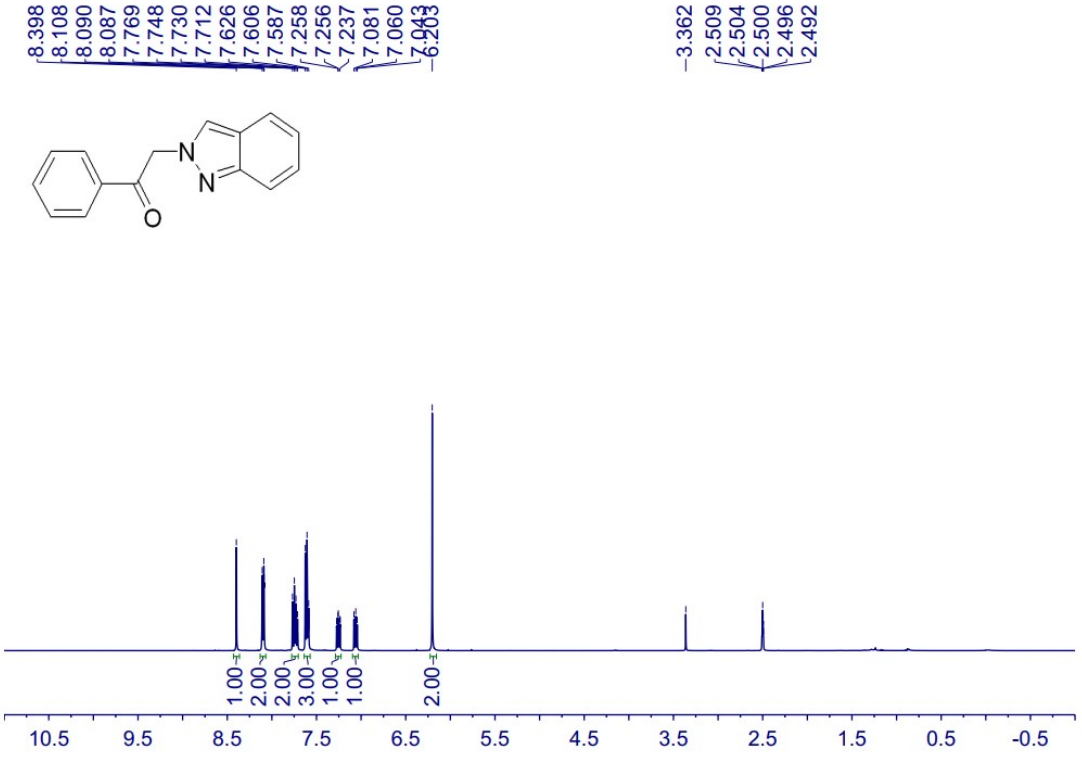
7.7 Hz, 2H), 7.47 (dt, J = 15.3, 7.1 Hz, 4H), 6.58 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 192.1, 147.8, 135.2, 134.2, 129.6, 128.9, 127.9, 126.4, 125.8, 119.1, 118.8, 111.2, 108.7, 60.1; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{16}H_{12}N_3O^+$: 262.0975; found: 262.0975.

2-(3-chloro-2*H*-indazol-2-yl)-1-phenylethan-1-one (3aw)

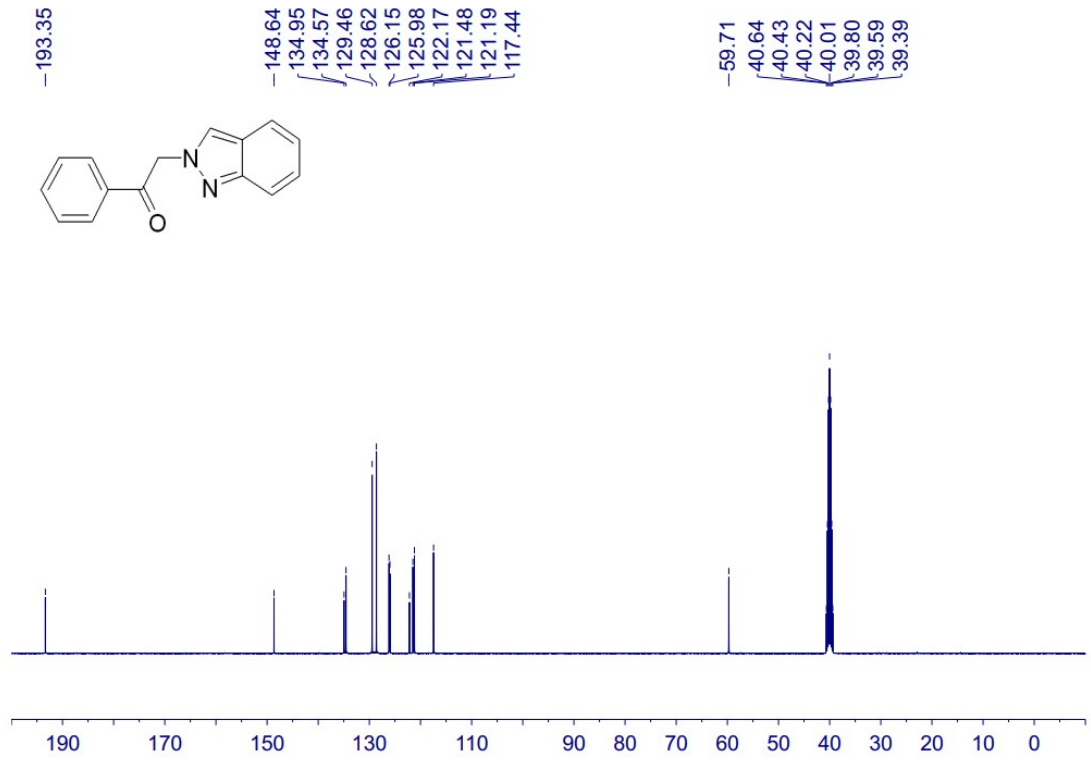


Yellow solid, m.p.: 104-105 °C, yield: 72%
^{1}H NMR (400 MHz, DMSO-d_6): δ = .13 (d, J = 7.4 Hz, 2H), 7.76 (t, J = 7.4 Hz, 1H), 7.63 (dd, J = 13.2, 5.7 Hz, 4H), 7.39 – 7.31 (m, 1H), 7.18 (dd, J = 8.3, 6.9 Hz, 1H), 6.29 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 192.2, 147.8, 134.9, 134.5, 129.5, 128.8, 127.4, 122.9, 120.3, 119.0, 118.8, 118.2, 57.6; HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{15}H_{12}ClN_2O^+$: 271.0633; found: 271.0631.

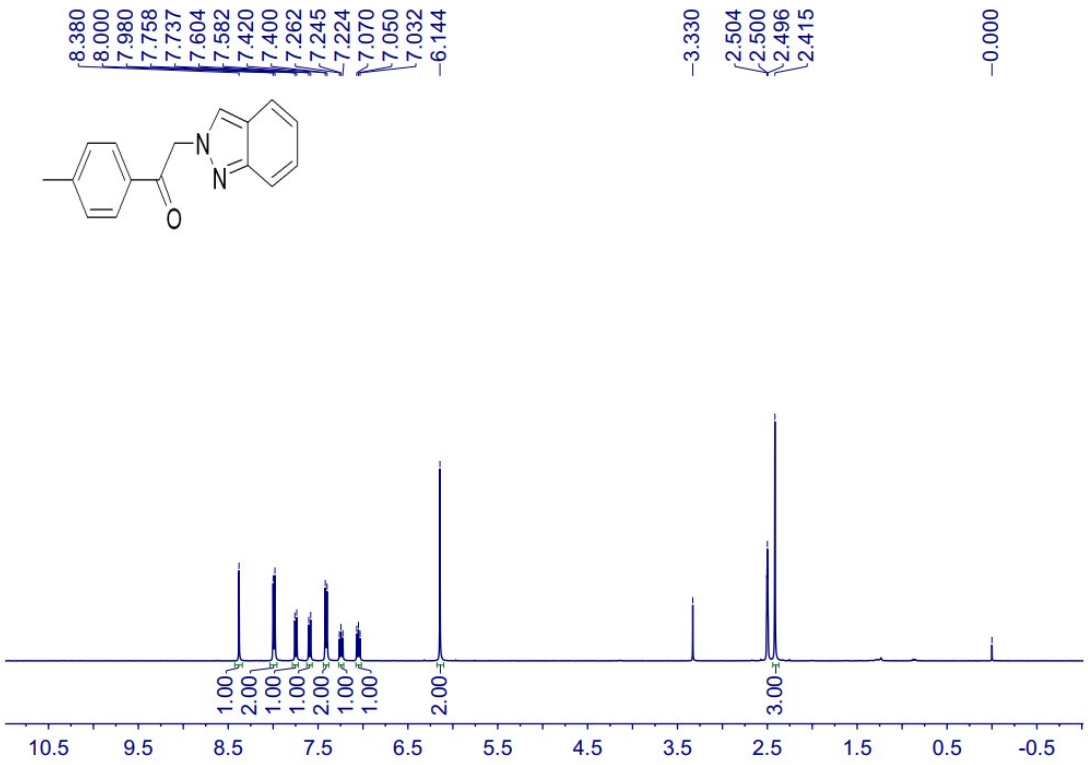
5. NMR Spectra of Compounds



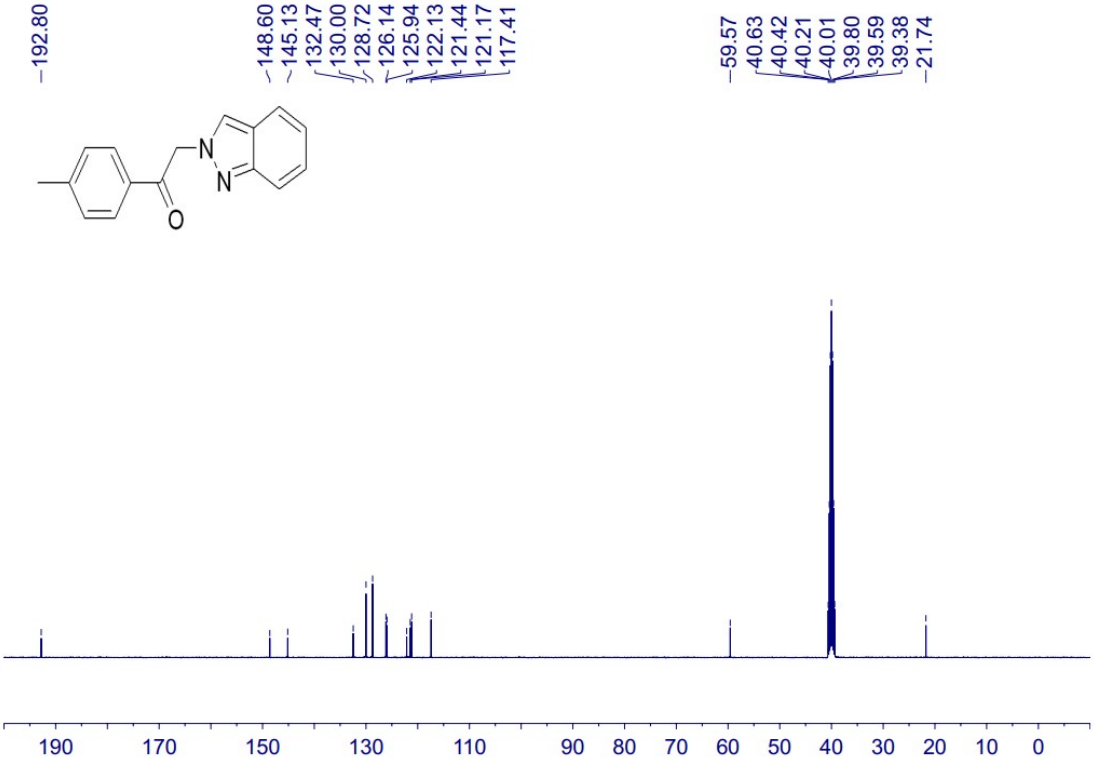
^{1}H NMR Spectrum of Compound **3a** (400 MHz, DMSO-d_6).



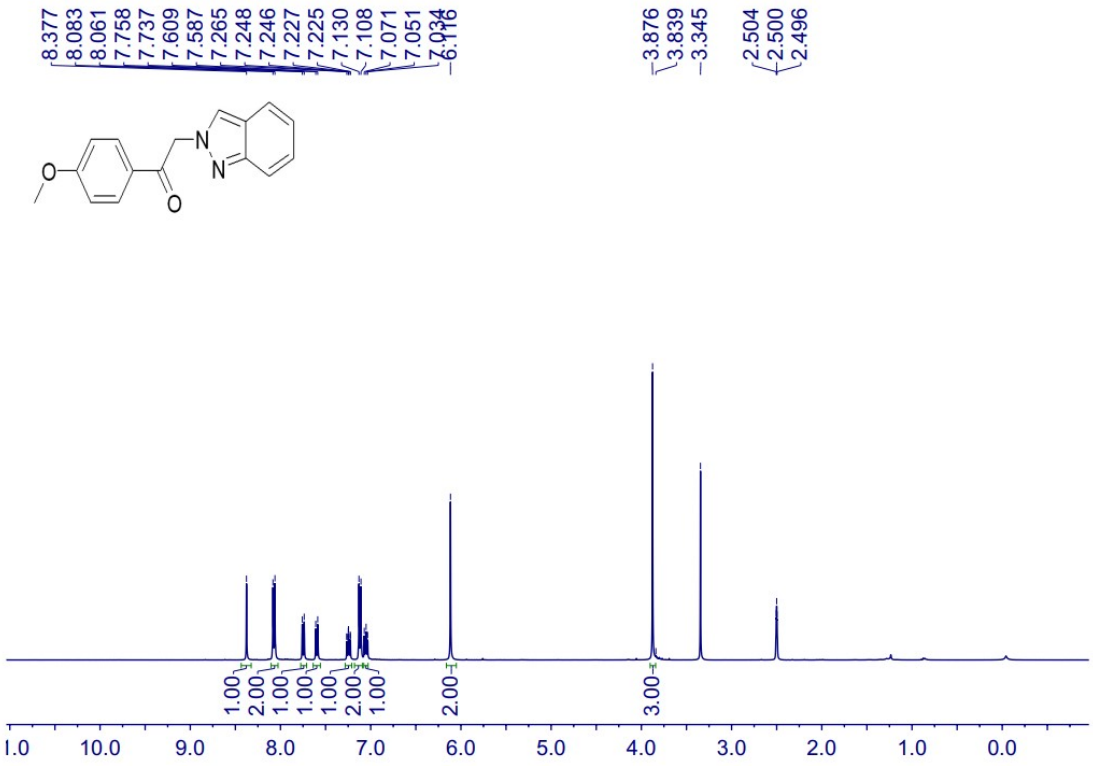
^{13}C NMR Spectrum of Compound **3a** (100 MHz, DMSO-d_6).



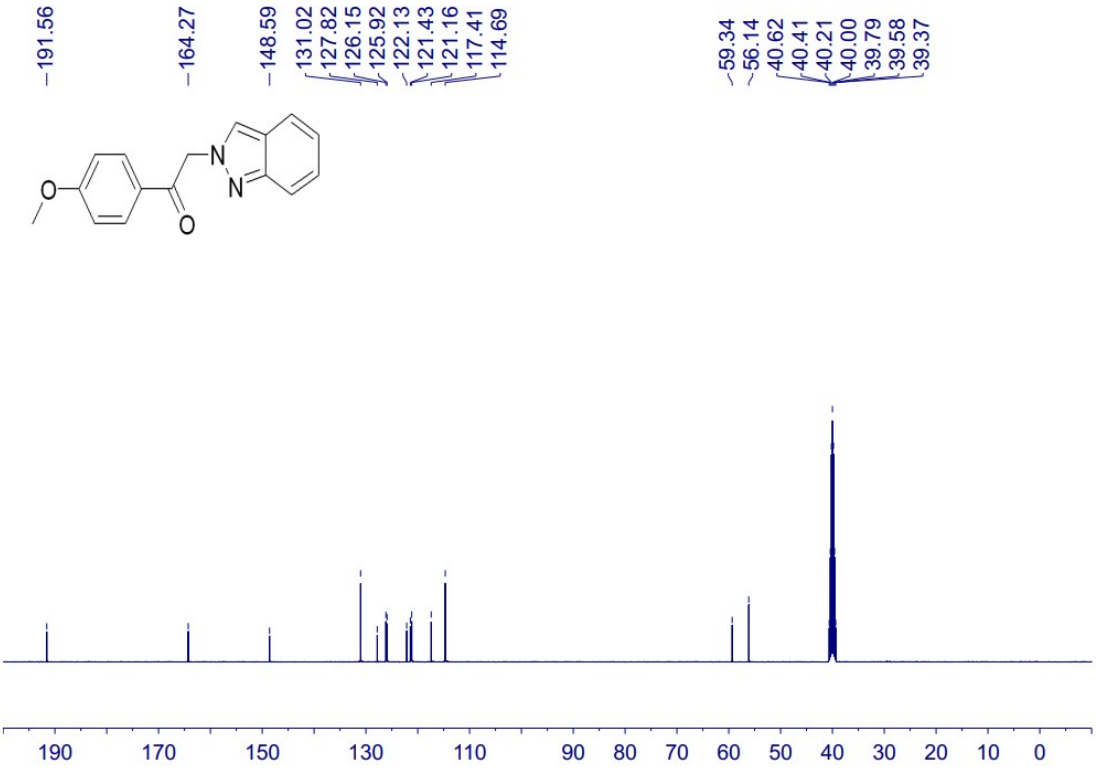
^{1}H NMR Spectrum of Compound **3b** (400 MHz, DMSO-d_6)



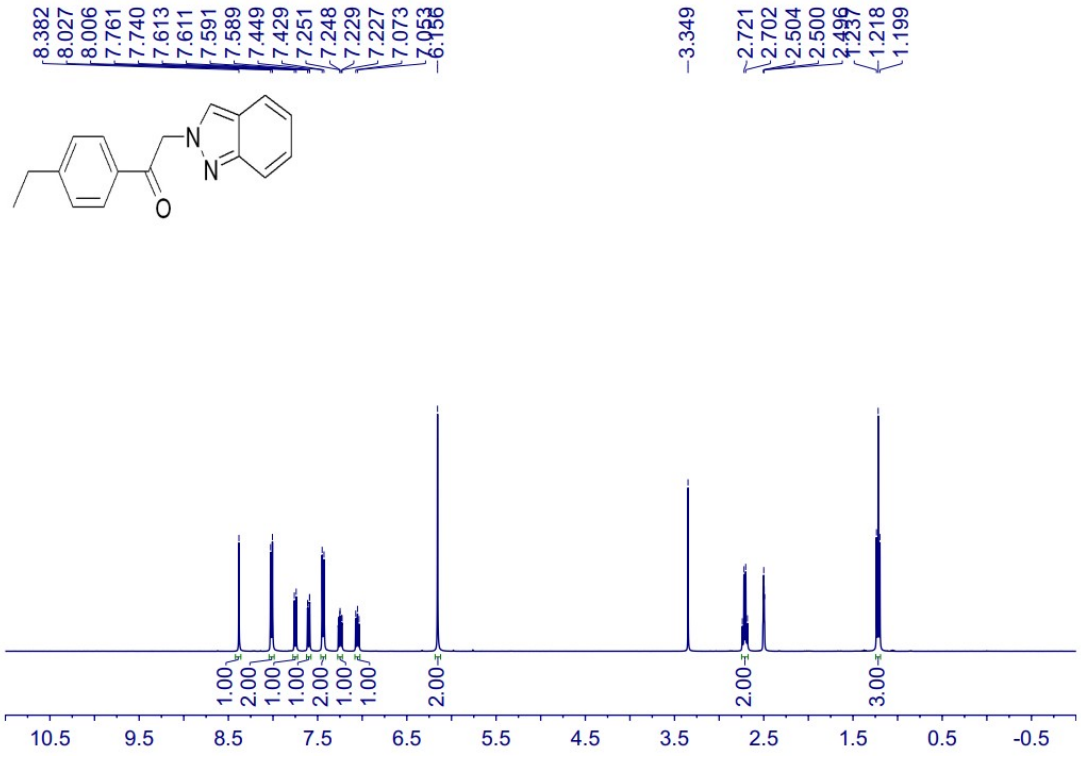
^{13}C NMR Spectrum of Compound **3b** (100 MHz, DMSO-d_6)



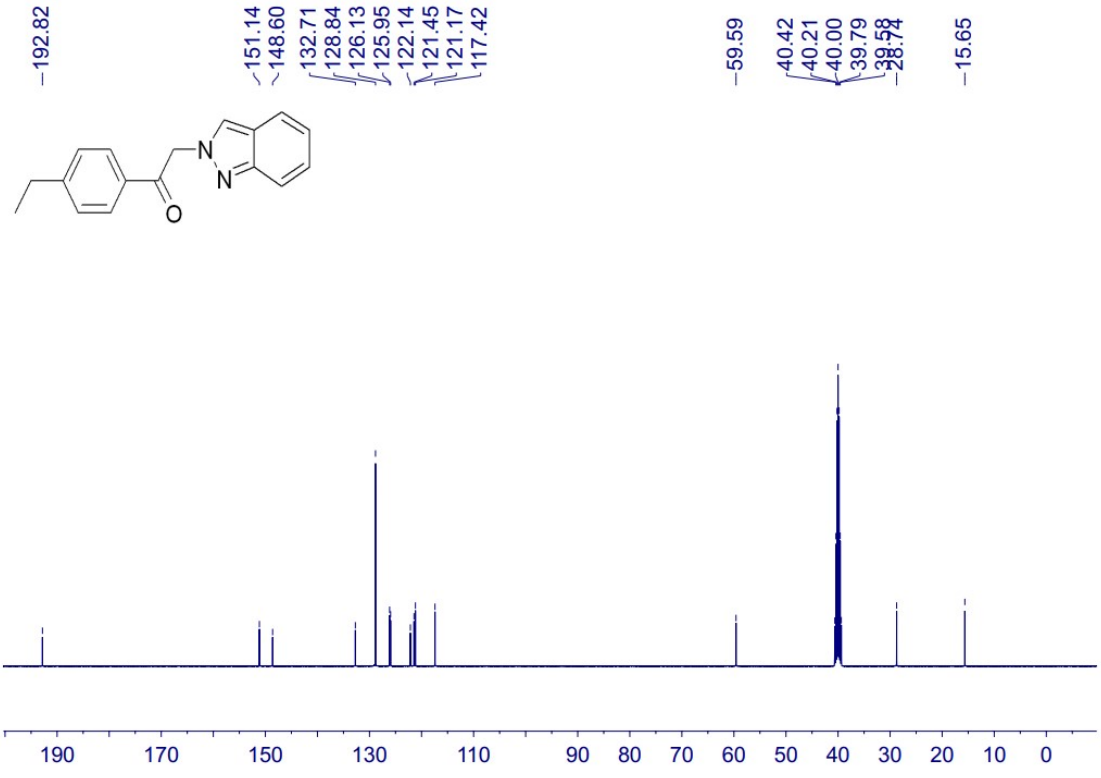
^{1}H NMR Spectrum of Compound **3c** (400 MHz, DMSO-d_6)



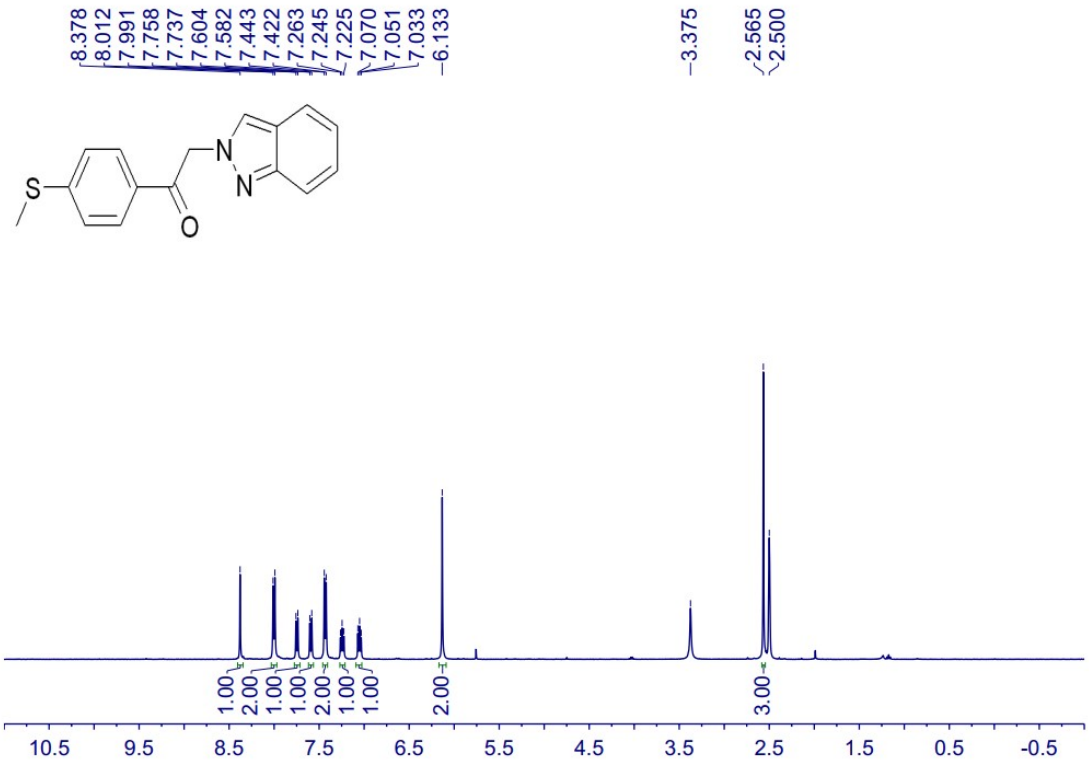
^{13}C NMR Spectrum of Compound **3c** (100 MHz, DMSO-d_6)



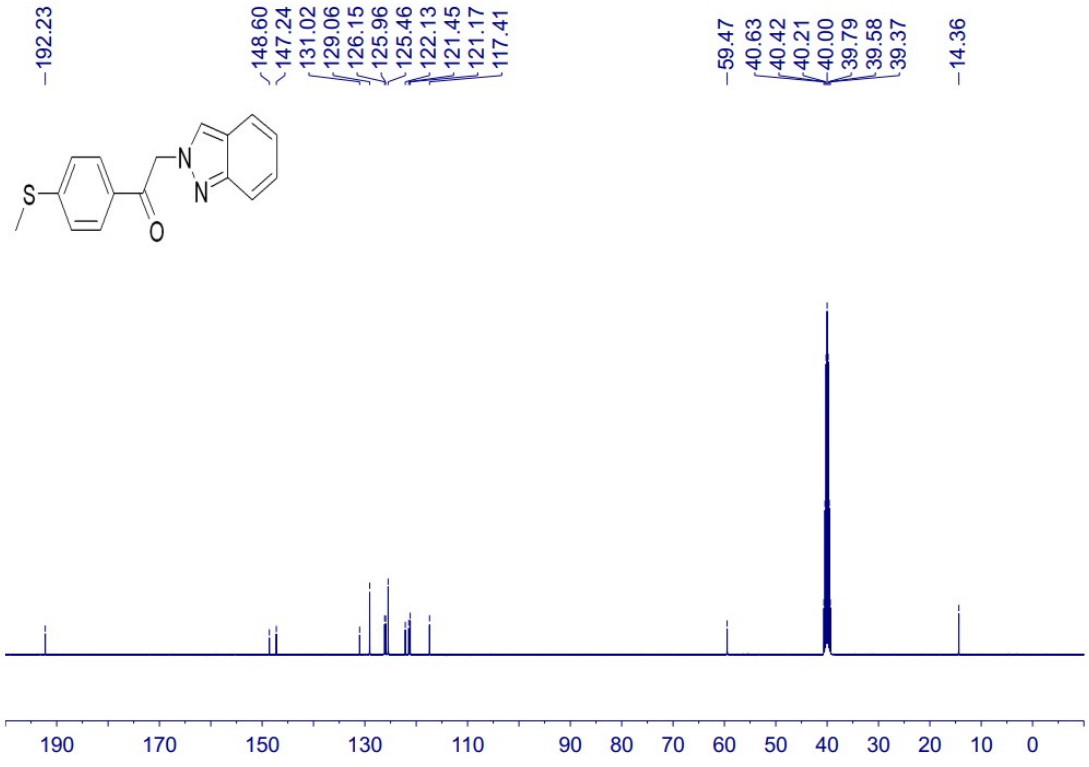
^{1}H NMR Spectrum of Compound **3d** (400 MHz, DMSO-d_6)



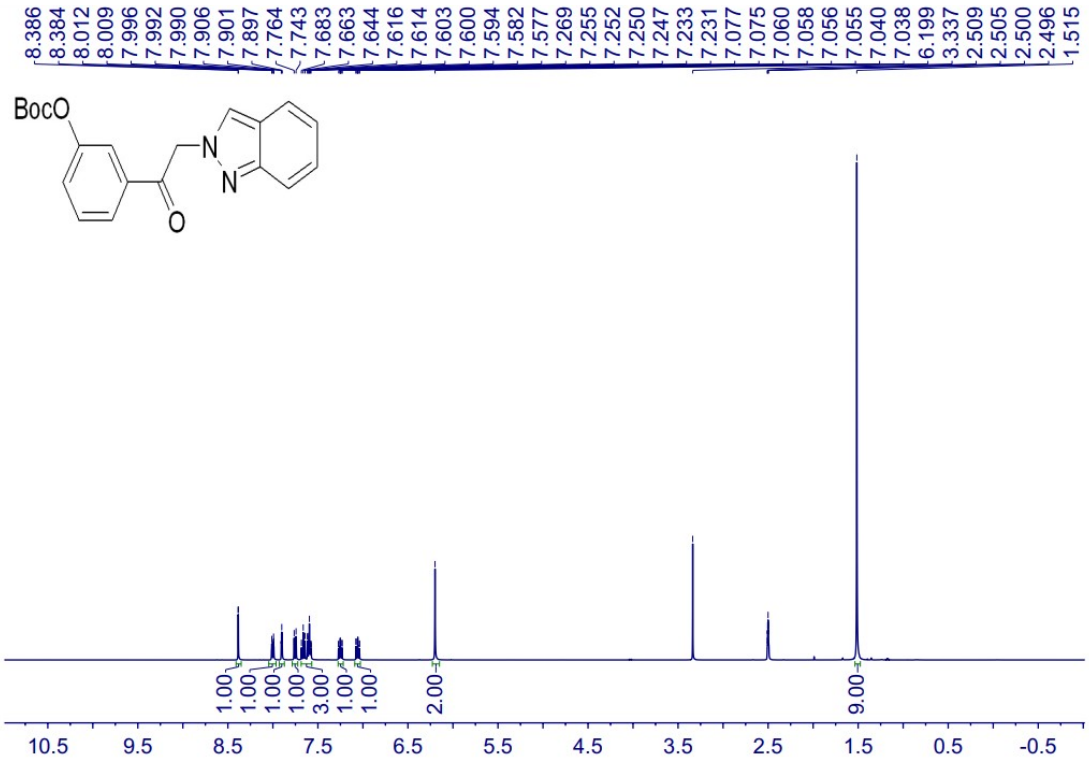
^{13}C NMR Spectrum of Compound **3d** (100 MHz, DMSO-d_6)



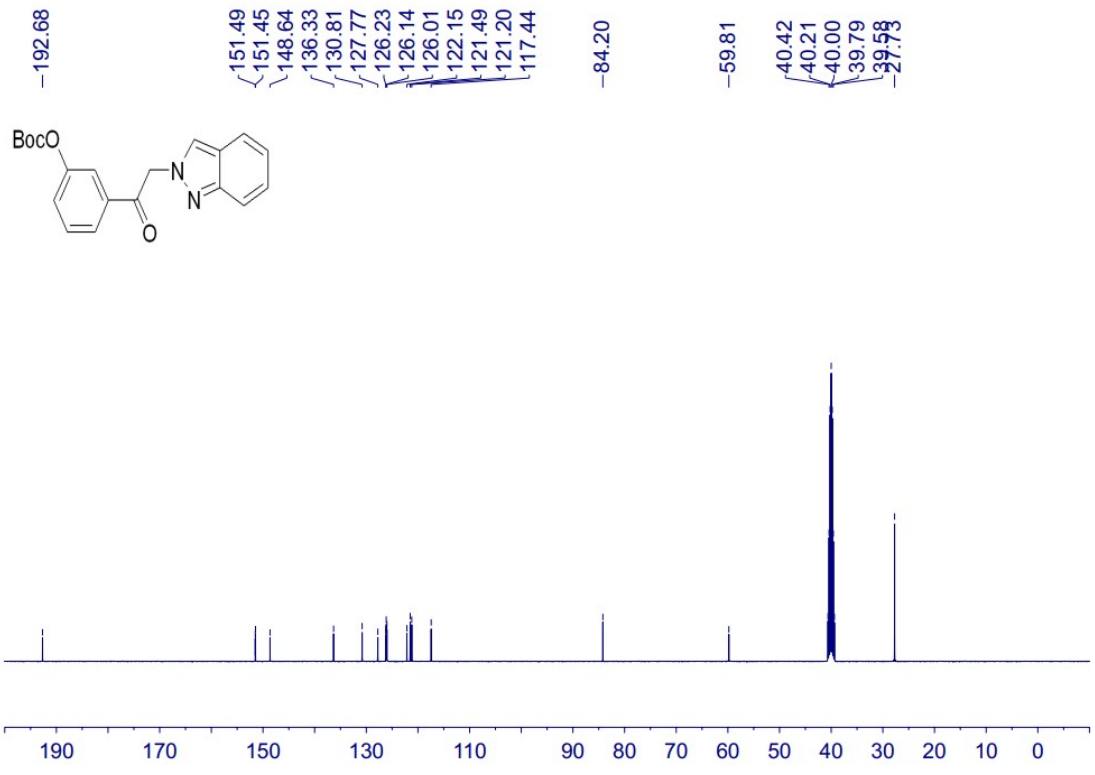
^{1}H NMR Spectrum of Compound **3e** (400 MHz, DMSO-d_6)



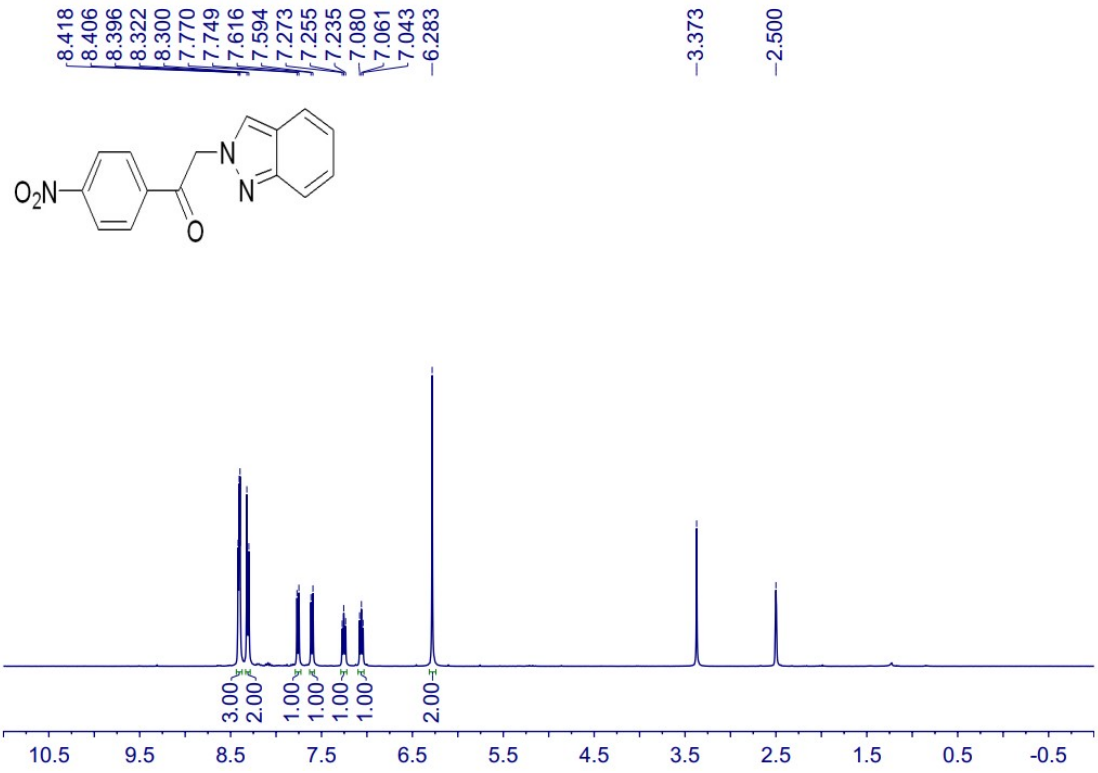
^{13}C NMR Spectrum of Compound **3e** (100 MHz, DMSO-d_6)



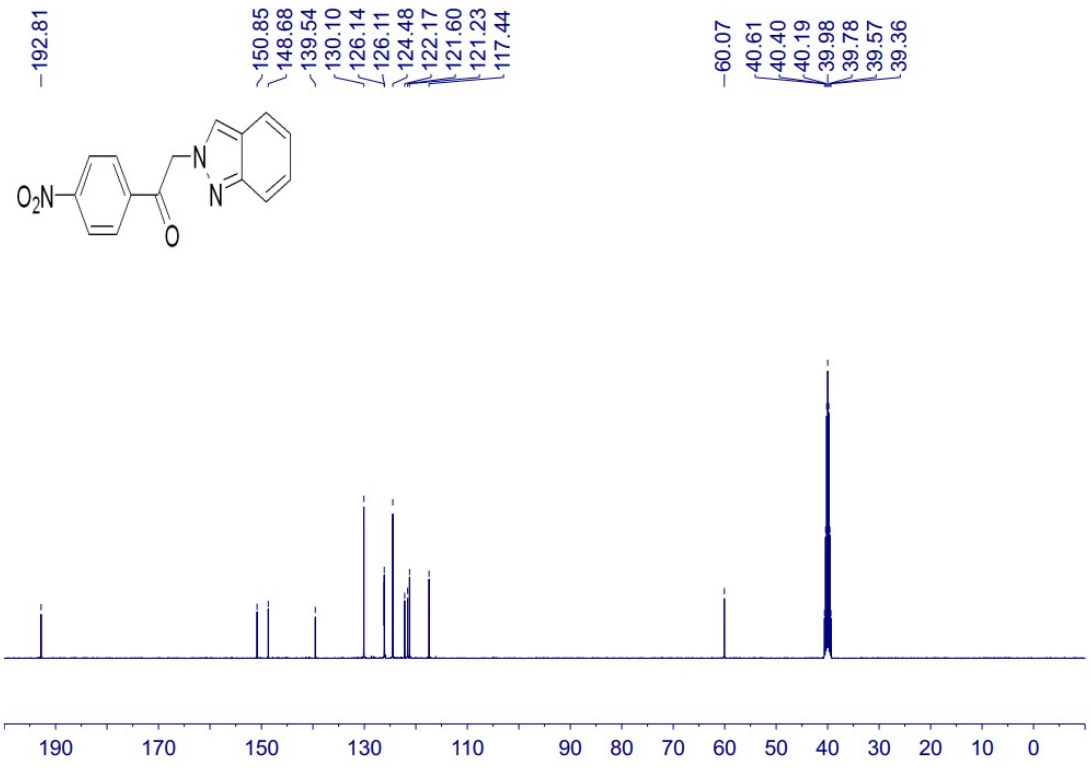
^{1}H NMR Spectrum of Compound **3f** (400 MHz, DMSO-d_6)



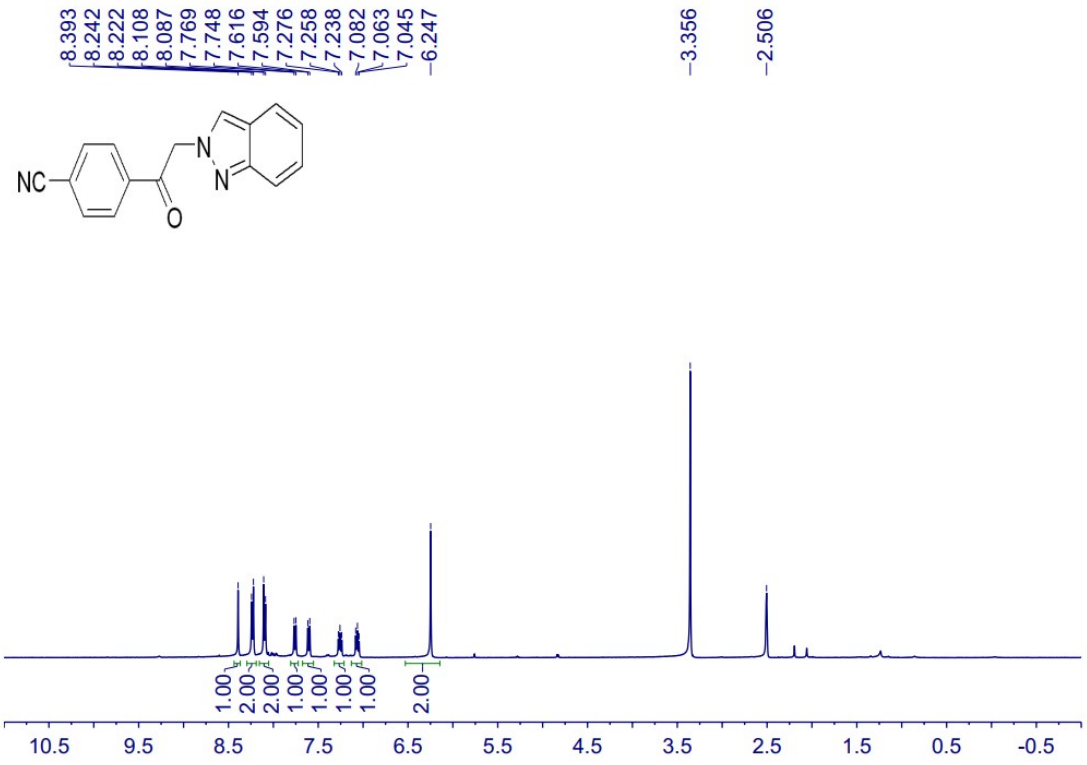
^{13}C NMR Spectrum of Compound **3f** (100 MHz, DMSO-d_6)



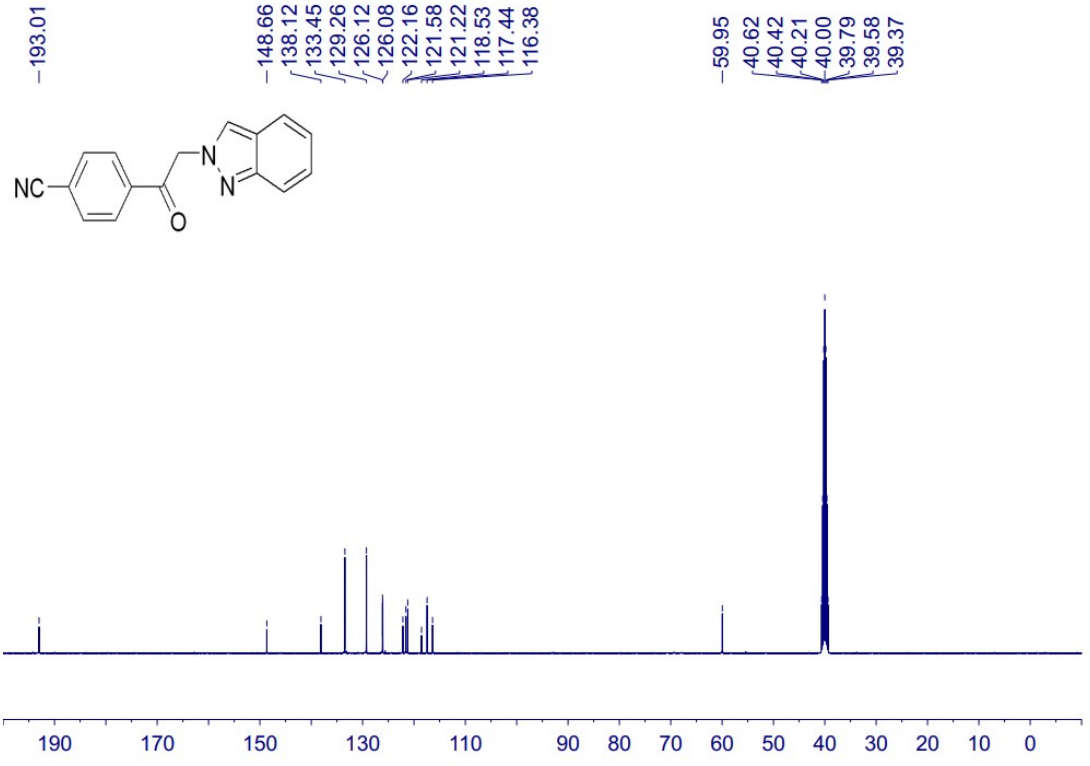
^{1}H NMR Spectrum of Compound **3g** (400 MHz, DMSO-d_6)



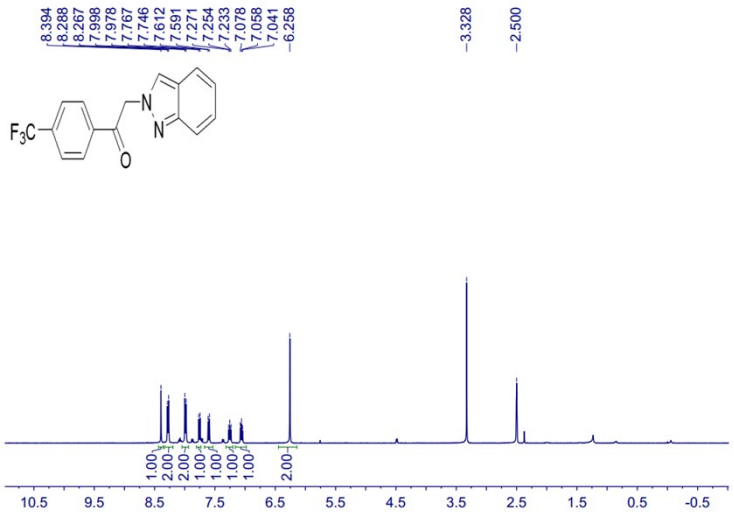
^{13}C NMR Spectrum of Compound **3g** (100 MHz, DMSO-d_6)



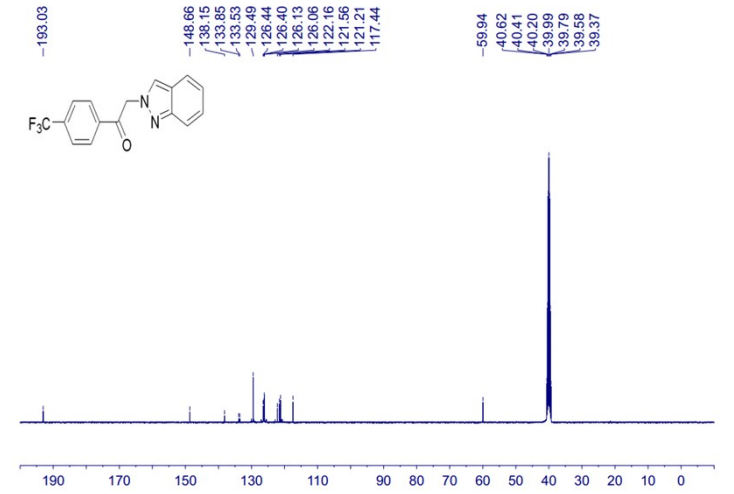
^{1}H NMR Spectrum of Compound **3h** (400 MHz, DMSO-d_6)



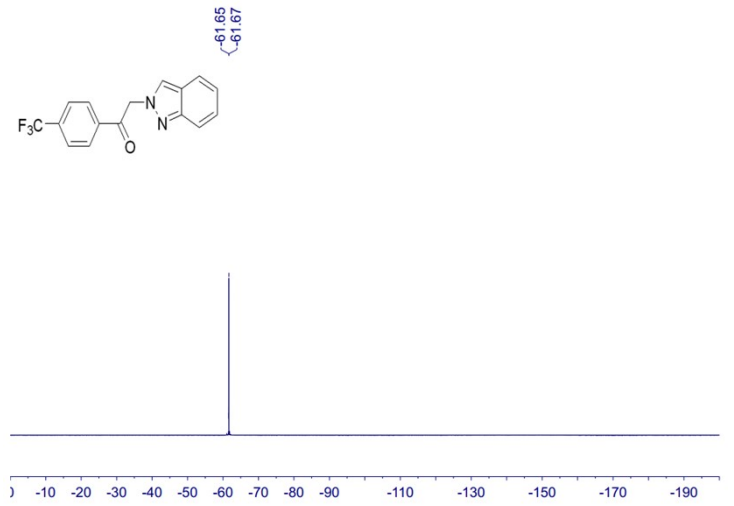
^{13}C NMR Spectrum of Compound **3h** (100 MHz, DMSO-d_6)



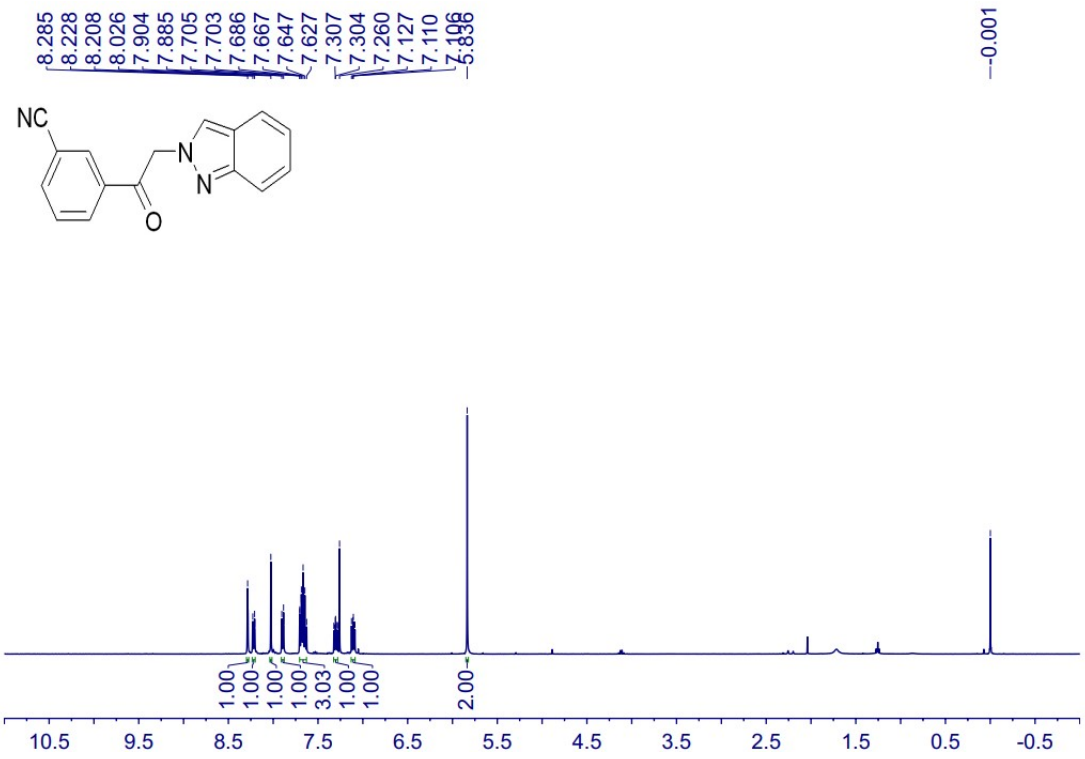
^{1}H NMR Spectrum of Compound **3i** (400 MHz, DMSO-d_6)



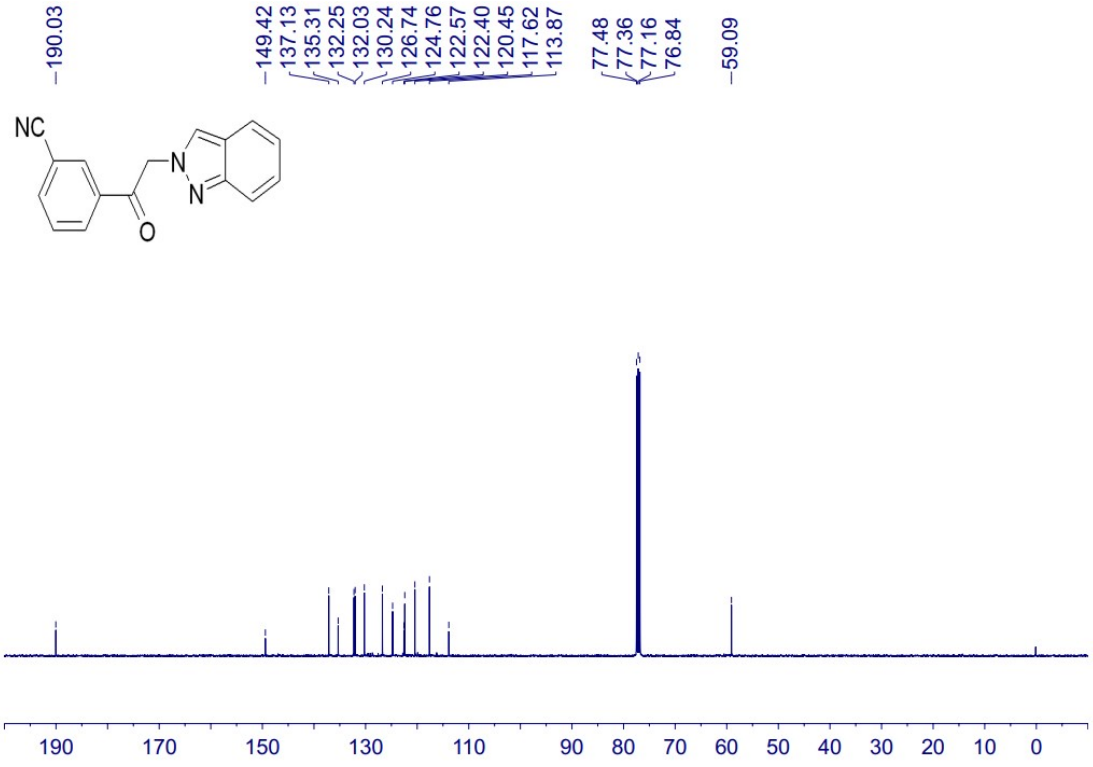
^{13}C NMR Spectrum of Compound **3i** (100 MHz, DMSO-d_6)



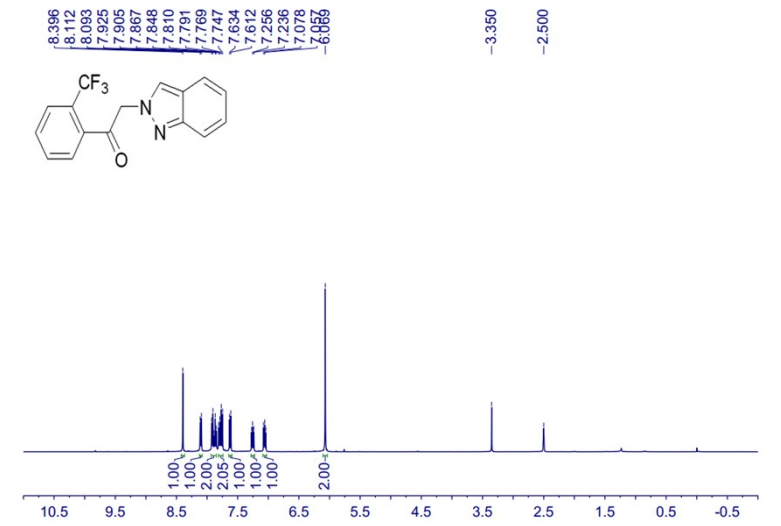
^{19}F NMR Spectrum of Compound **3i** (376 MHz, DMSO-d_6)



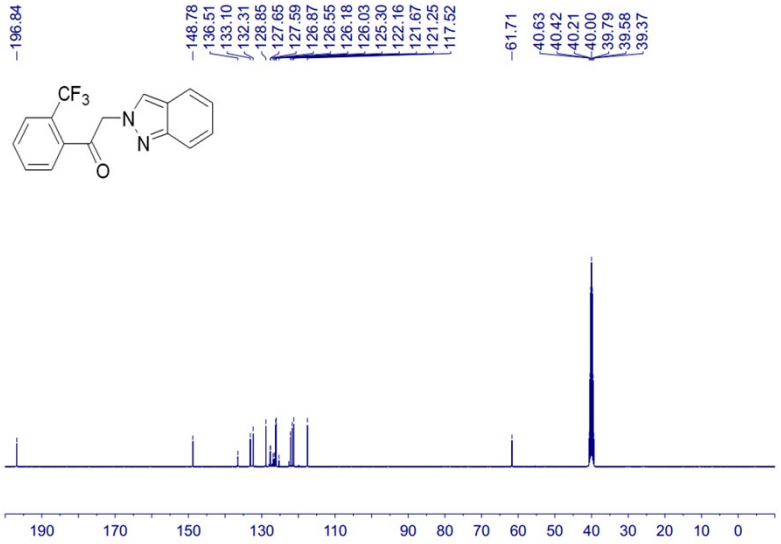
^{1}H NMR Spectrum of Compound **3j** (400 MHz, $CDCl_3$)



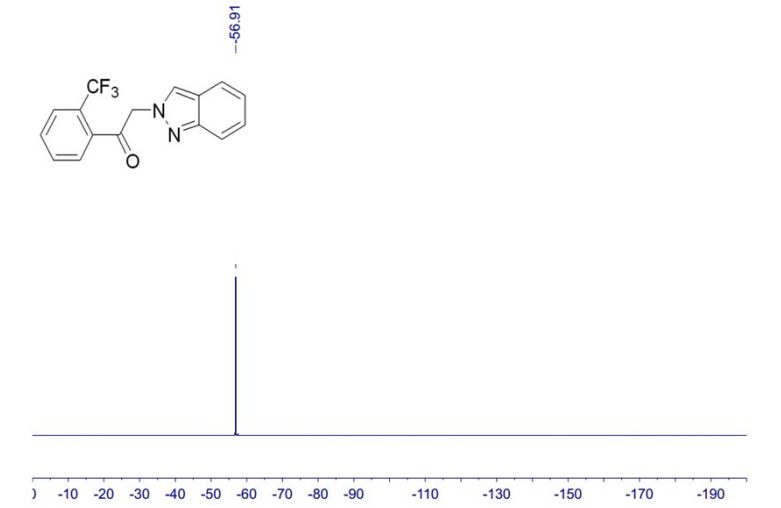
^{13}C NMR Spectrum of Compound **3j** (100 MHz, $CDCl_3$)



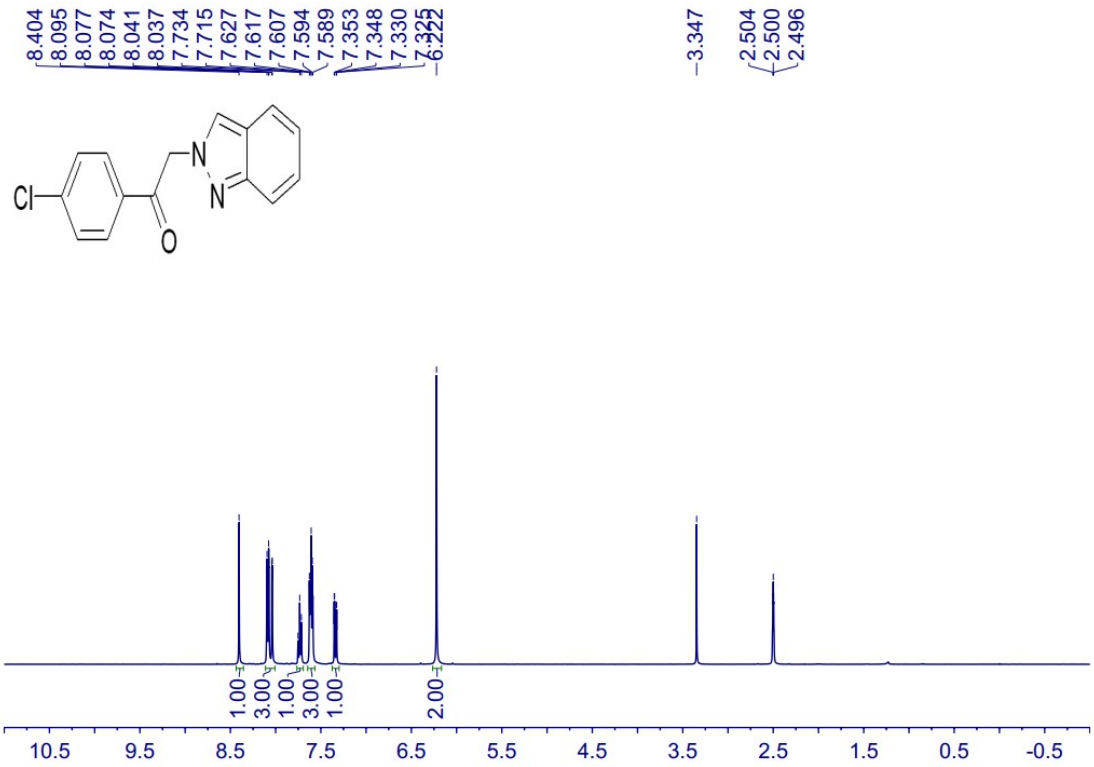
^{1}H NMR Spectrum of Compound **3k** (400 MHz, DMSO-d_6)



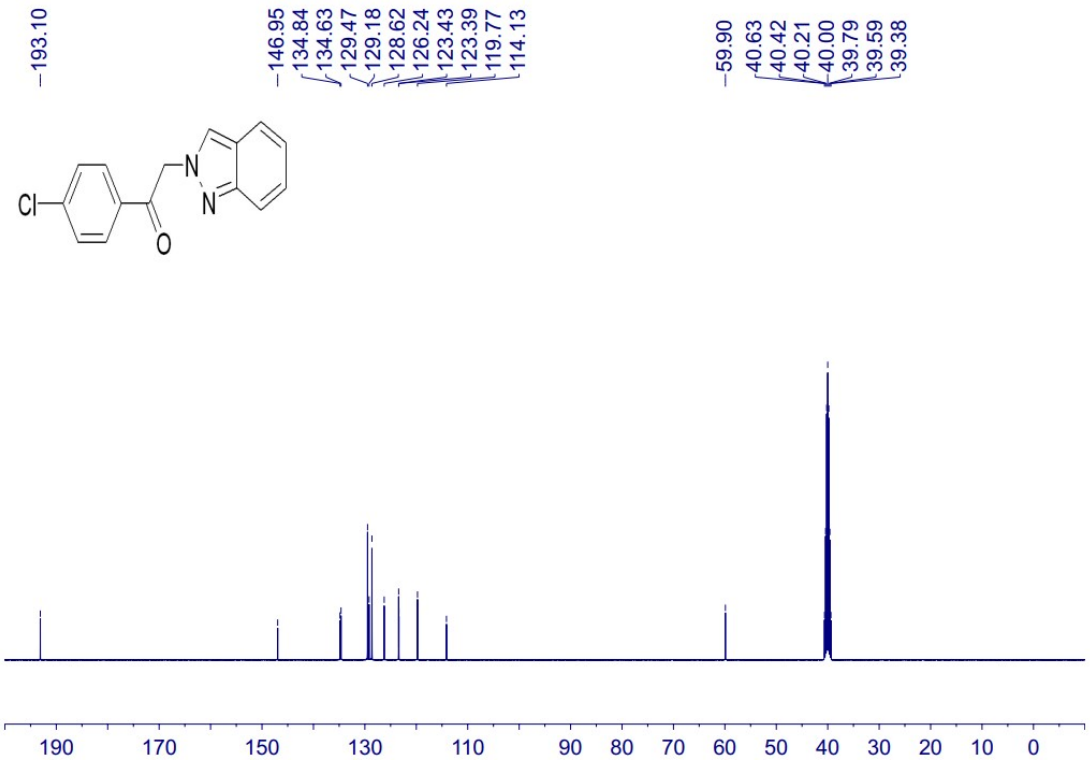
^{13}C NMR Spectrum of Compound **3k** (100 MHz, DMSO-d_6)



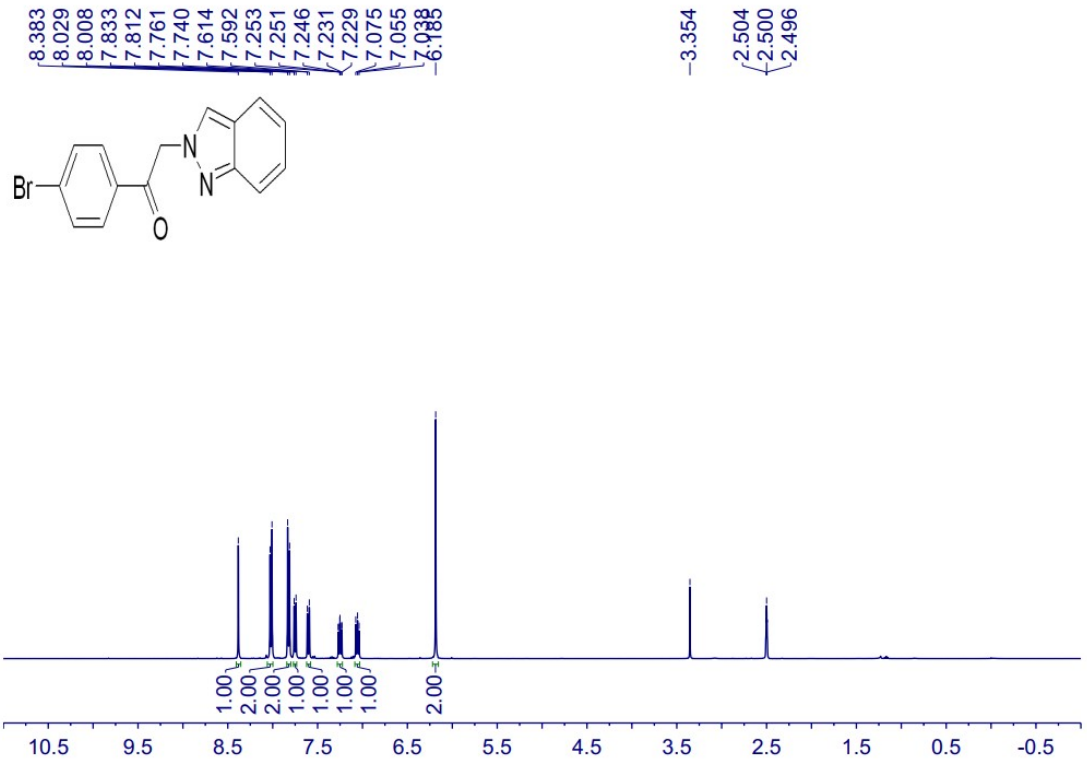
^{19}F NMR Spectrum of Compound **3k** (376 MHz, DMSO-d_6)



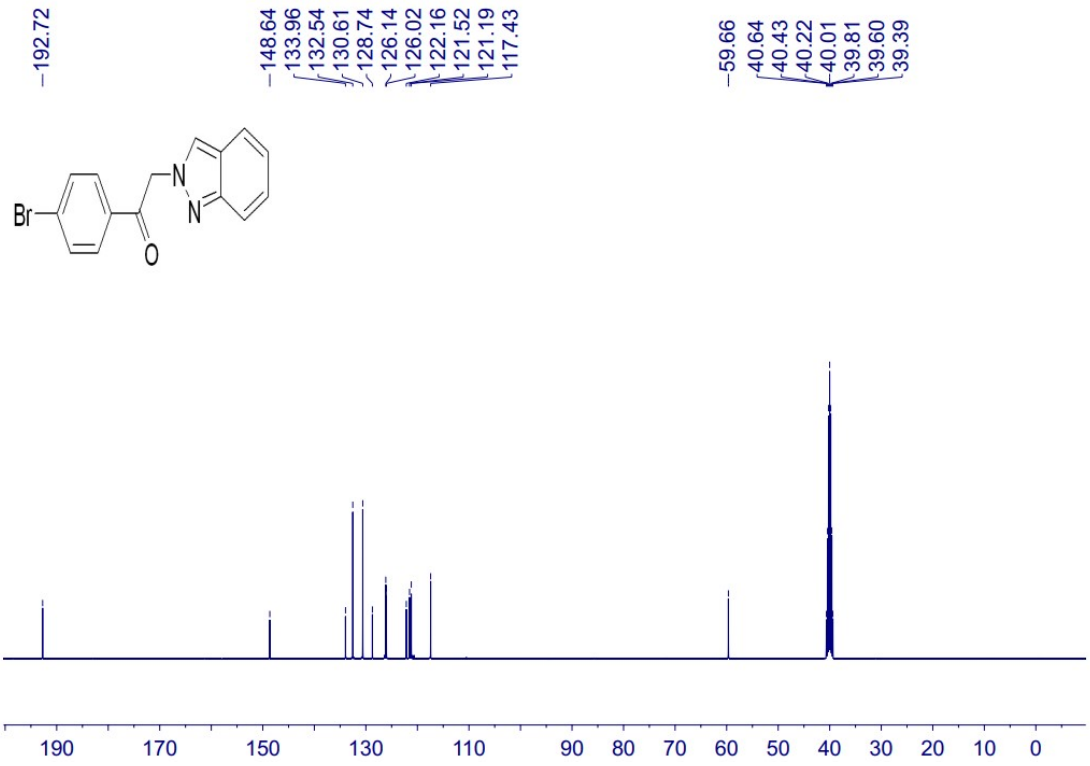
^{1}H NMR Spectrum of Compound **3l** (400 MHz, DMSO-d_6)



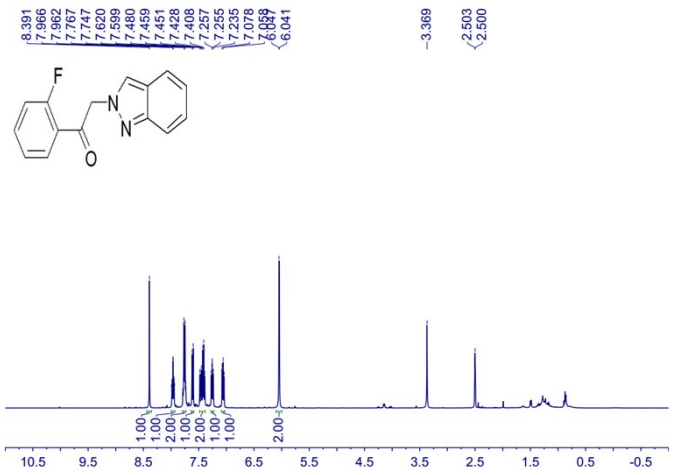
^{13}C NMR Spectrum of Compound **3l** (100 MHz, DMSO-d_6)



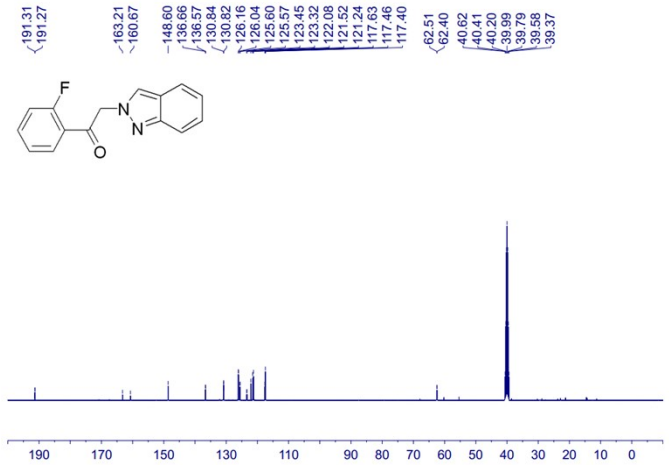
^{1}H NMR Spectrum of Compound **3m** (400 MHz, DMSO-d_6)



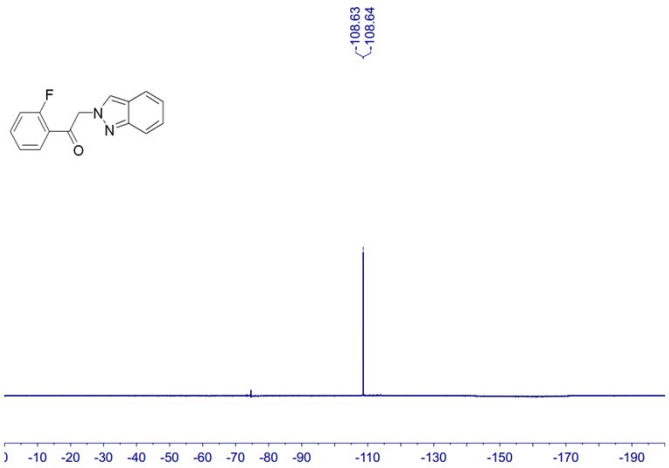
^{13}C NMR Spectrum of Compound **3m** (100 MHz, DMSO-d_6)



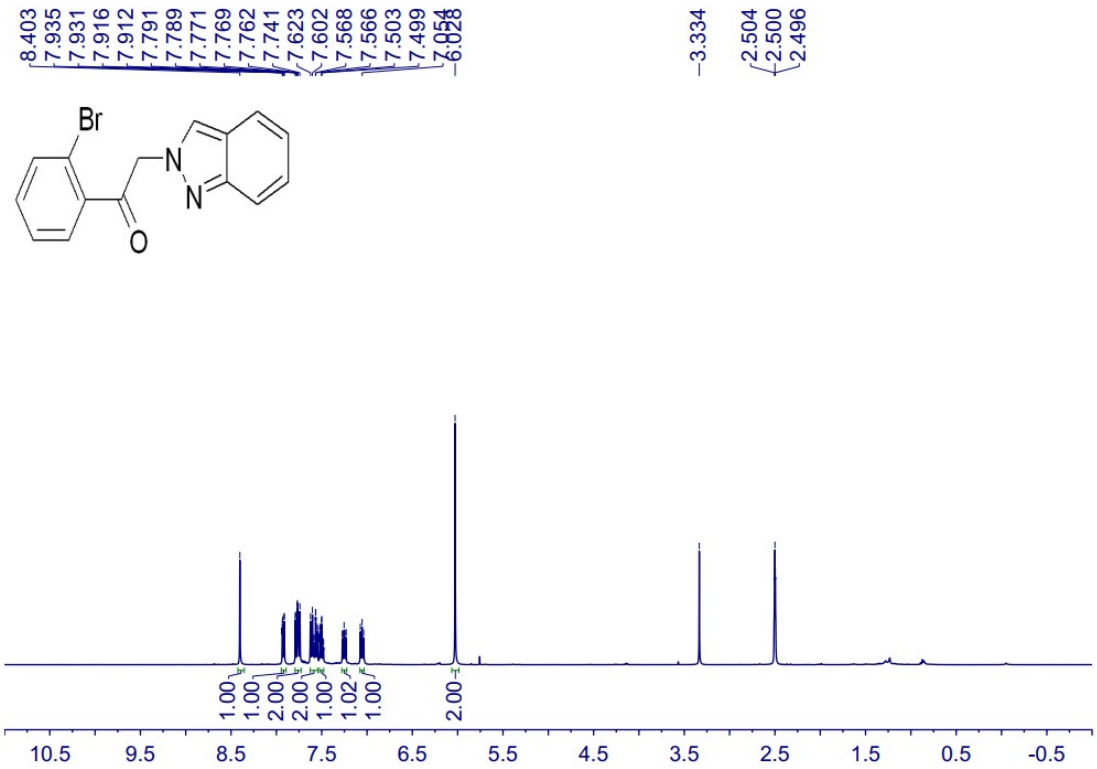
^{1}H NMR Spectrum of Compound **3n** (400 MHz, DMSO-d_6)



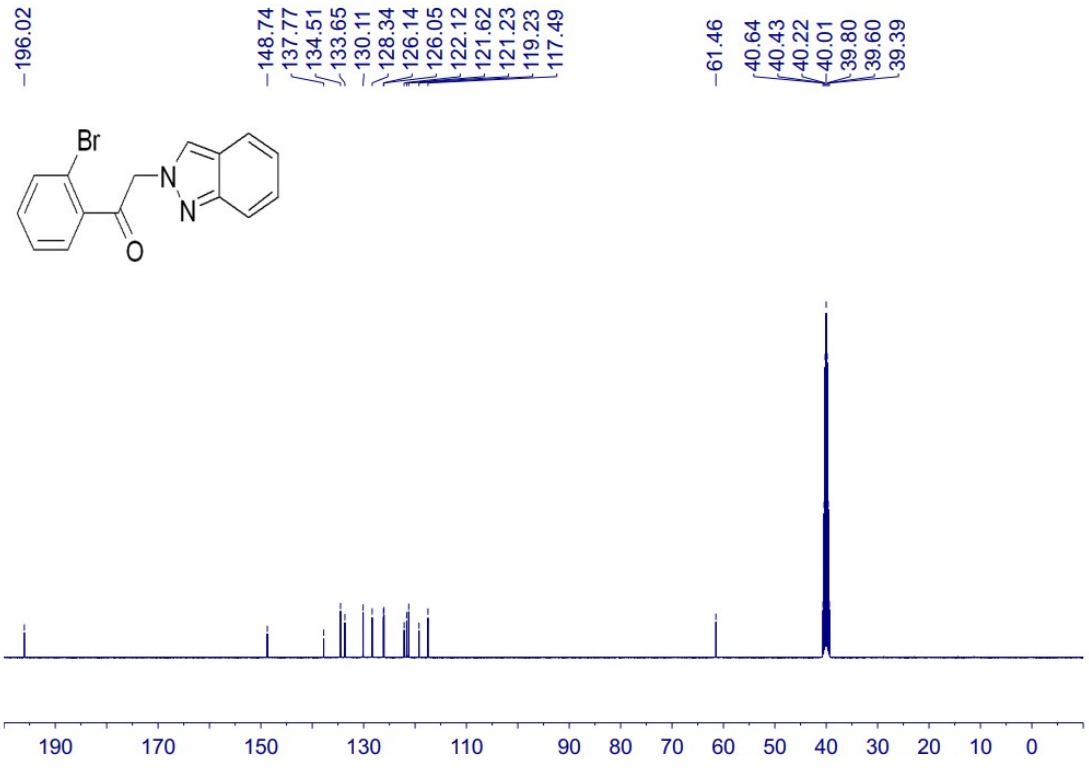
^{13}C NMR Spectrum of Compound **3n** (100 MHz, DMSO-d_6)



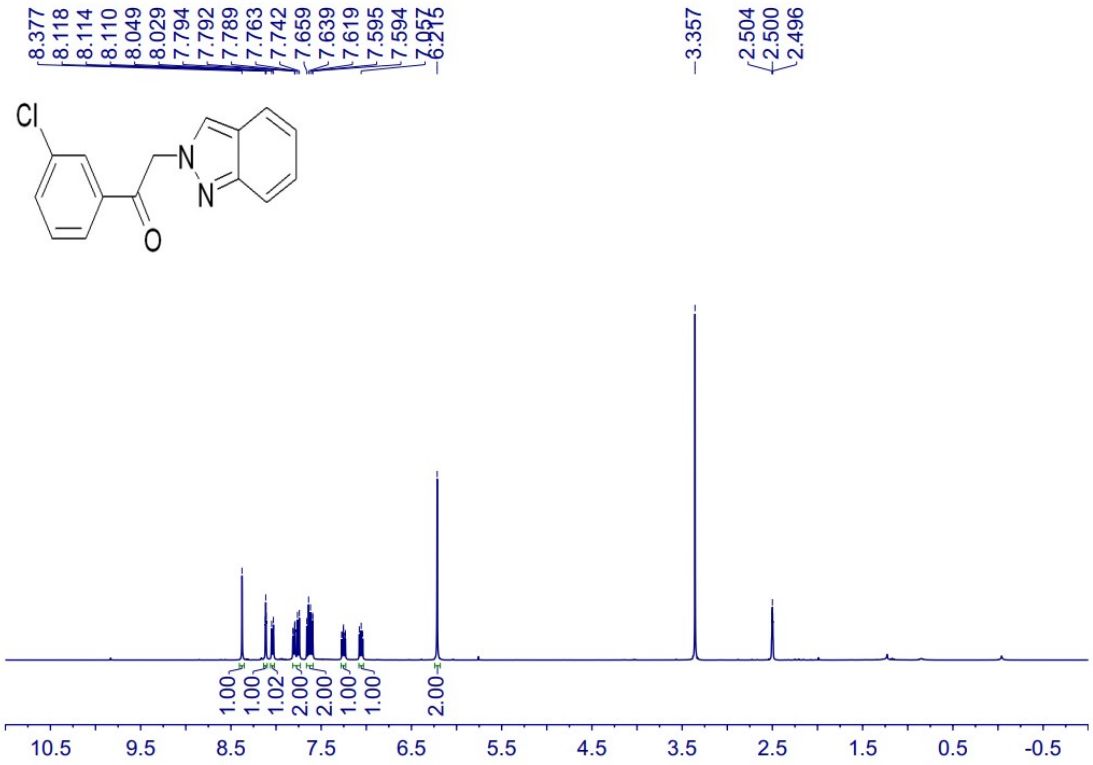
^{19}F NMR Spectrum of Compound **3n** (376 MHz, DMSO-d_6)



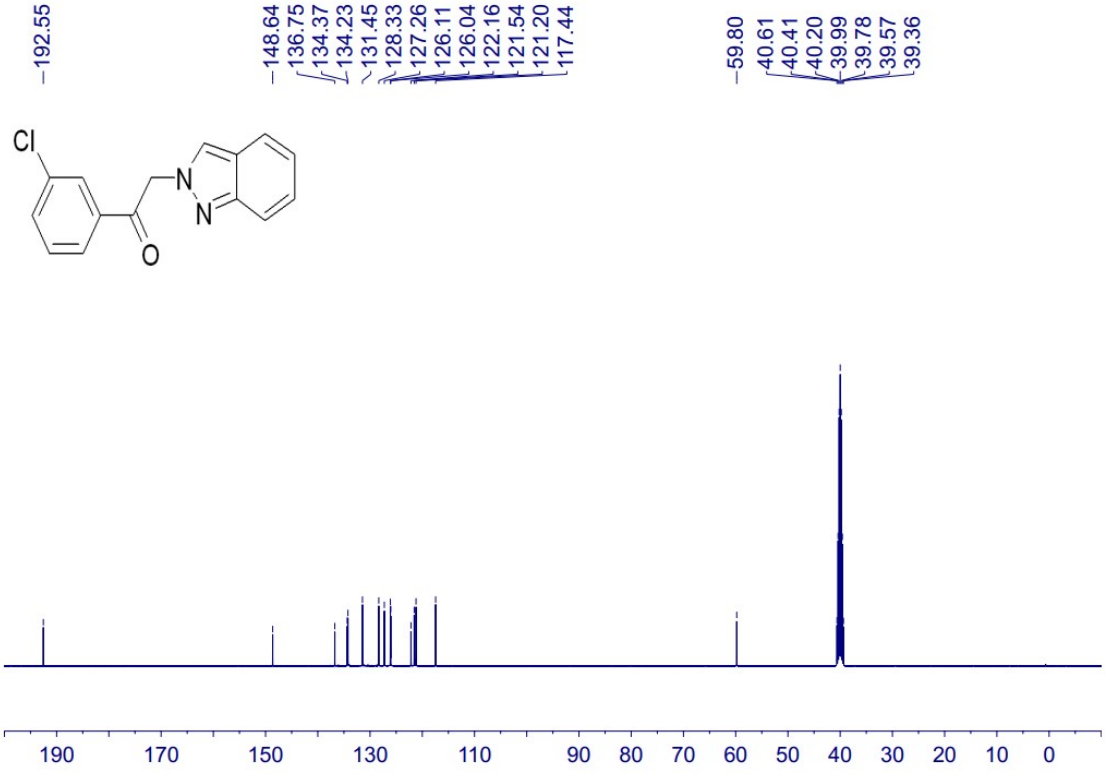
^{1}H NMR Spectrum of Compound **3o** (400 MHz, DMSO-d_6)



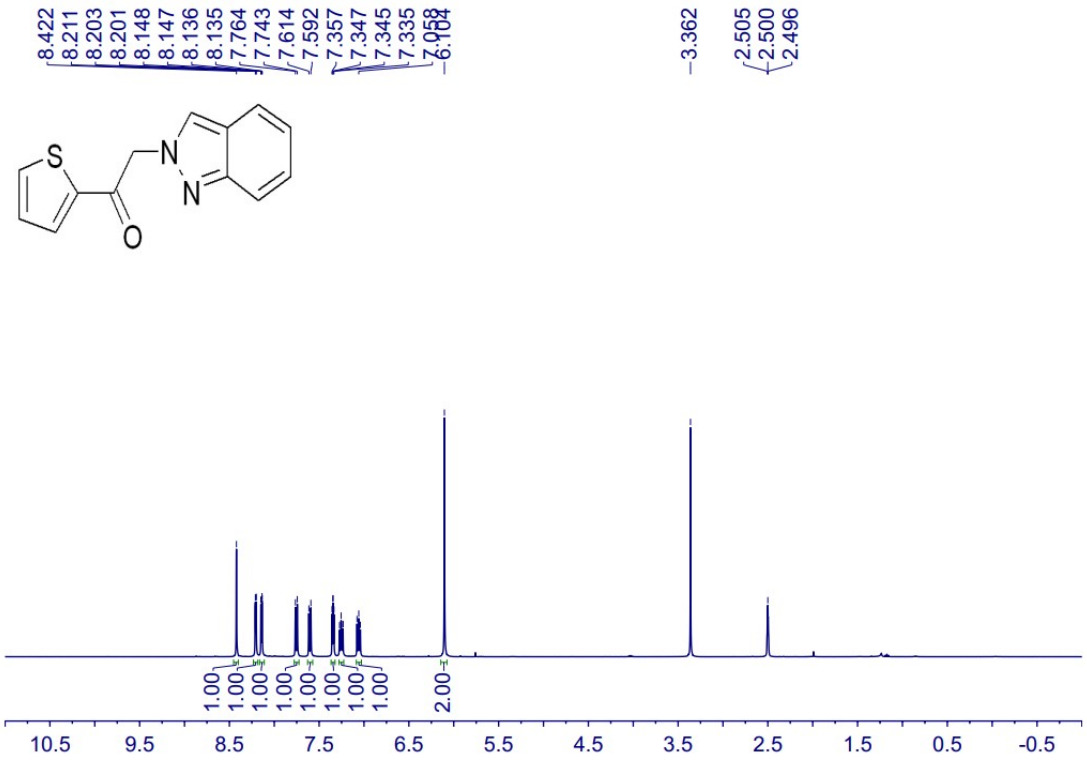
^{13}C NMR Spectrum of Compound **3o** (100 MHz, DMSO-d_6)



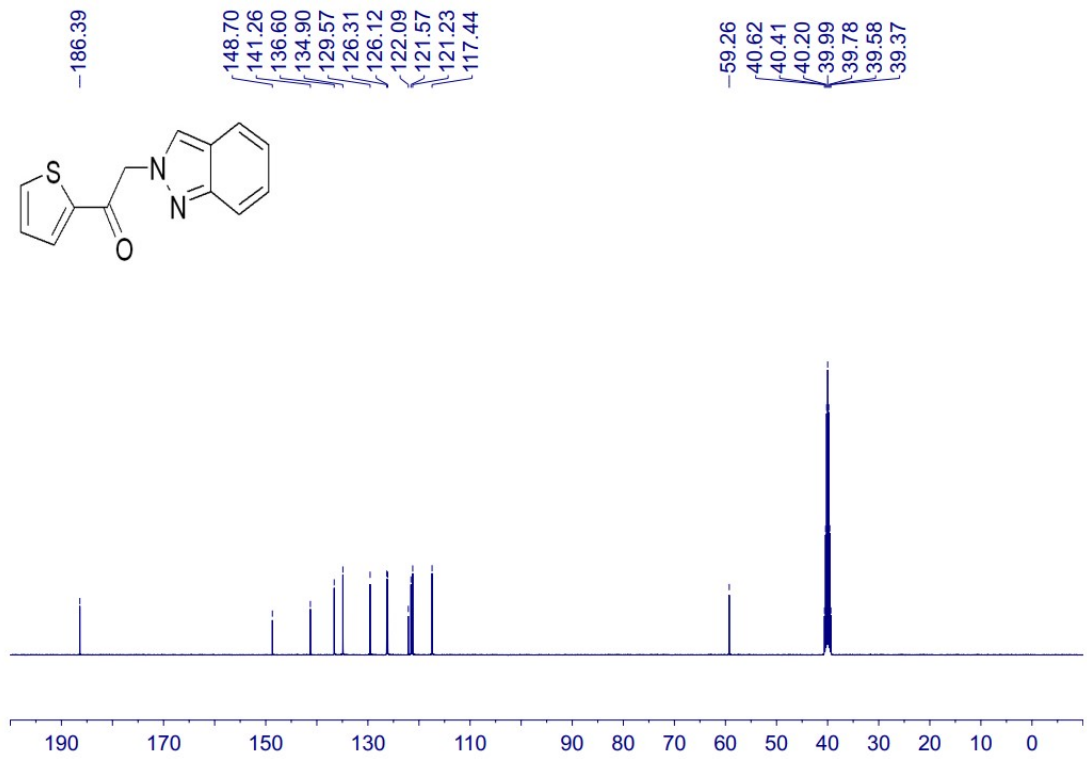
^{1}H NMR Spectrum of Compound **3p** (400 MHz, DMSO-d_6)



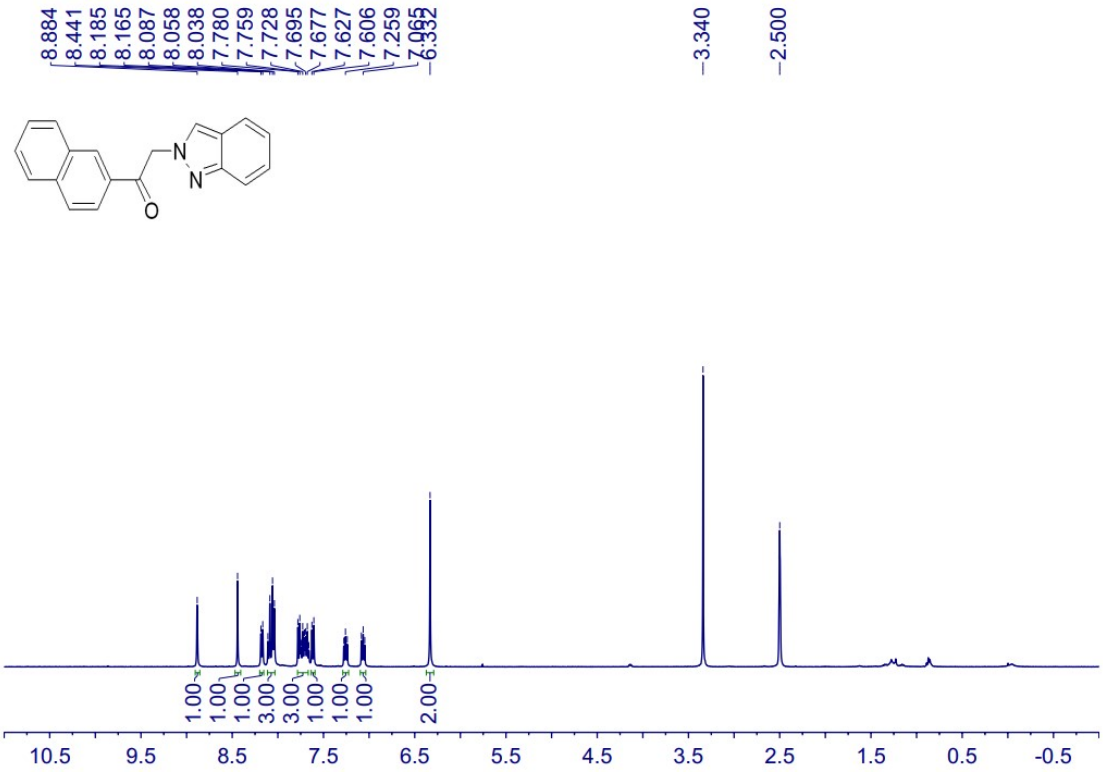
^{13}C NMR Spectrum of Compound **3p** (100 MHz, DMSO-d_6)



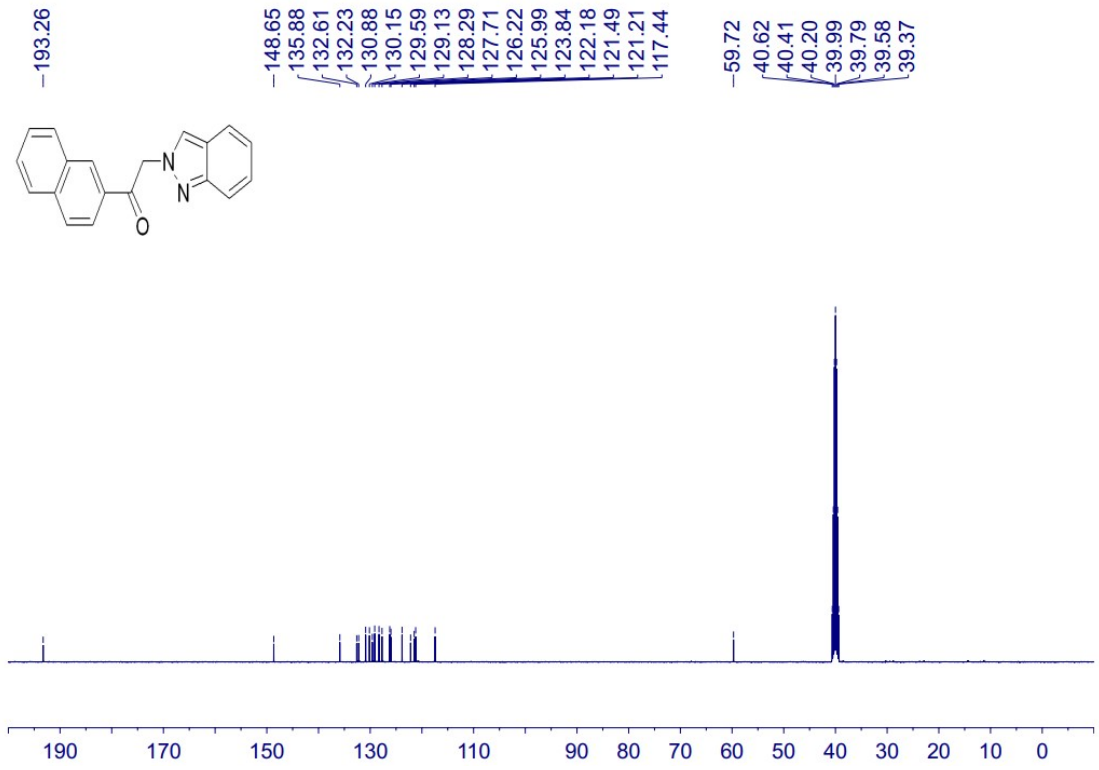
^{1}H NMR Spectrum of Compound **3q** (400 MHz, DMSO-d_6)



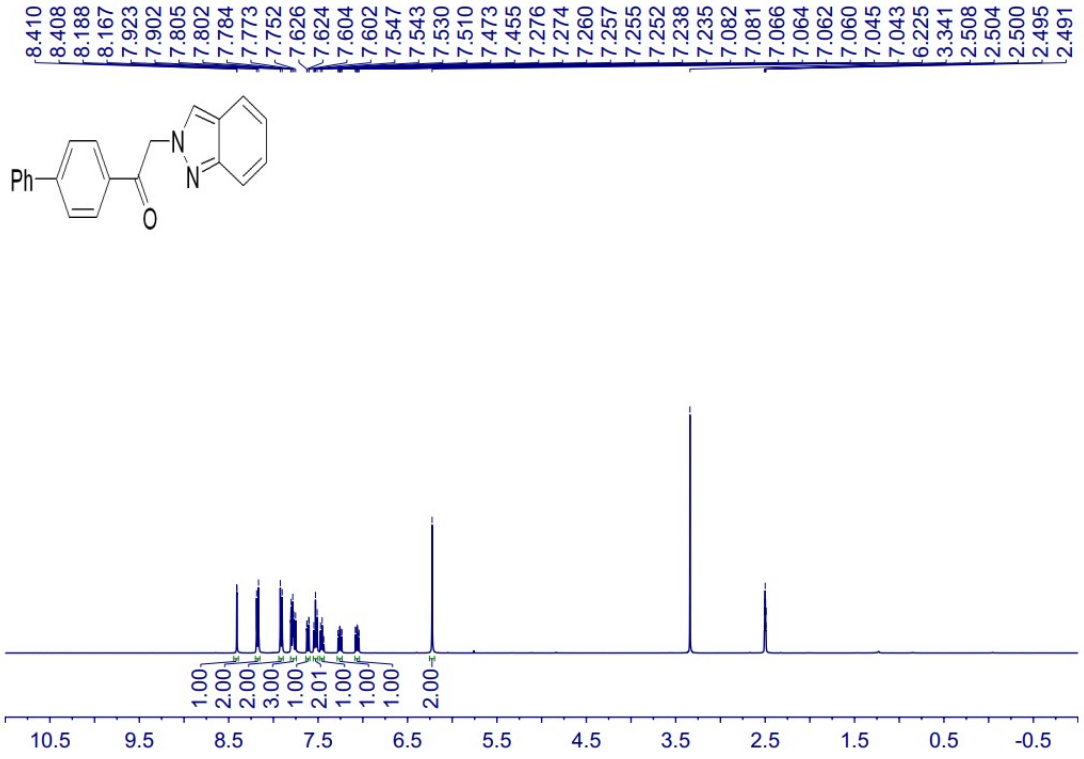
^{13}C NMR Spectrum of Compound **3q** (100 MHz, DMSO-d_6)



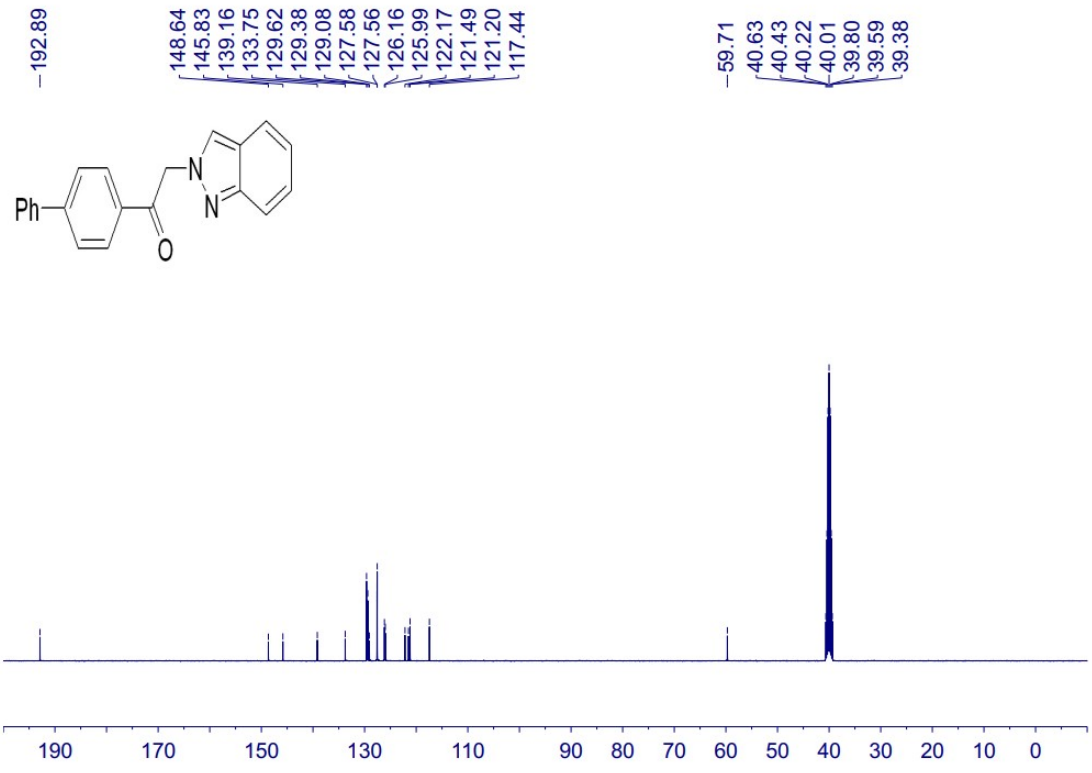
^{1}H NMR Spectrum of Compound **3r** (400 MHz, DMSO-d_6)



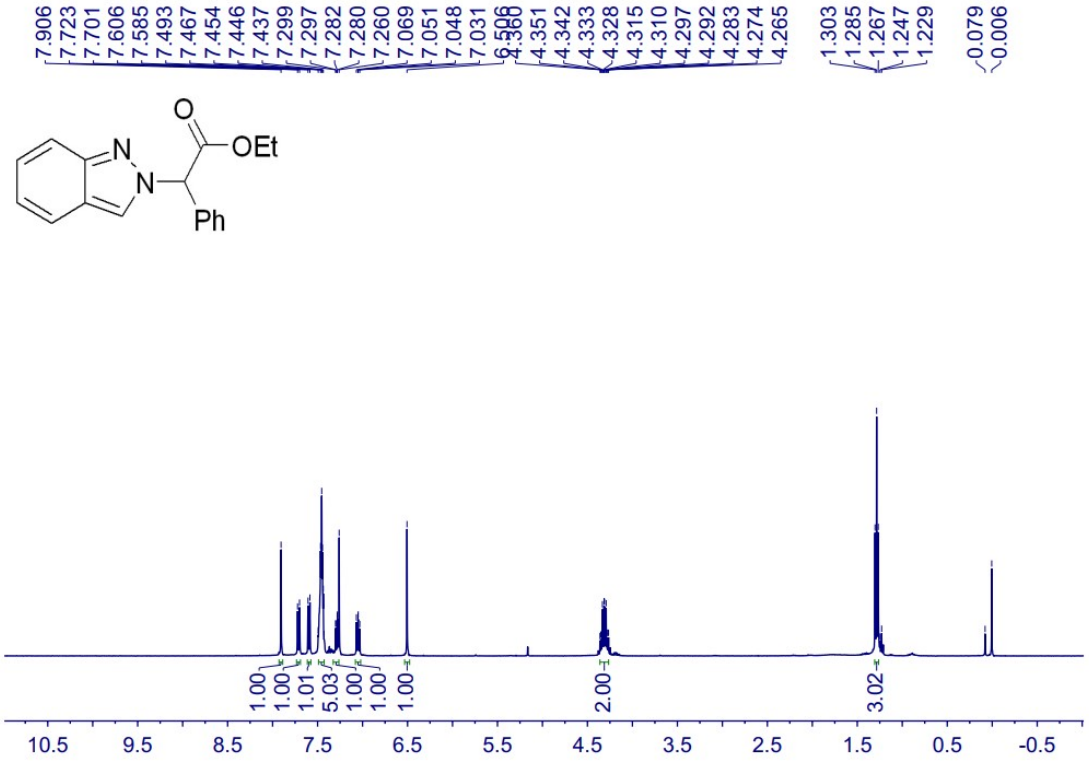
^{13}C NMR Spectrum of Compound **3r** (100 MHz, DMSO-d_6)



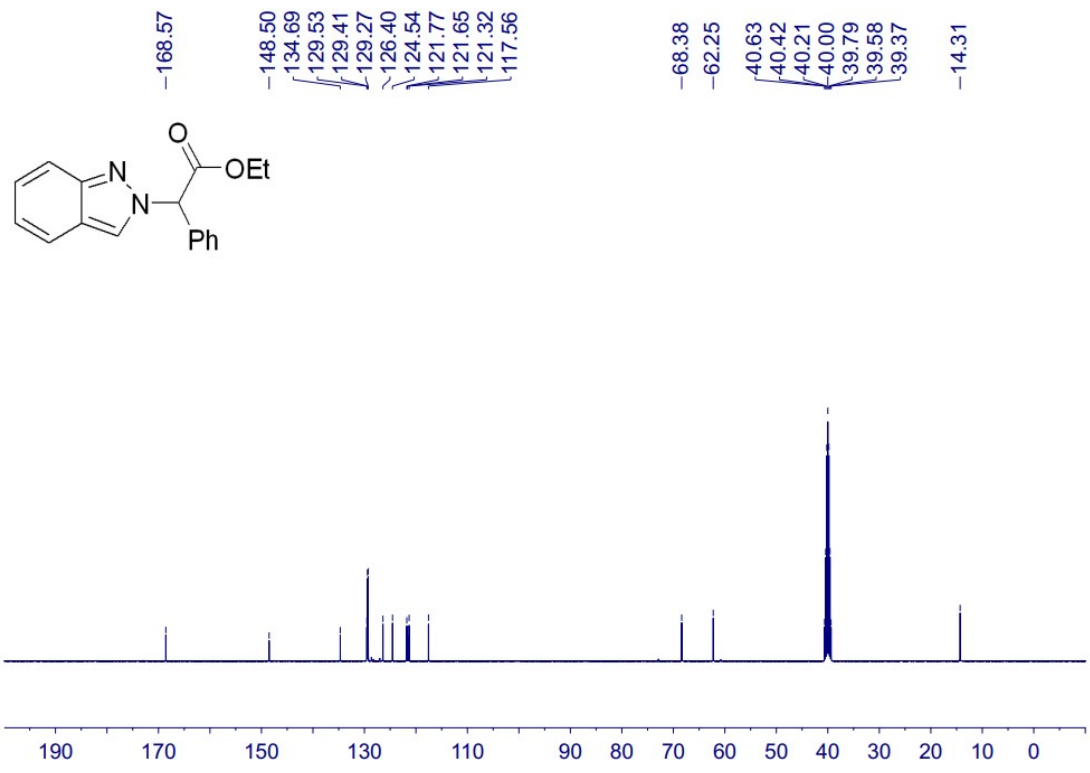
^{1}H NMR Spectrum of Compound **3s** (400 MHz, DMSO-d_6)



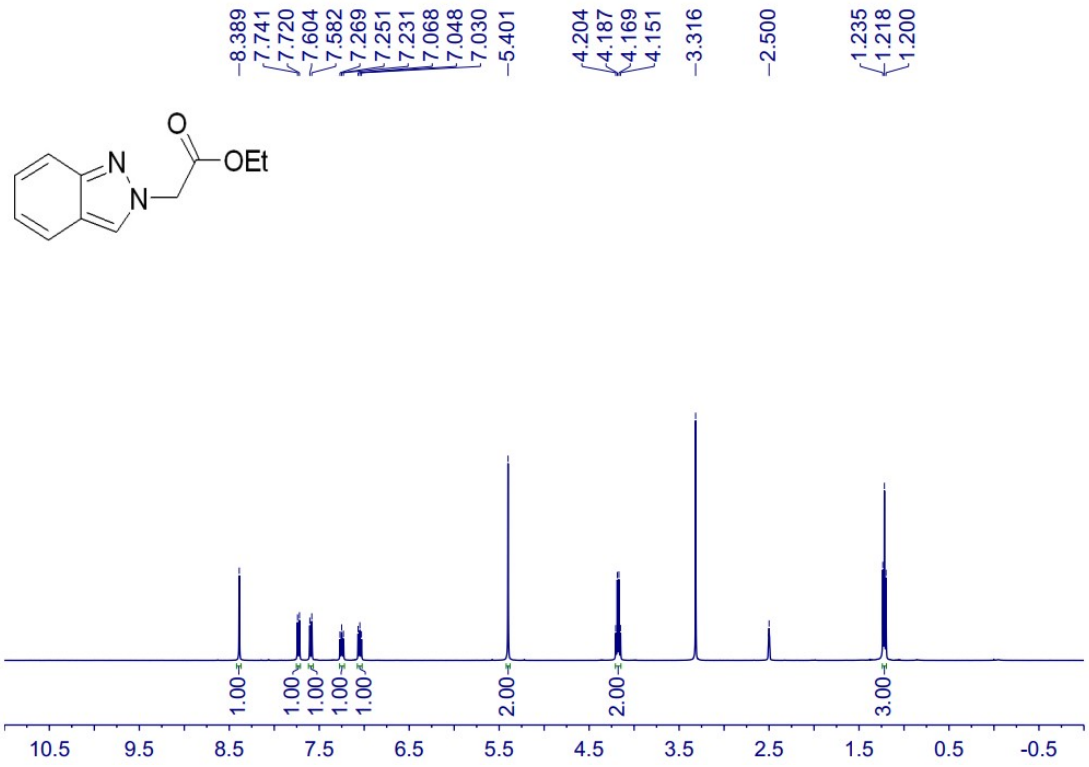
^{13}C NMR Spectrum of Compound **3s** (100 MHz, DMSO-d_6)



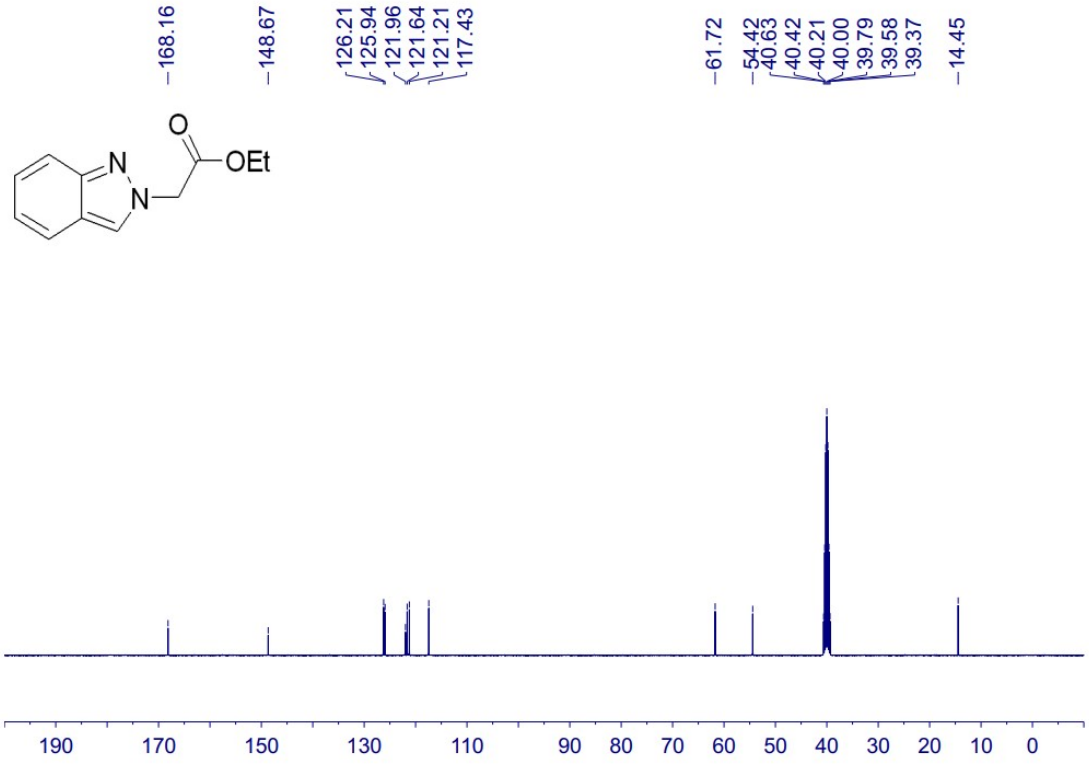
^{1}H NMR Spectrum of Compound **3t** (400 MHz, $CDCl_3$)



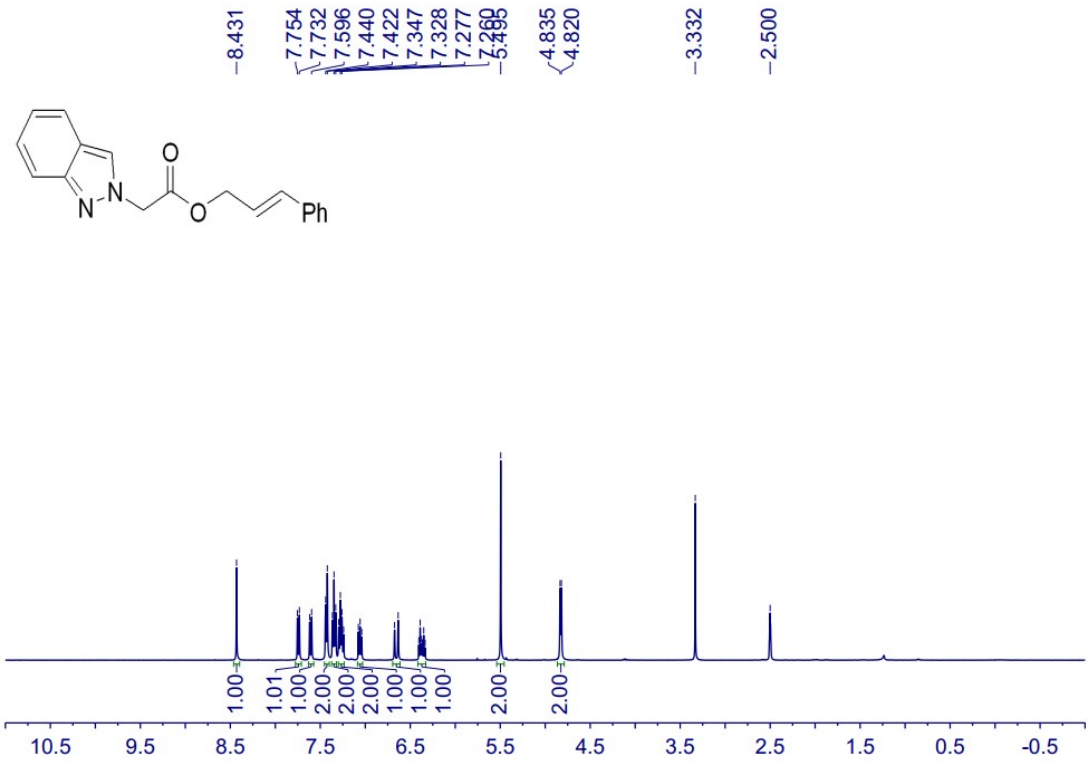
^{13}C NMR Spectrum of Compound **3t** (100 MHz, DMSO-d_6)



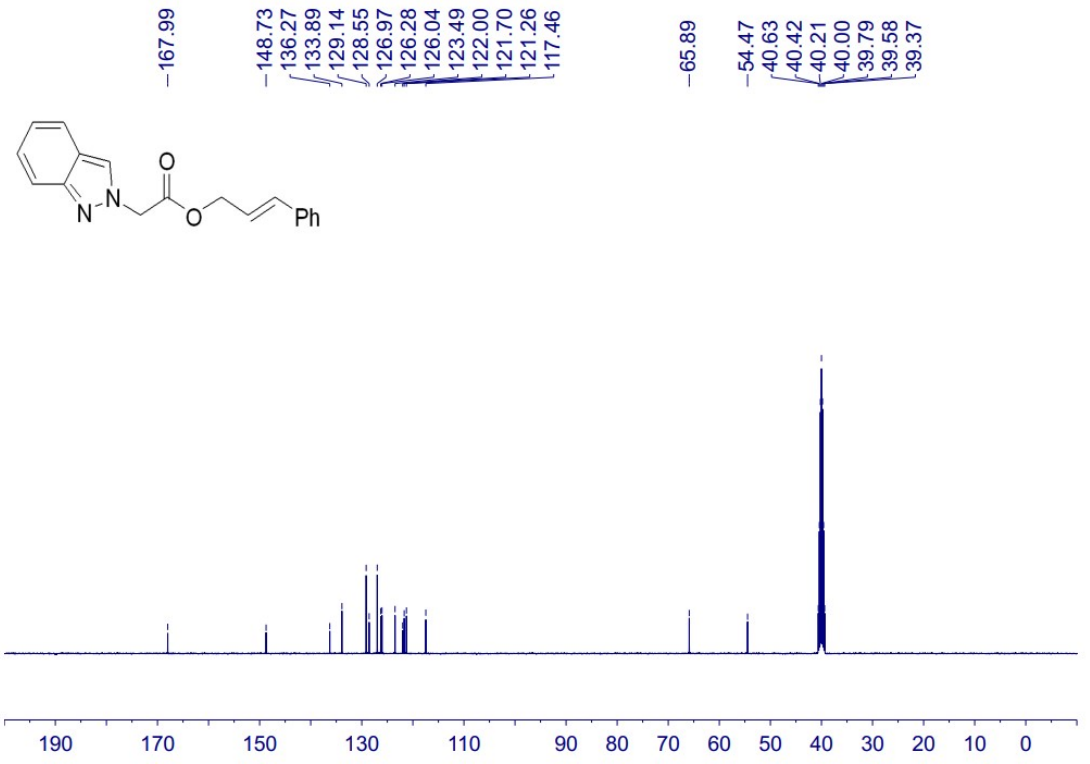
^{1}H NMR Spectrum of Compound **3u** (400 MHz, DMSO-d_6)



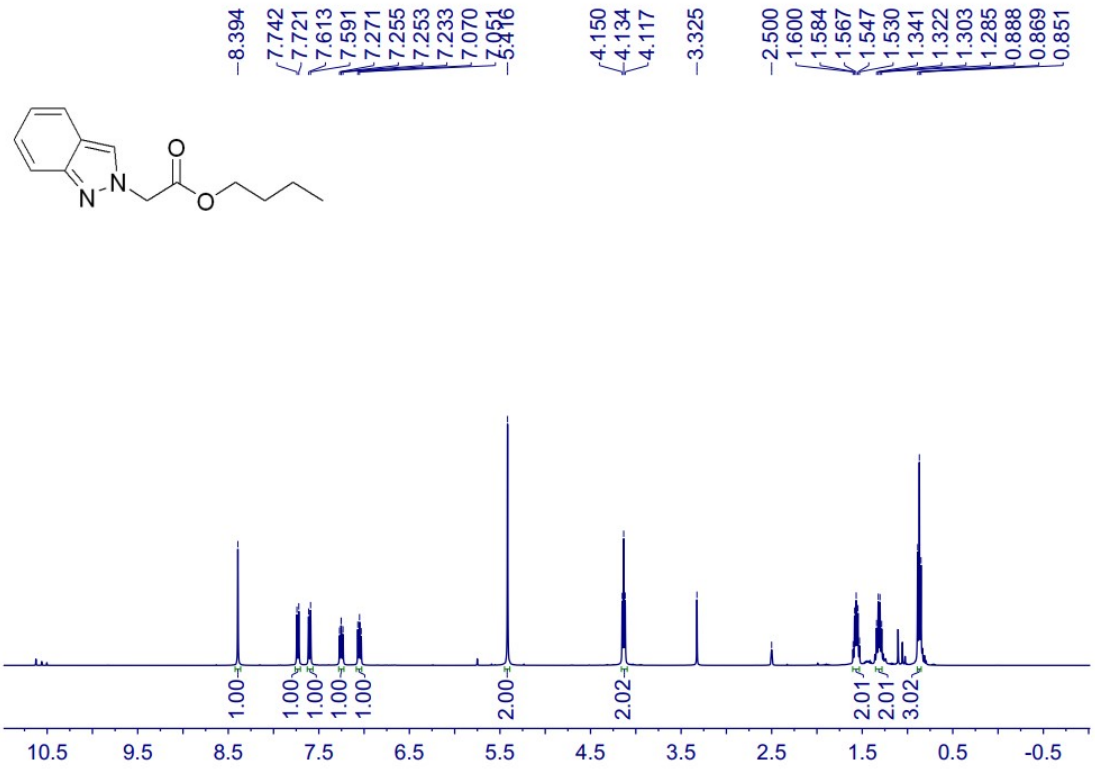
^{13}C NMR Spectrum of Compound **3u** (100 MHz, DMSO-d_6)



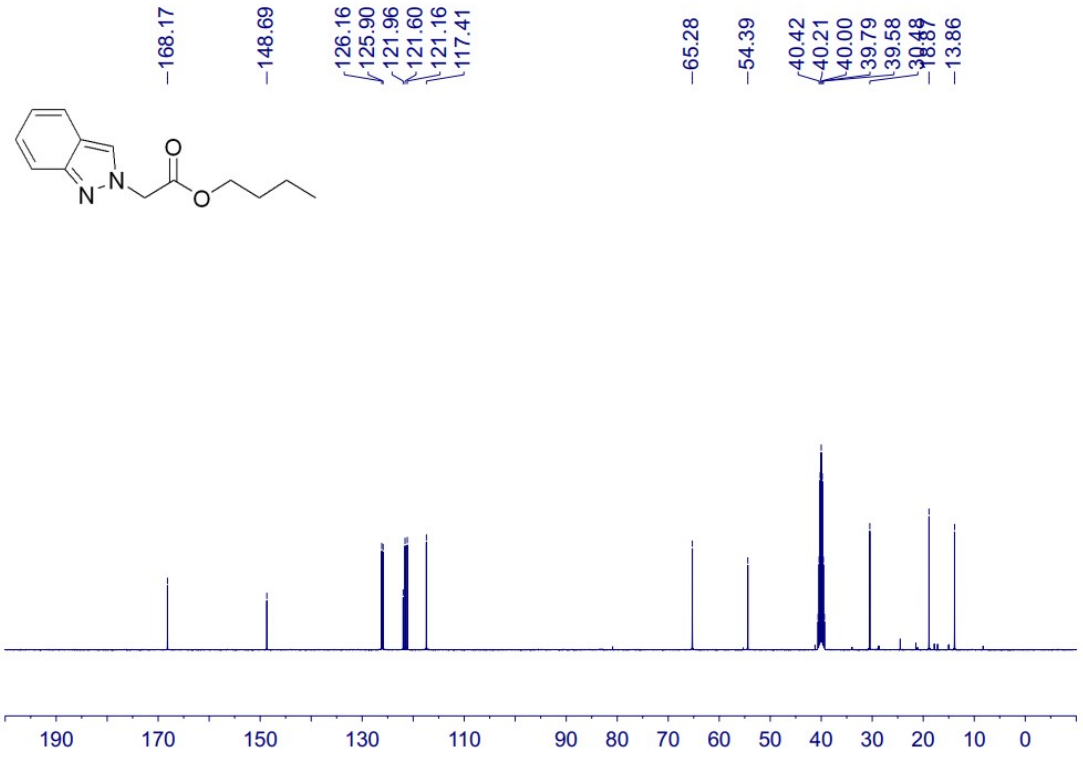
^{1}H NMR Spectrum of Compound **3v** (400 MHz, DMSO-d_6)



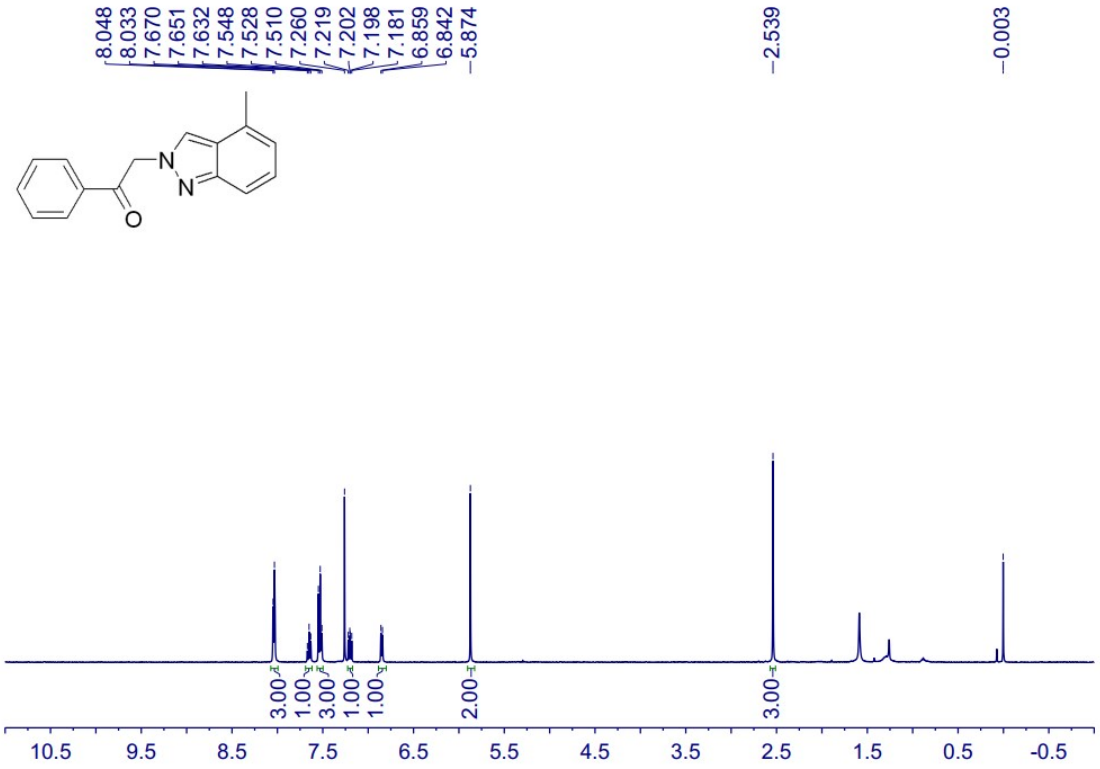
^{13}C NMR Spectrum of Compound **3v** (100 MHz, DMSO-d_6)



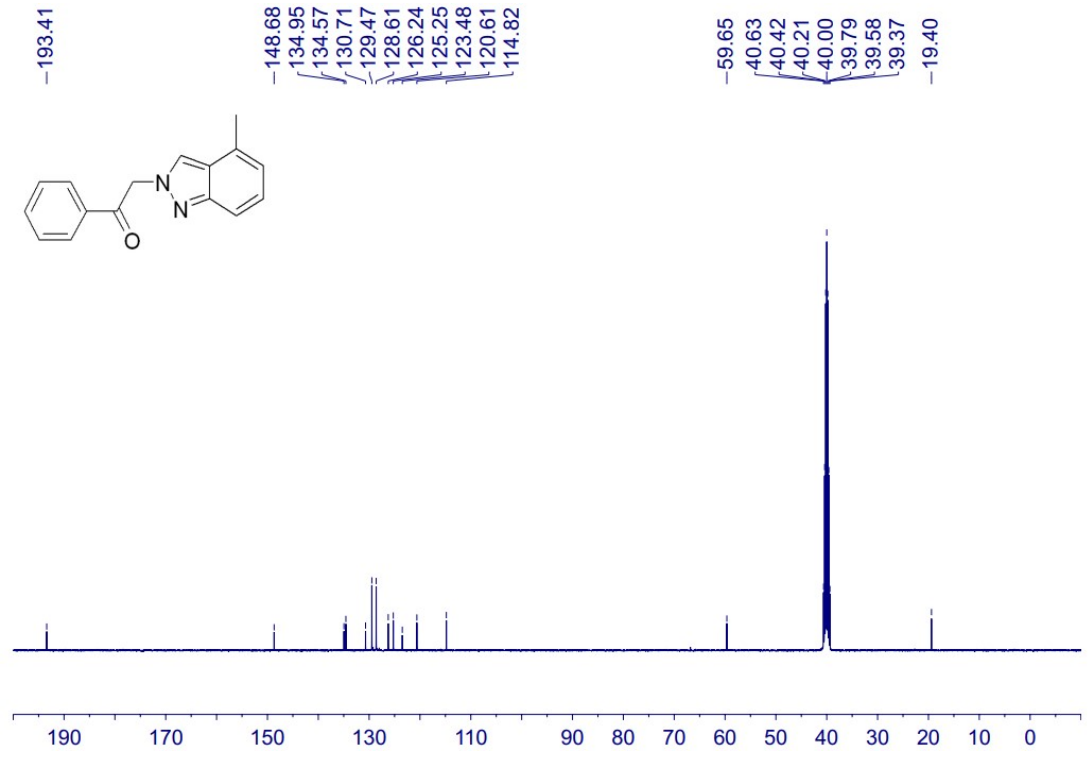
^{1}H NMR Spectrum of Compound **3w** (400 MHz, DMSO-d_6)



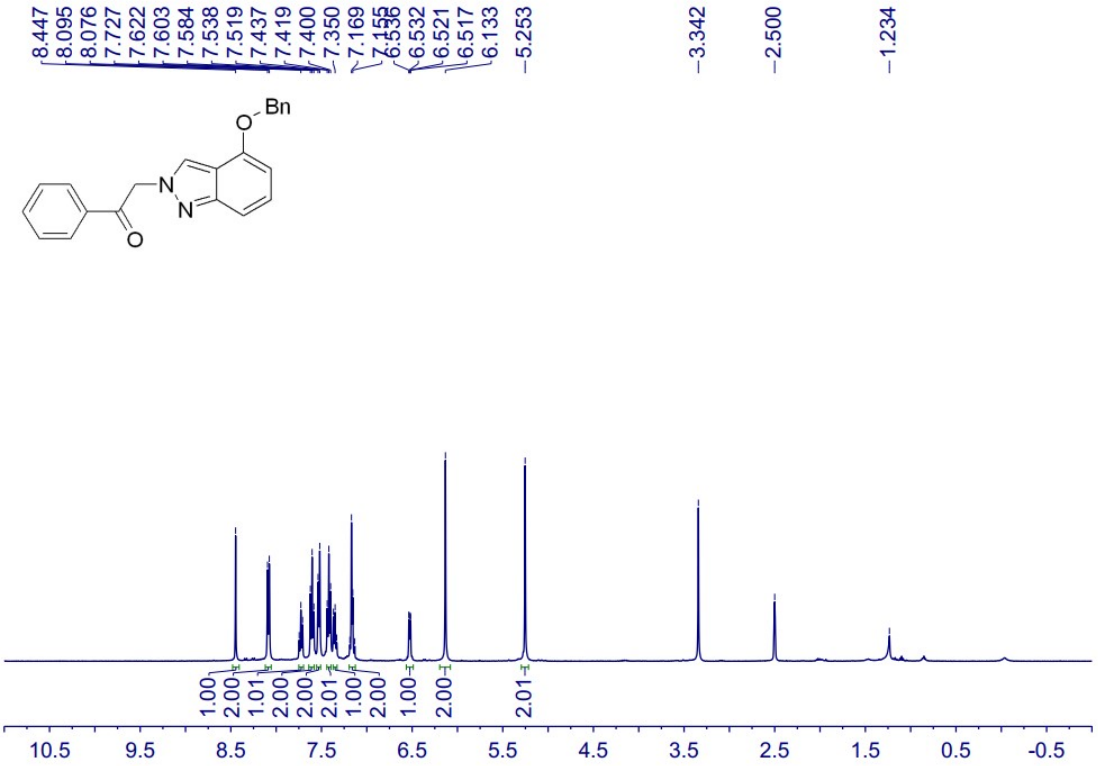
^{13}C NMR Spectrum of Compound **3w** (100 MHz, DMSO-d_6)



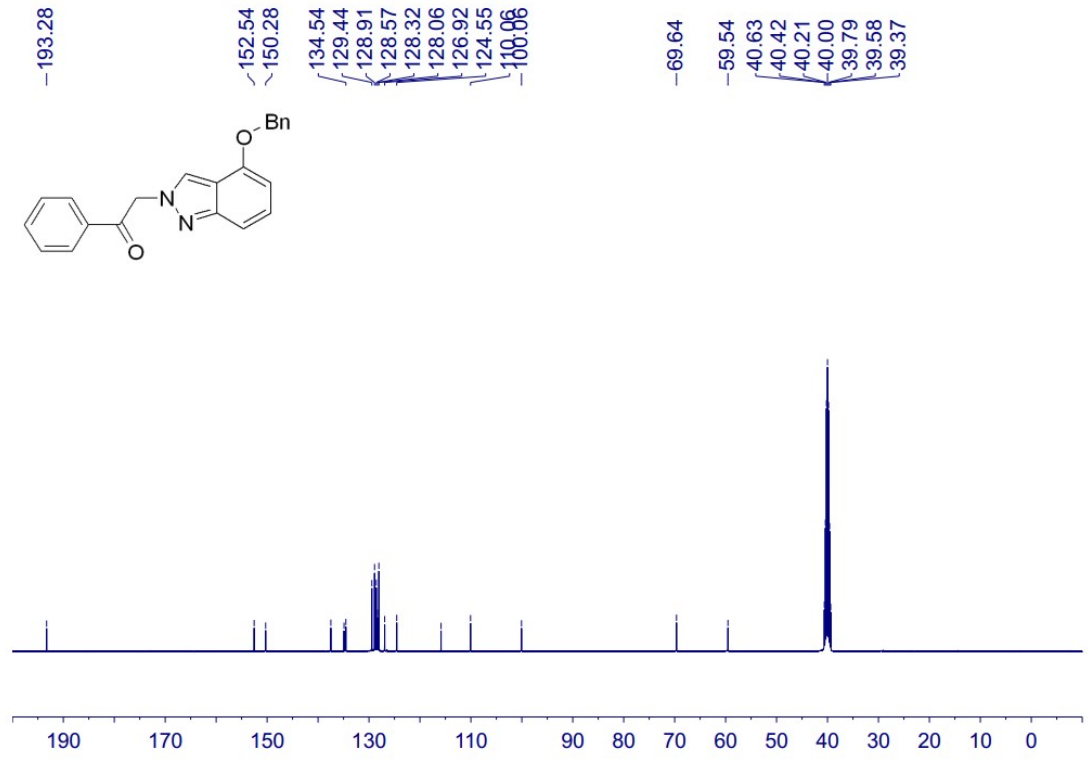
^{1}H NMR Spectrum of Compound **3ab** (400 MHz, $CDCl_3$)



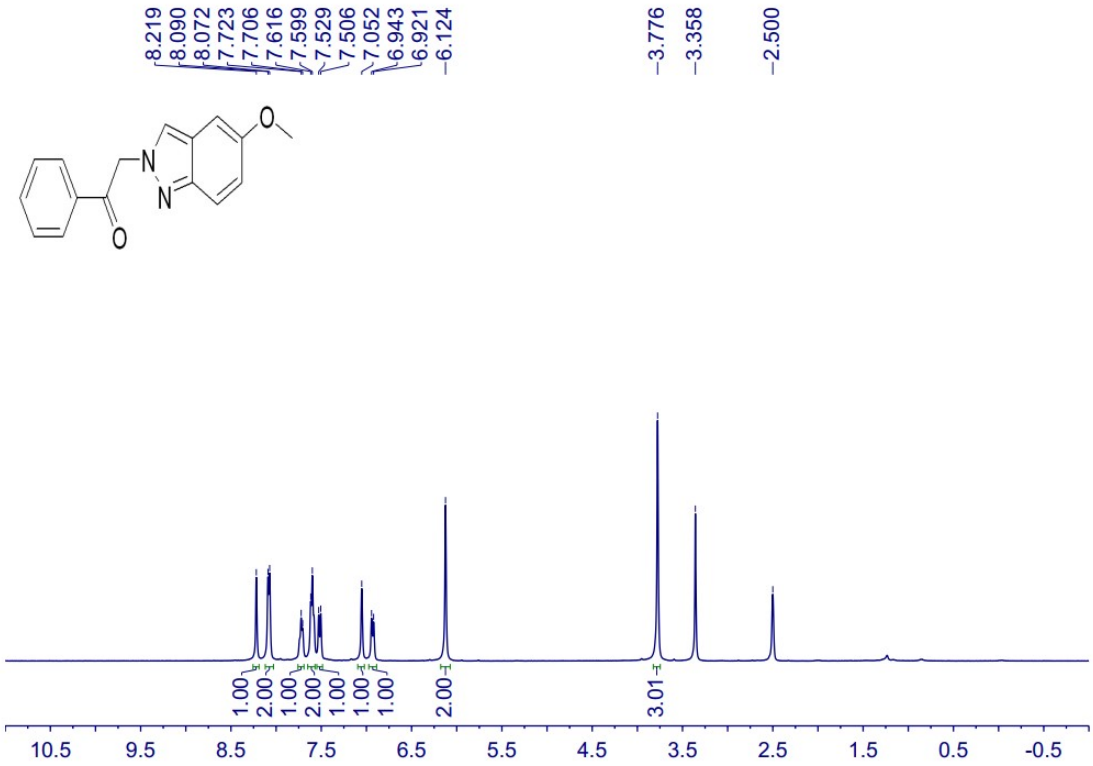
^{13}C NMR Spectrum of Compound **3ab** (100 MHz, DMSO-d_6)



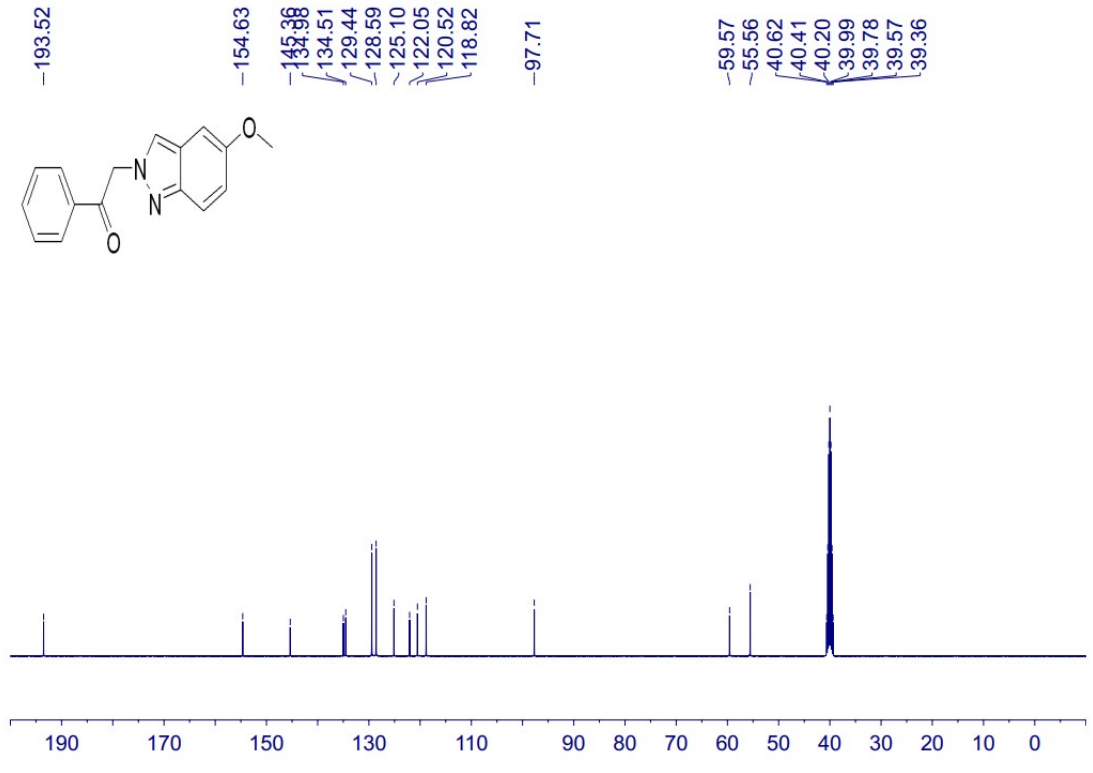
^{1}H NMR Spectrum of Compound **3ac** (400 MHz, DMSO-d_6)



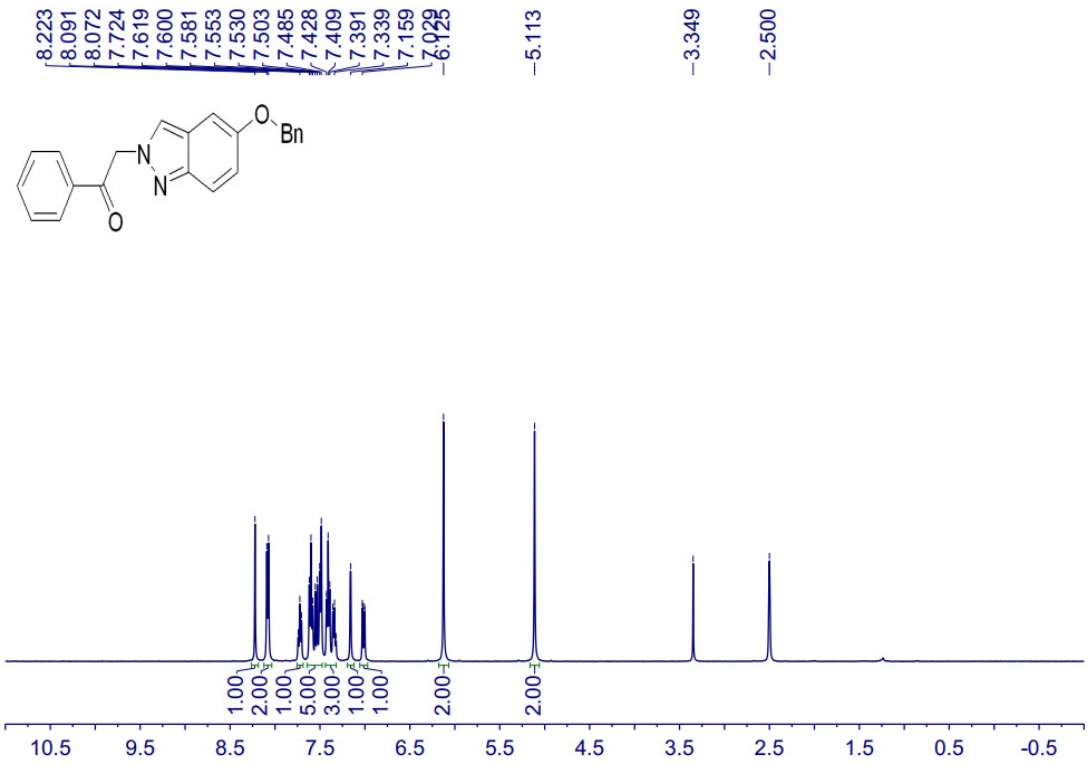
^{13}C NMR Spectrum of Compound **3ac** (100 MHz, DMSO-d_6)



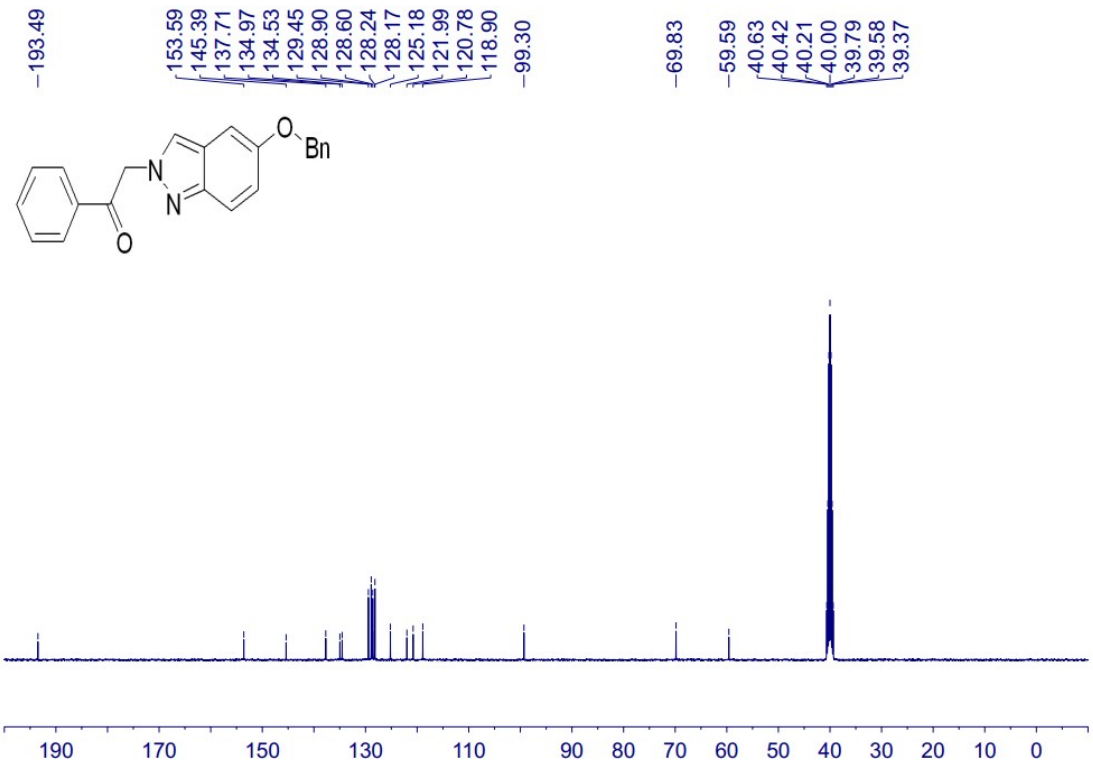
^{1}H NMR Spectrum of Compound **3ad** (400 MHz, DMSO-d_6)



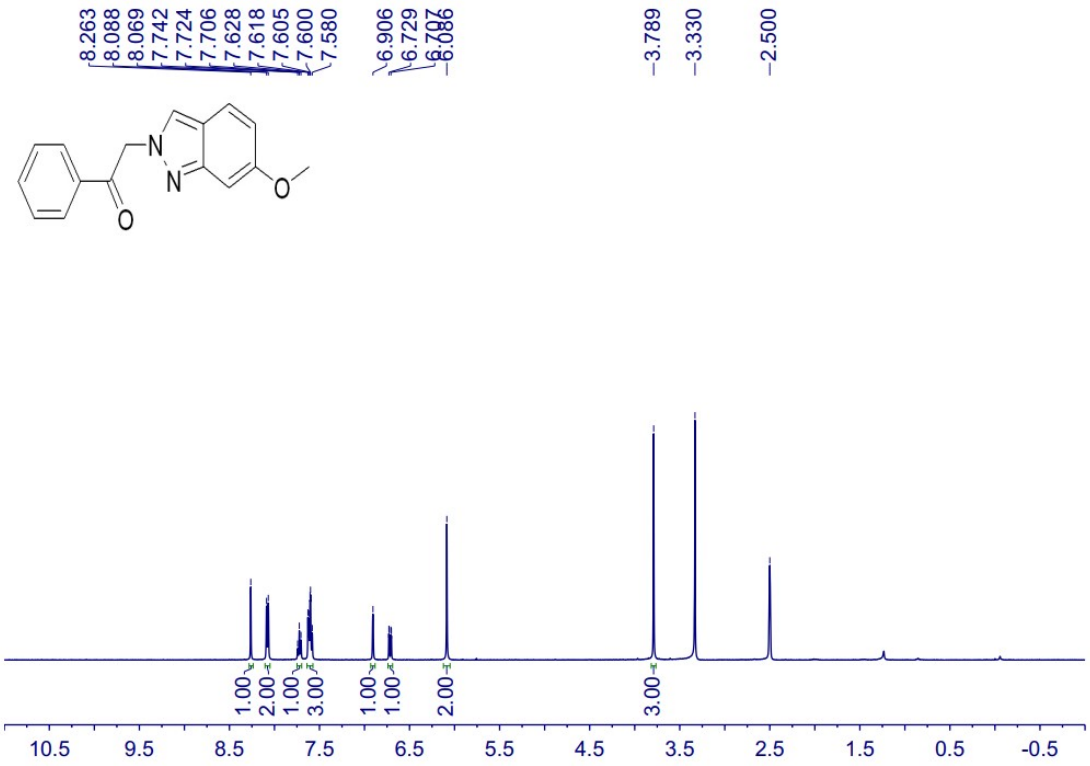
^{13}C NMR Spectrum of Compound **3ad** (100 MHz, DMSO-d_6)



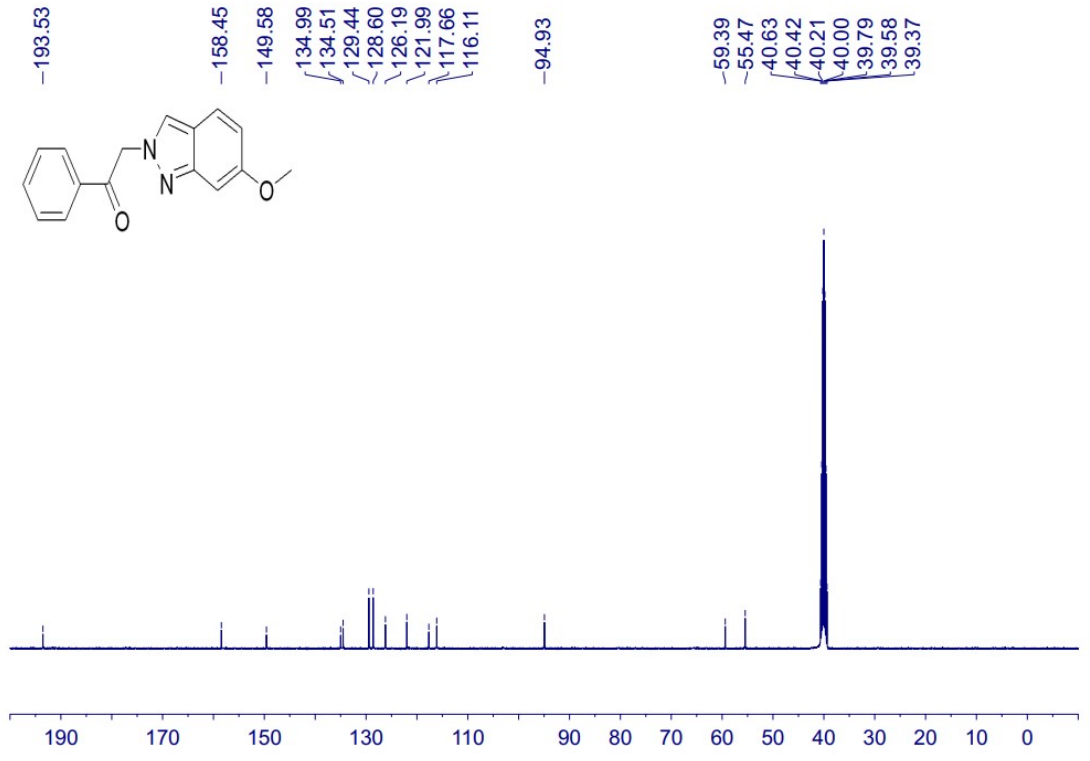
^{1}H NMR Spectrum of Compound **3ae** (400 MHz, DMSO-d_6)



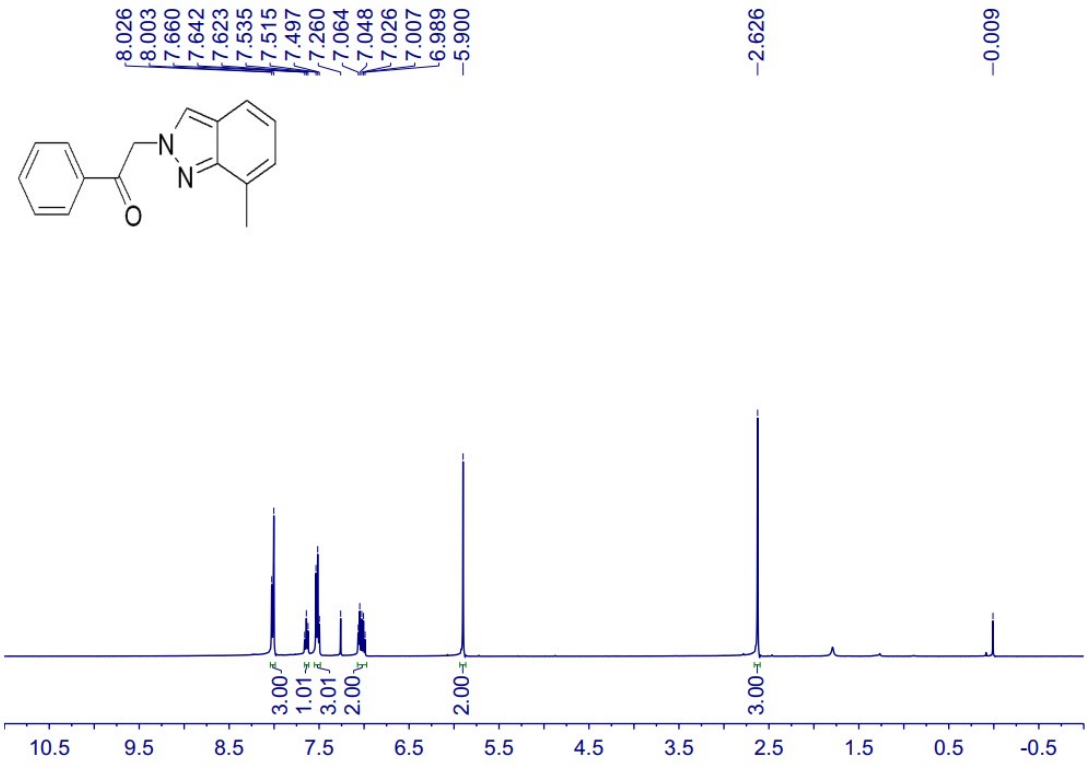
^{13}C NMR Spectrum of Compound **3ae** (100 MHz, DMSO-d_6)



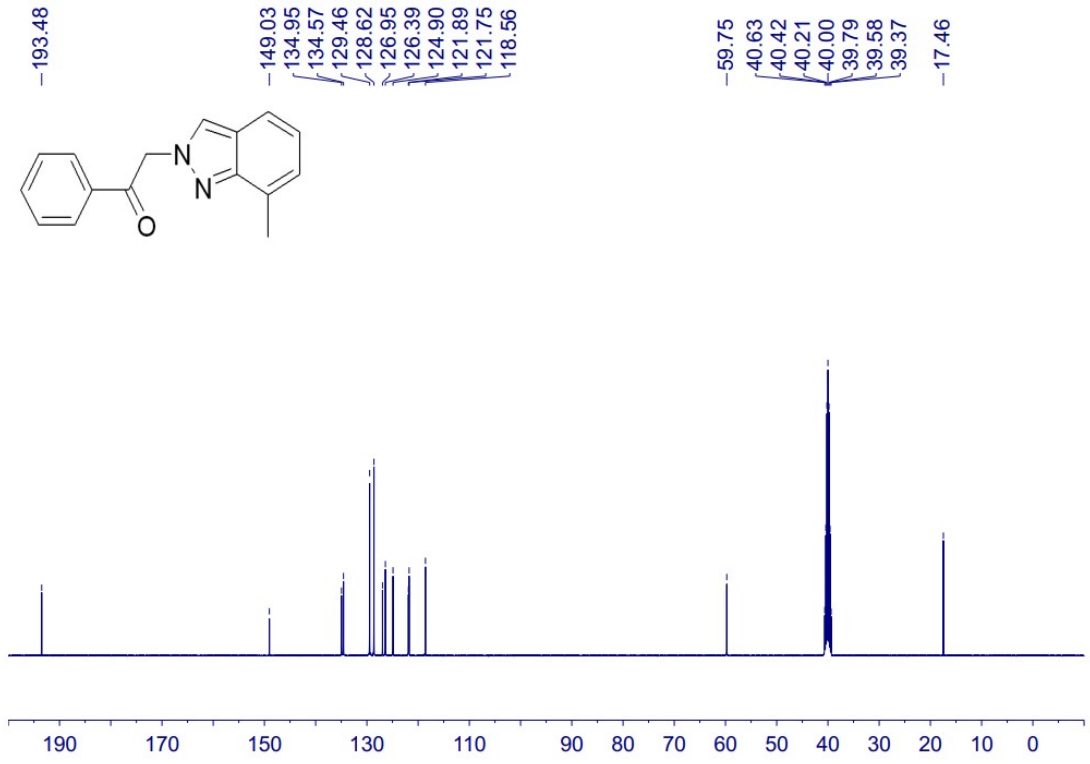
^{1}H NMR Spectrum of Compound **3af** (400 MHz, DMSO-d_6)



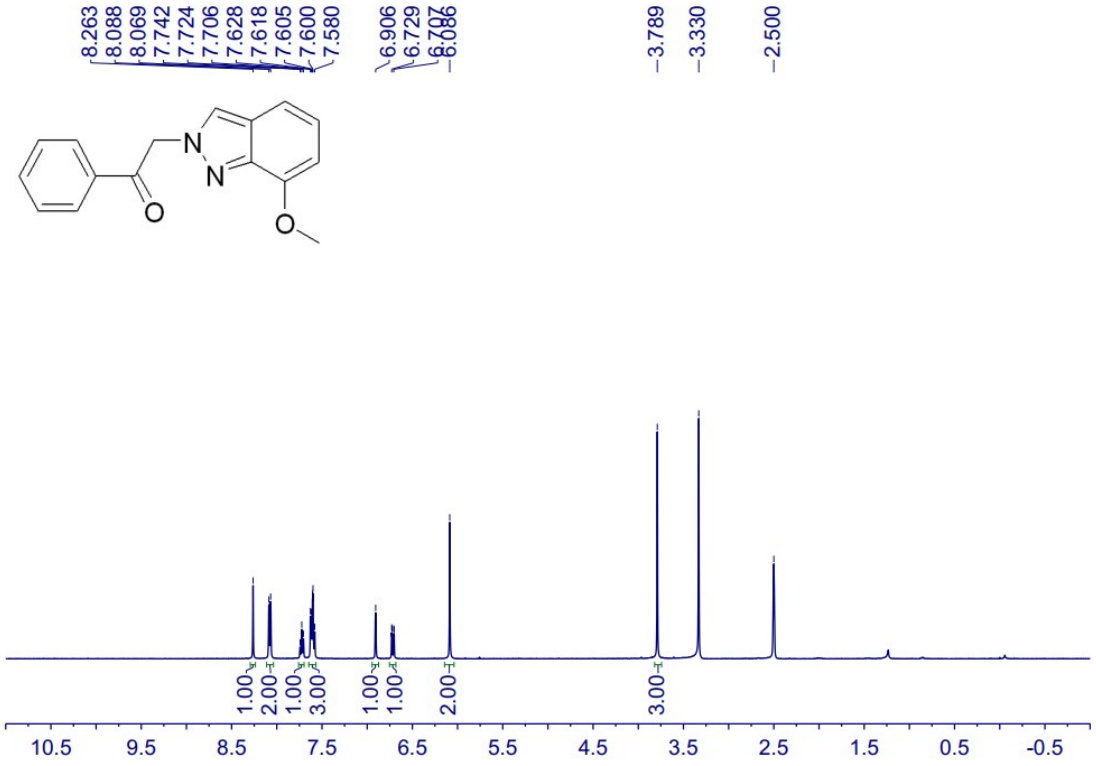
^{13}C NMR Spectrum of Compound **3af** (100 MHz, DMSO-d_6)



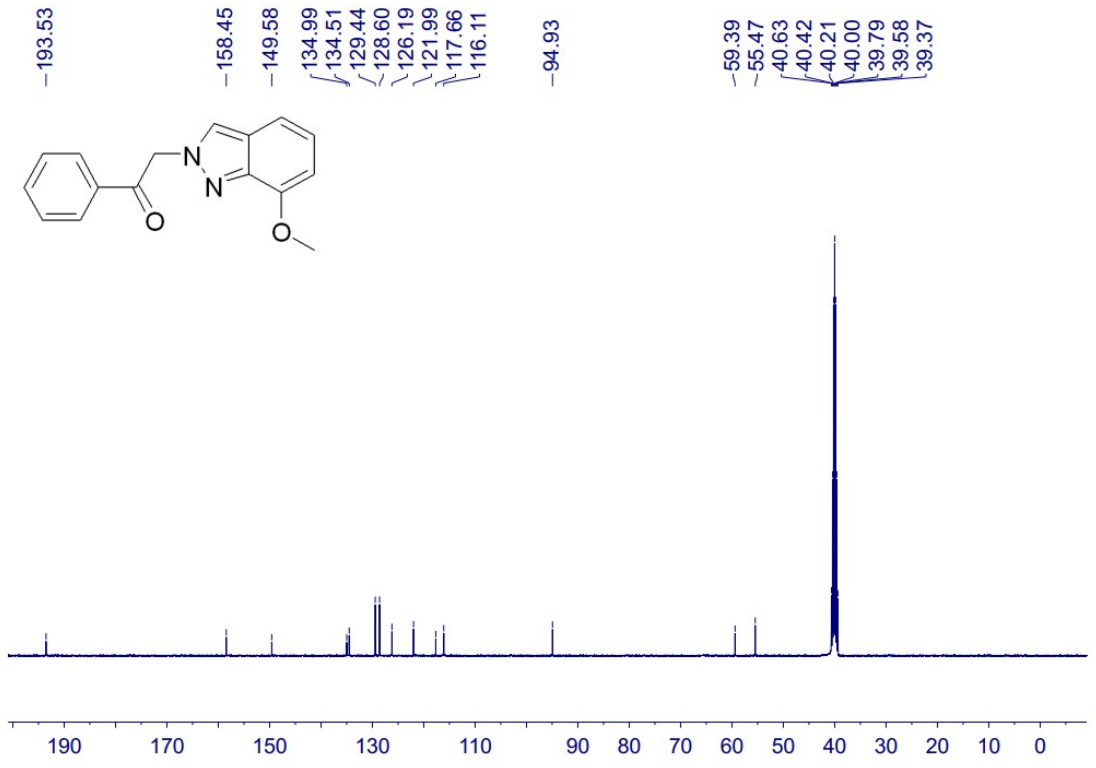
^{1}H NMR Spectrum of Compound **3ag** (400 MHz, $CDCl_3$)



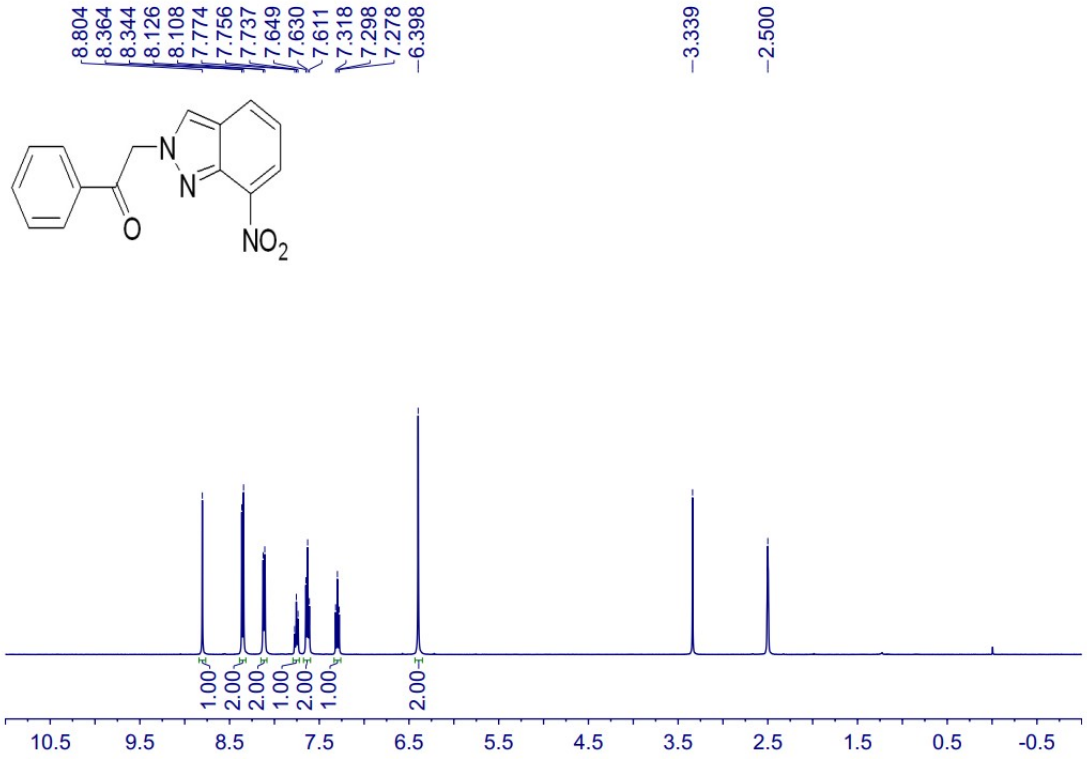
^{13}C NMR Spectrum of Compound **3ag** (100 MHz, DMSO-d_6)



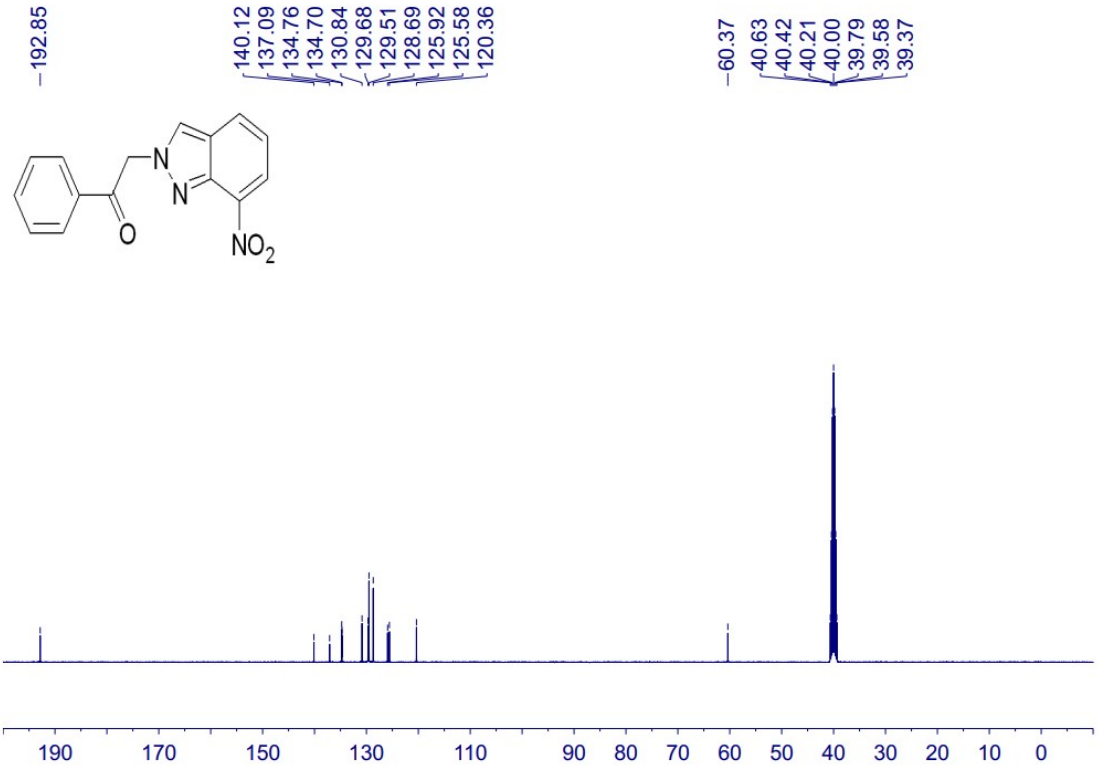
^{1}H NMR Spectrum of Compound **3ah** (400 MHz, DMSO-d_6)



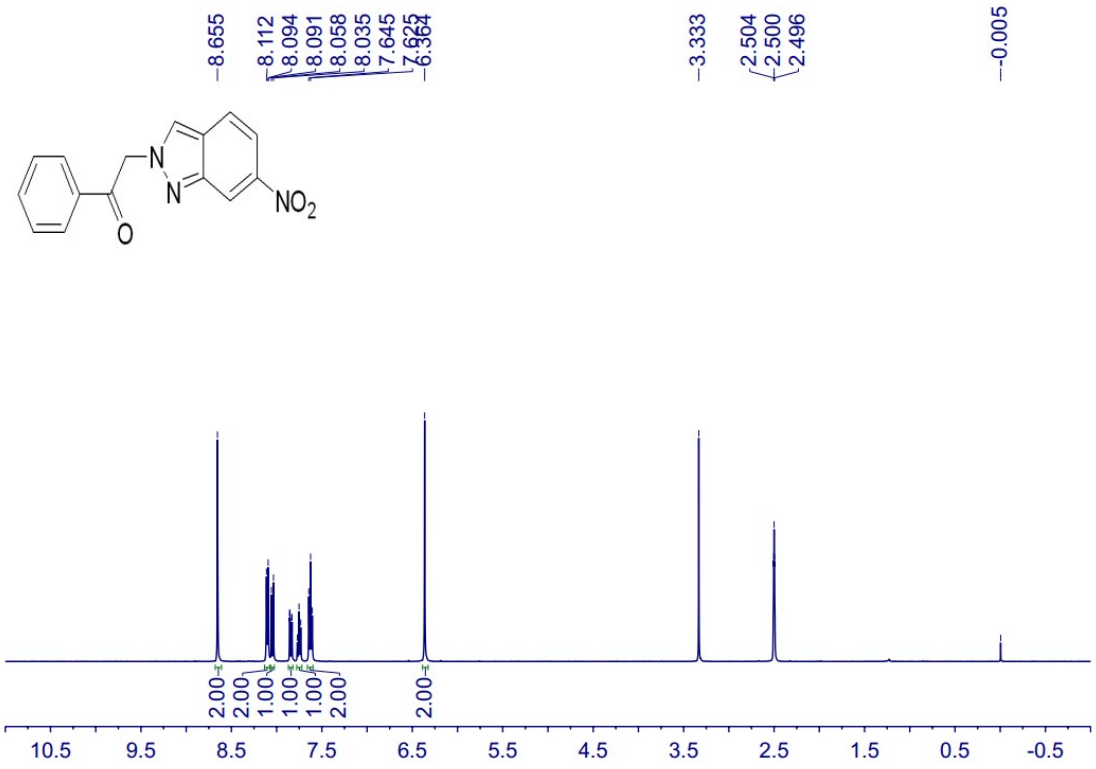
^{13}C NMR Spectrum of Compound **3ah** (100 MHz, DMSO-d_6)



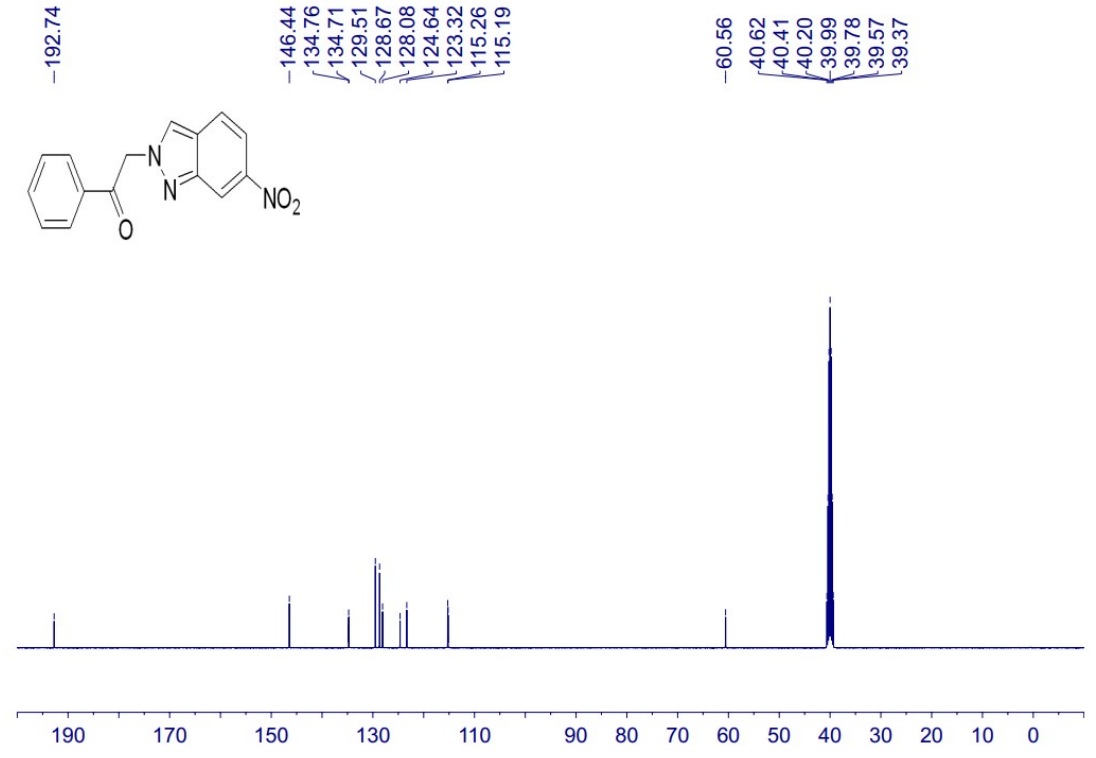
^{1}H NMR Spectrum of Compound **3ai** (400 MHz, DMSO-d_6)



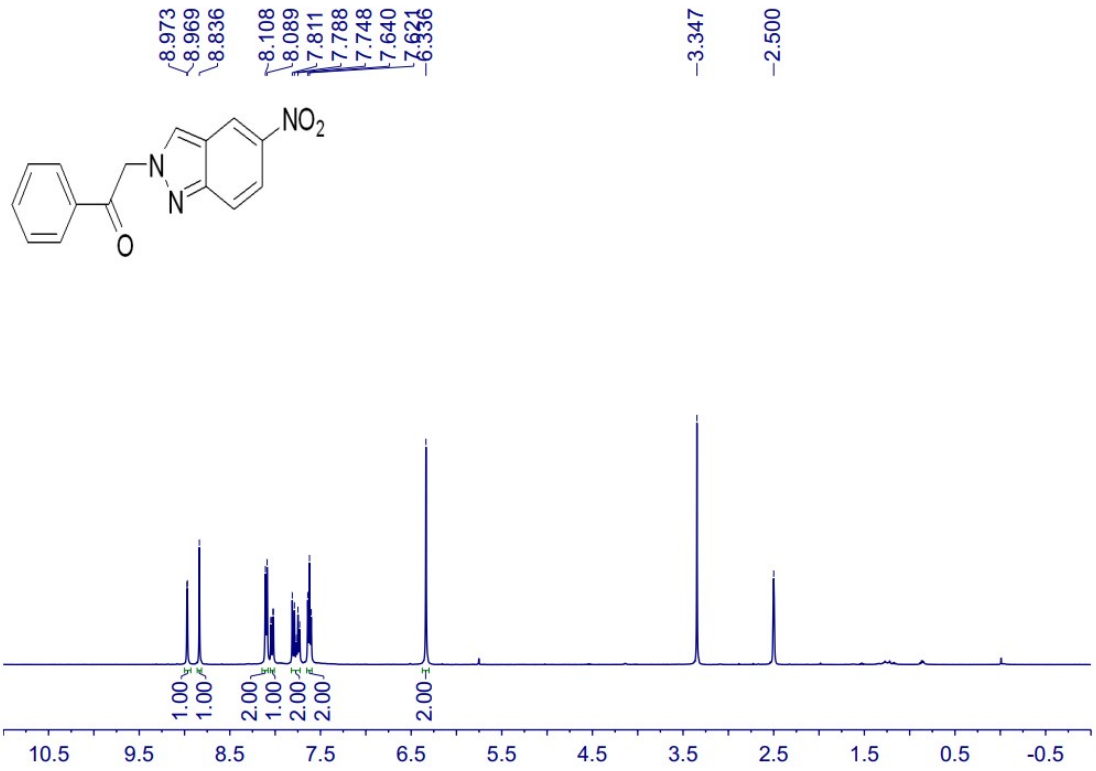
^{13}C NMR Spectrum of Compound **3ai** (100 MHz, DMSO-d_6)



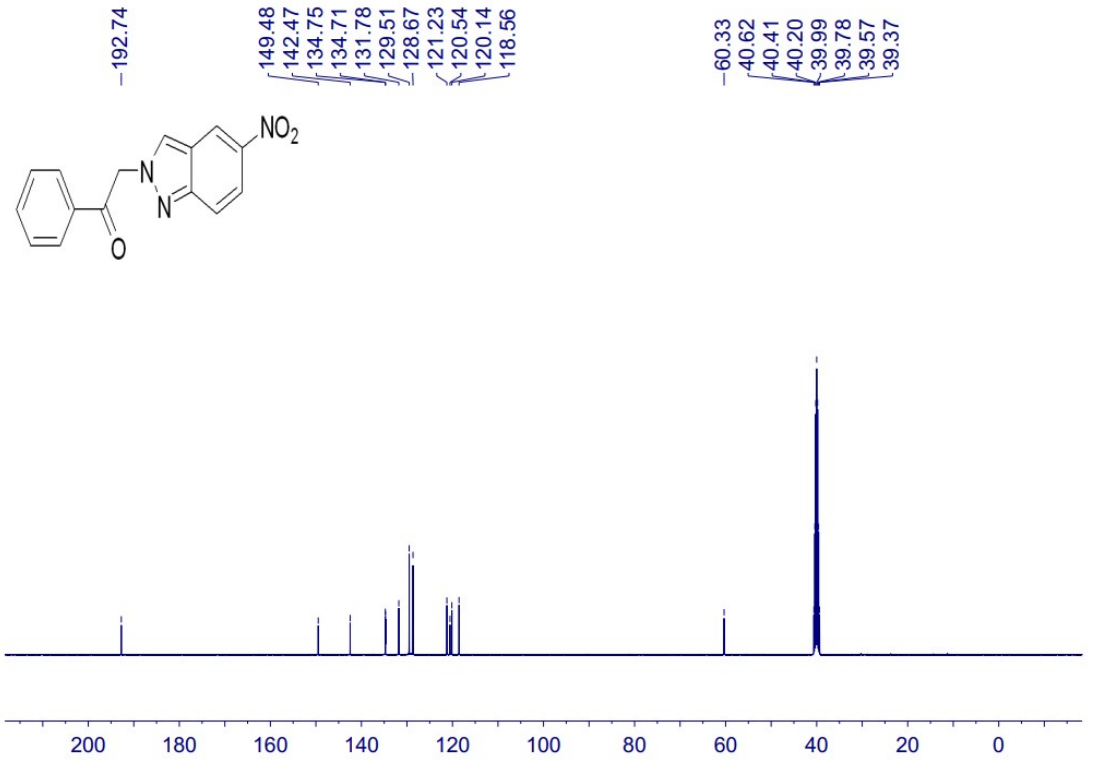
^{1}H NMR Spectrum of Compound **3aj** (400 MHz, DMSO-d_6)



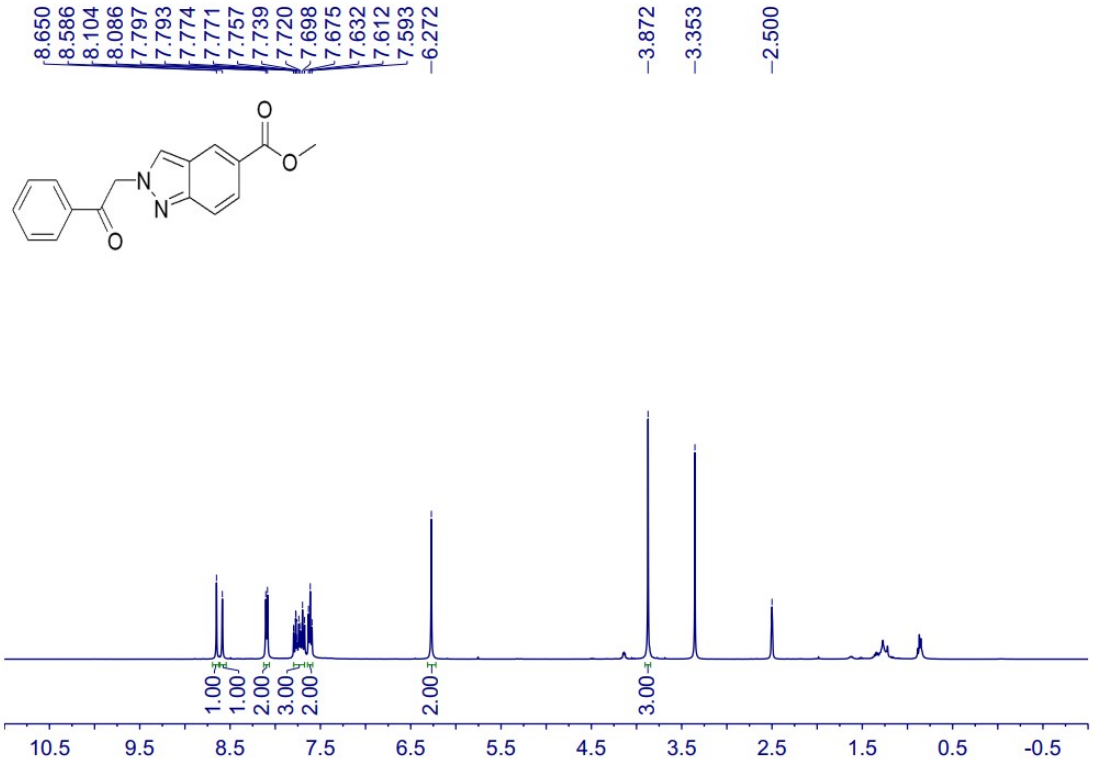
^{13}C NMR Spectrum of Compound **3aj** (100 MHz, DMSO-d_6)



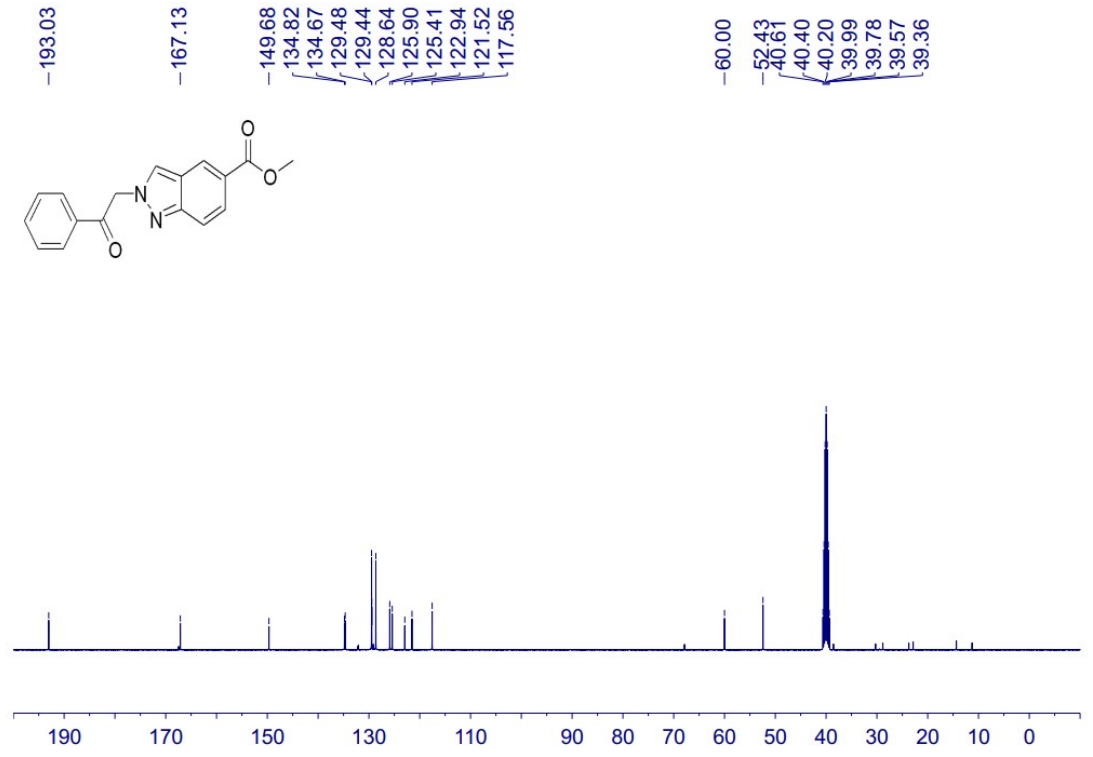
^{1}H NMR Spectrum of Compound **3ak** (400 MHz, DMSO-d_6)



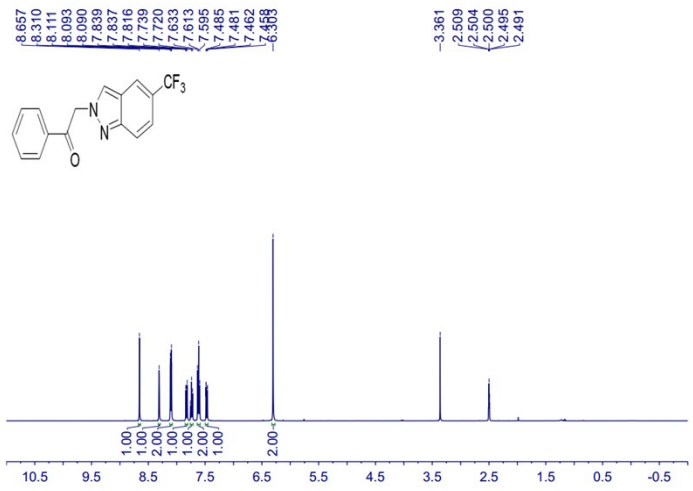
^{13}C NMR Spectrum of Compound **3ak** (100 MHz, DMSO-d_6)



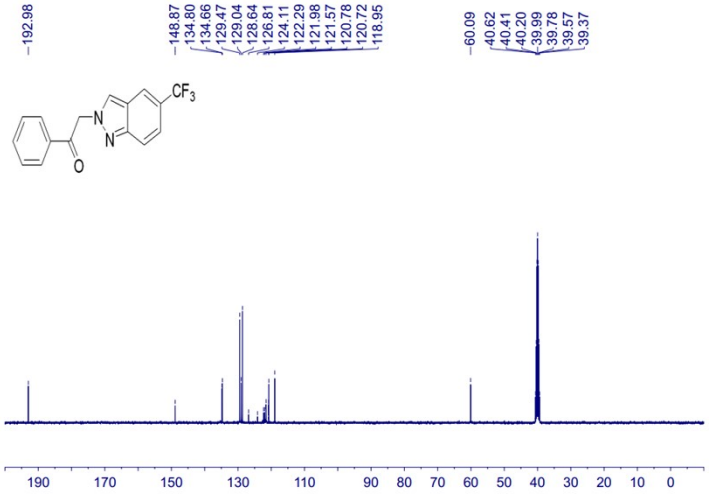
^{1}H NMR Spectrum of Compound **3al** (400 MHz, DMSO-d_6)



^{13}C NMR Spectrum of Compound **3al** (100 MHz, DMSO-d_6)

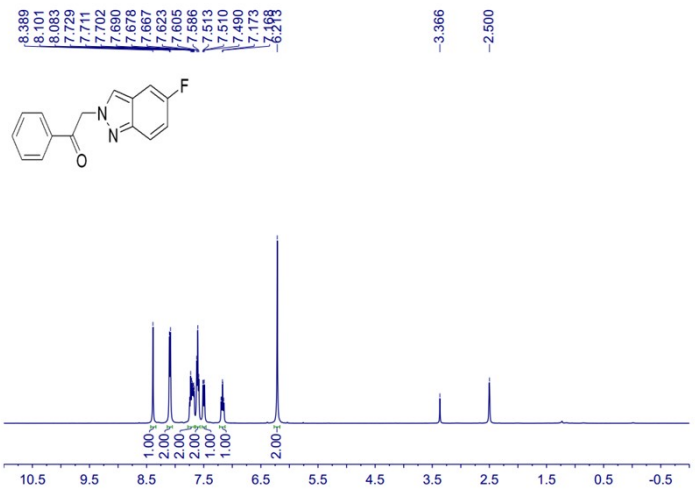


^{1}H NMR Spectrum of Compound **3am** (400 MHz, DMSO-d_6)

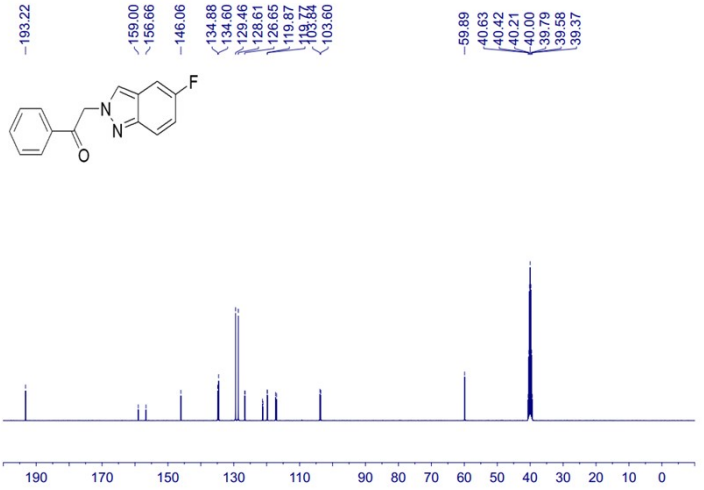


^{13}C NMR Spectrum of Compound **3am** (100 MHz, DMSO-d_6)

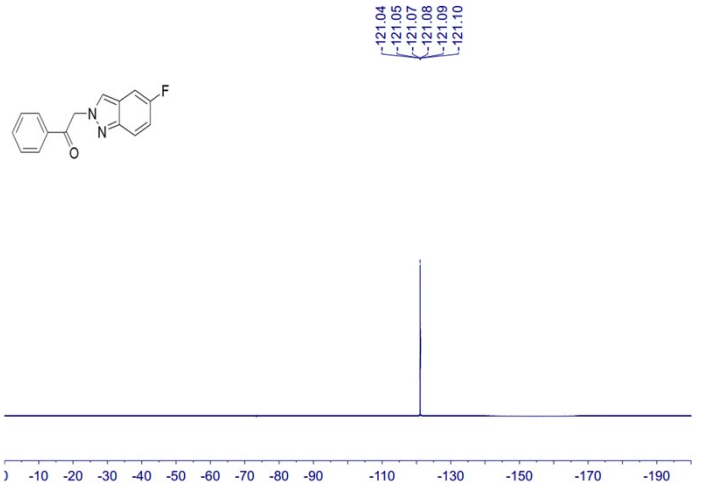
^{19}F NMR Spectrum of Compound **3am** (376 MHz, DMSO-d_6)



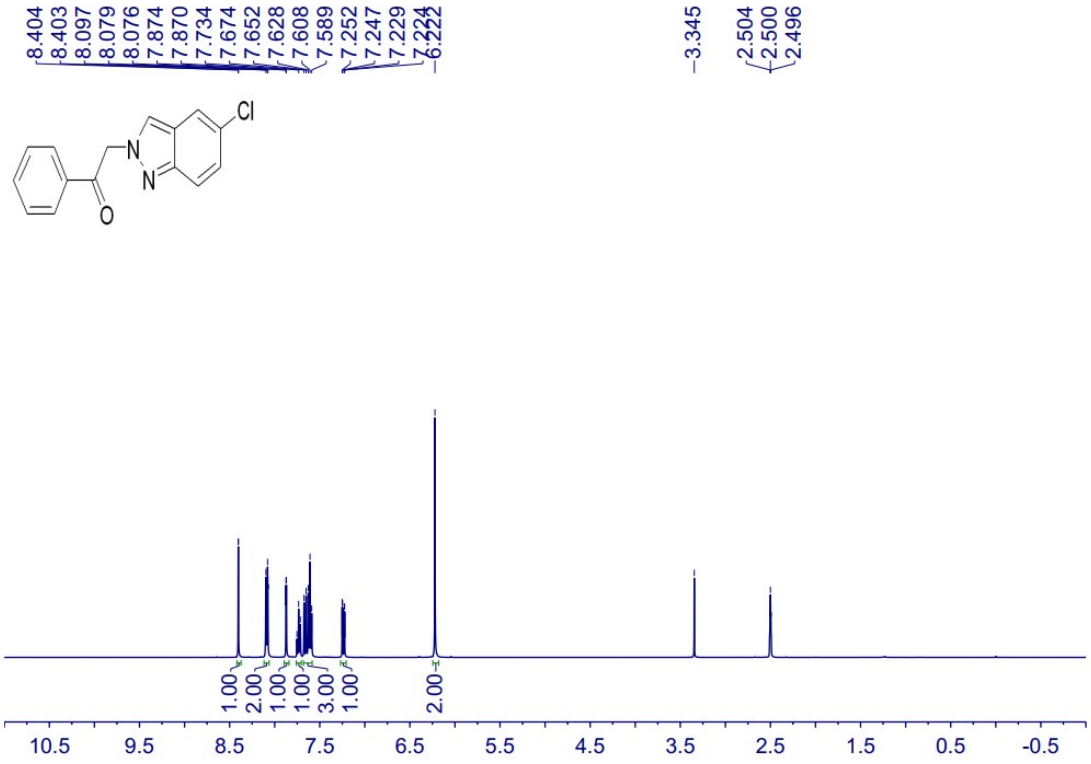
^{1}H NMR Spectrum of Compound **3an** (400 MHz, DMSO-d_6)



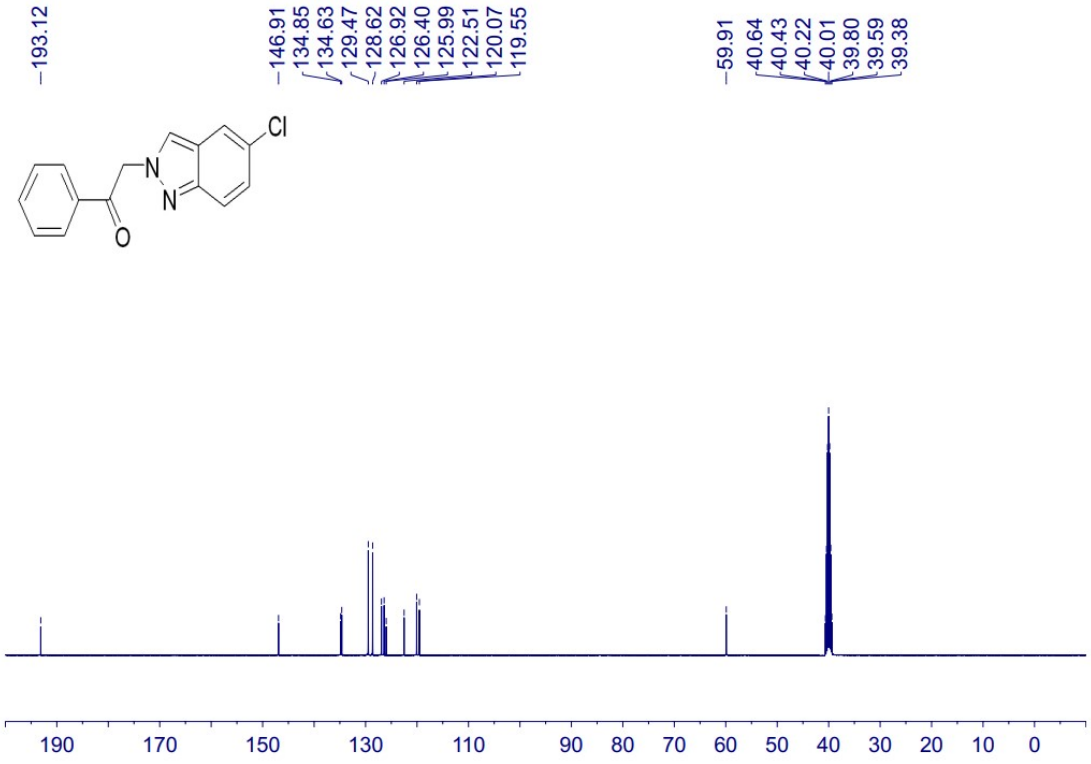
^{13}C NMR Spectrum of Compound **3an** (100 MHz, DMSO-d_6)



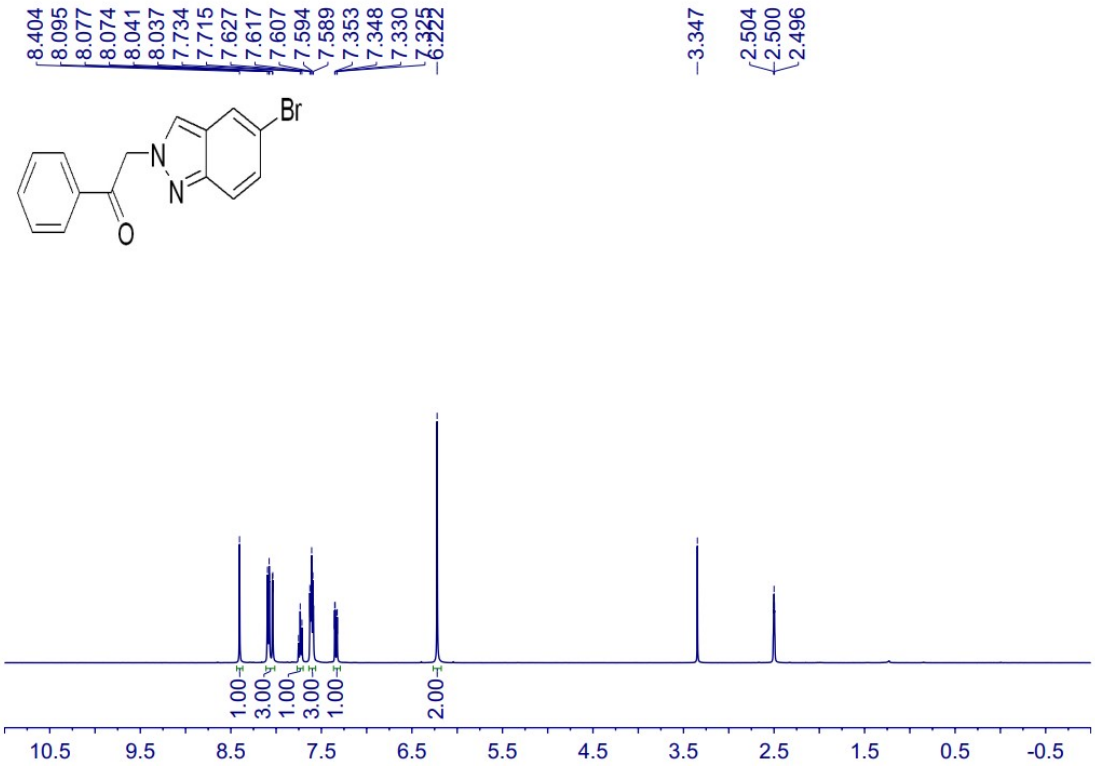
^{19}F NMR Spectrum of Compound **3an** (376 MHz, DMSO-d_6)



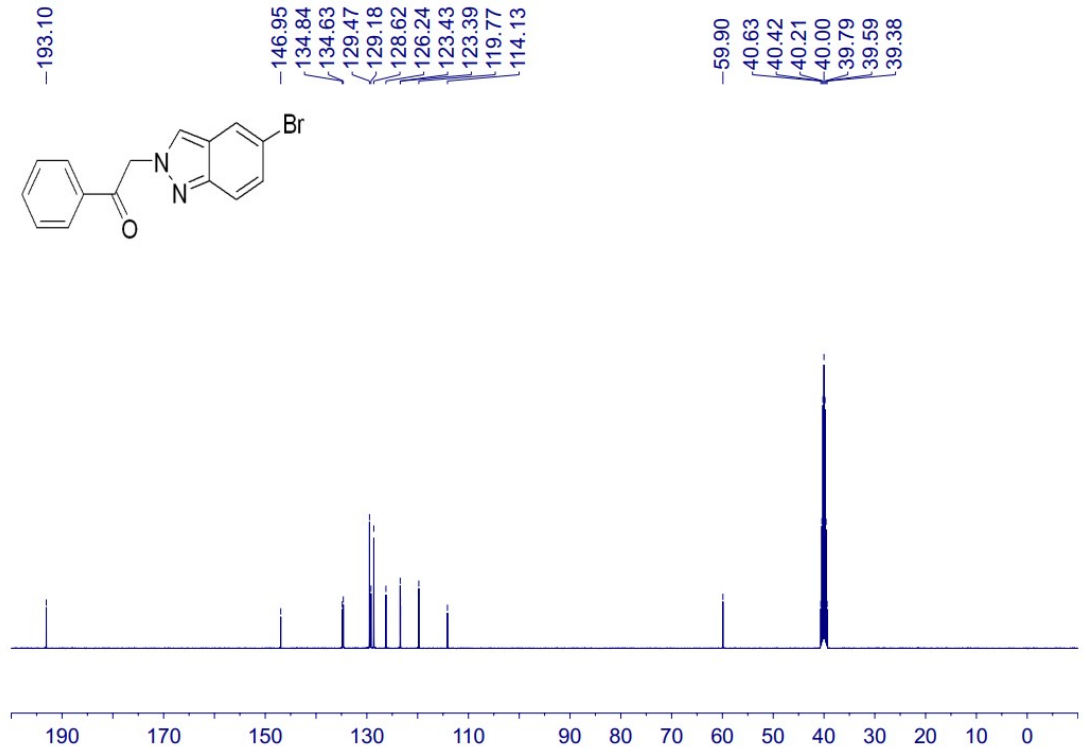
^{1}H NMR Spectrum of Compound **3ao** (400 MHz, DMSO-d_6)



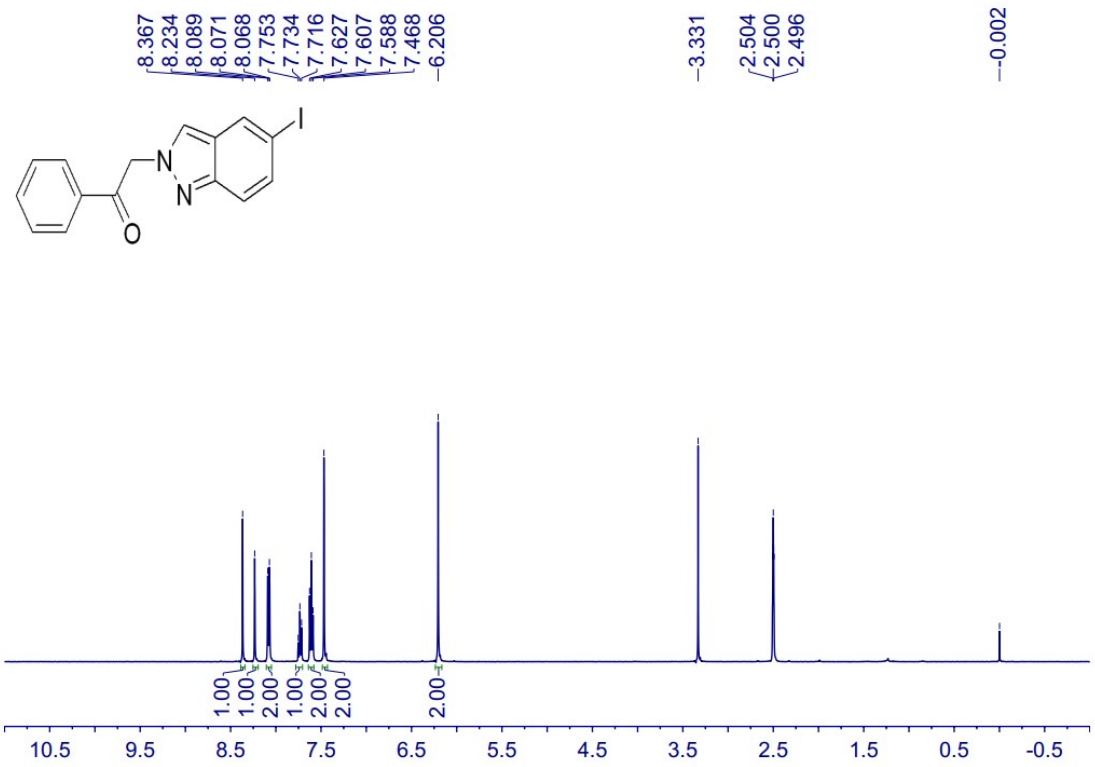
^{13}C NMR Spectrum of Compound **3ao** (100 MHz, DMSO-d_6)



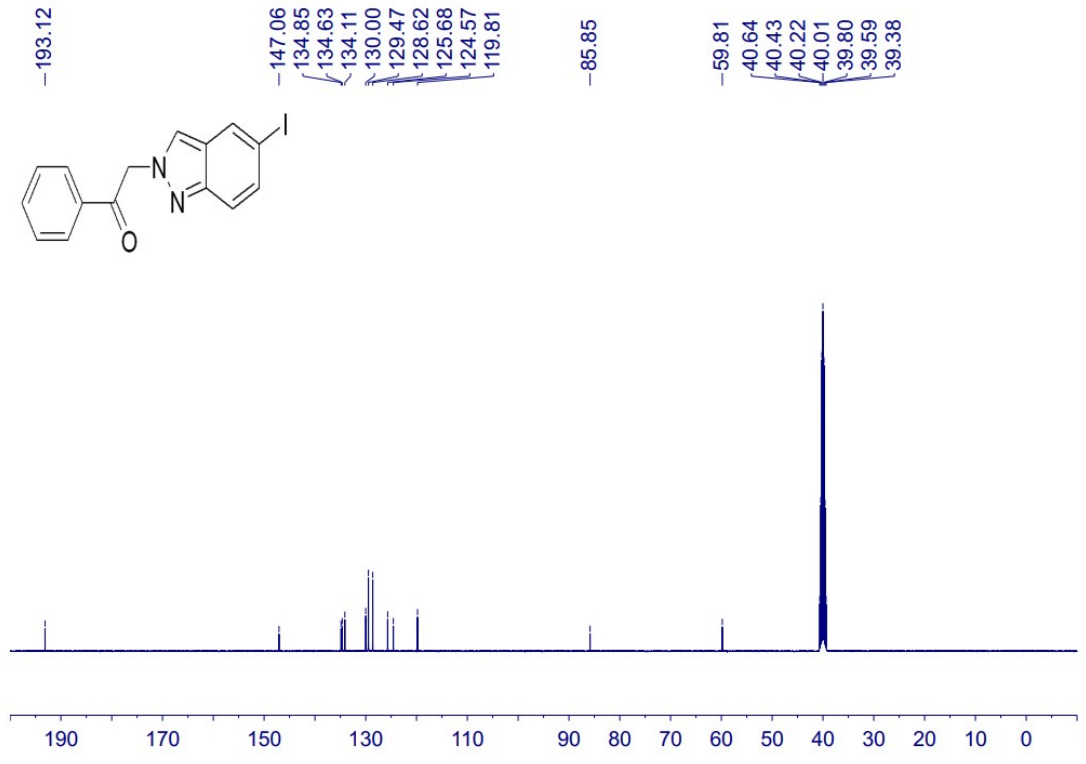
^{1}H NMR Spectrum of Compound **3ap** (400 MHz, DMSO-d_6)



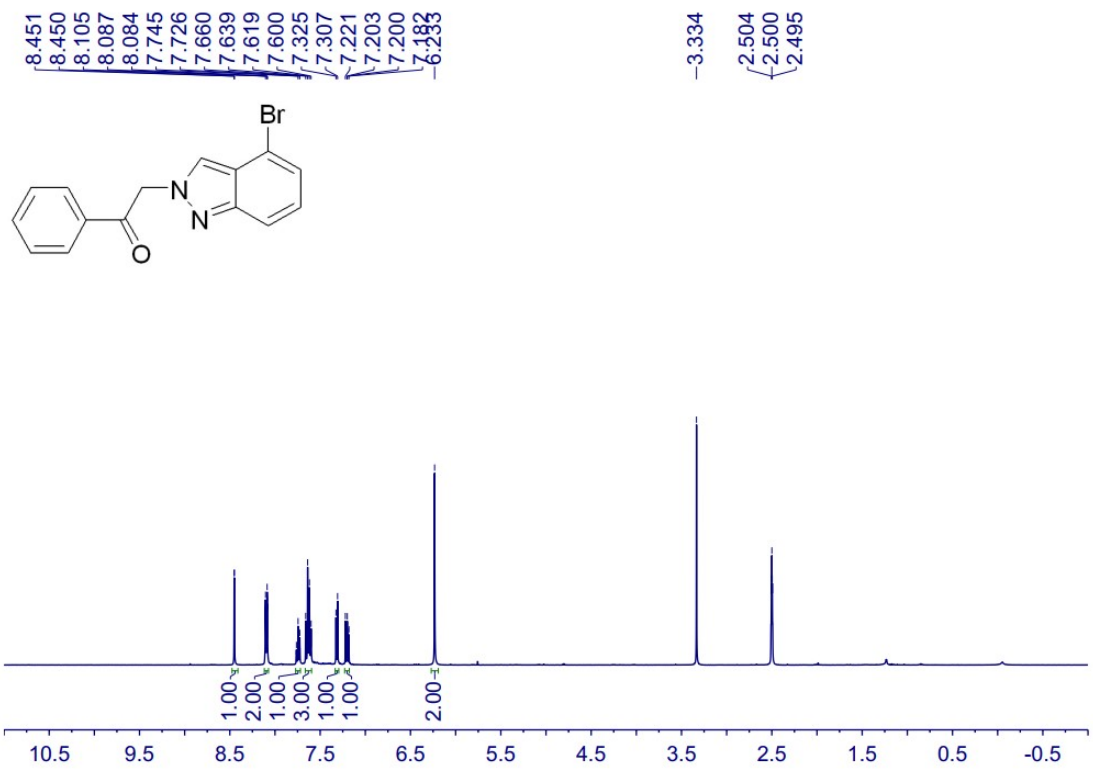
^{13}C NMR Spectrum of Compound **3ap** (100 MHz, DMSO-d_6)



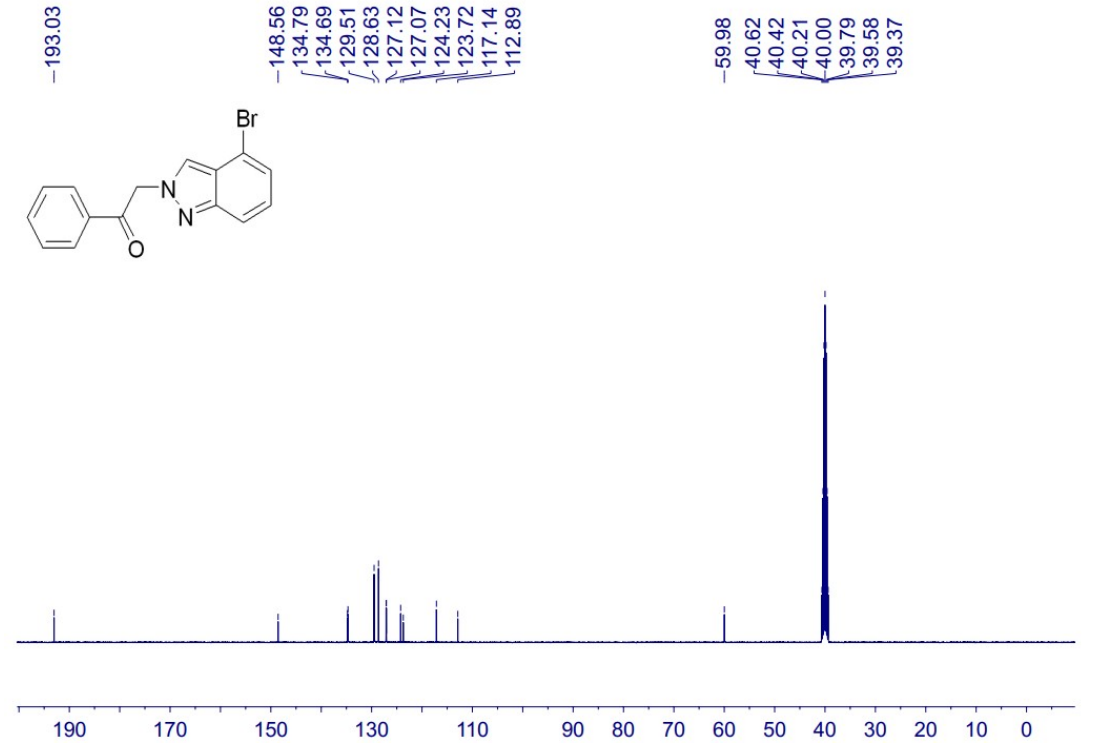
^{1}H NMR Spectrum of Compound **3aq** (400 MHz, DMSO-d_6)



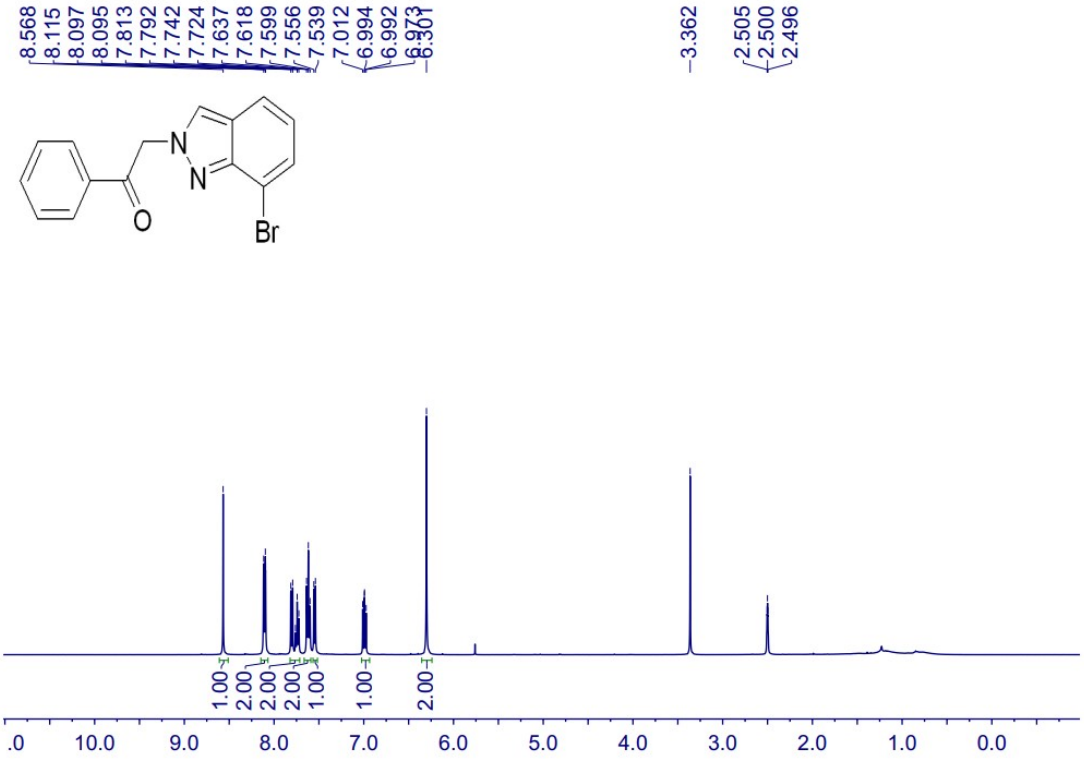
^{13}C NMR Spectrum of Compound **3aq** (100 MHz, DMSO-d_6)



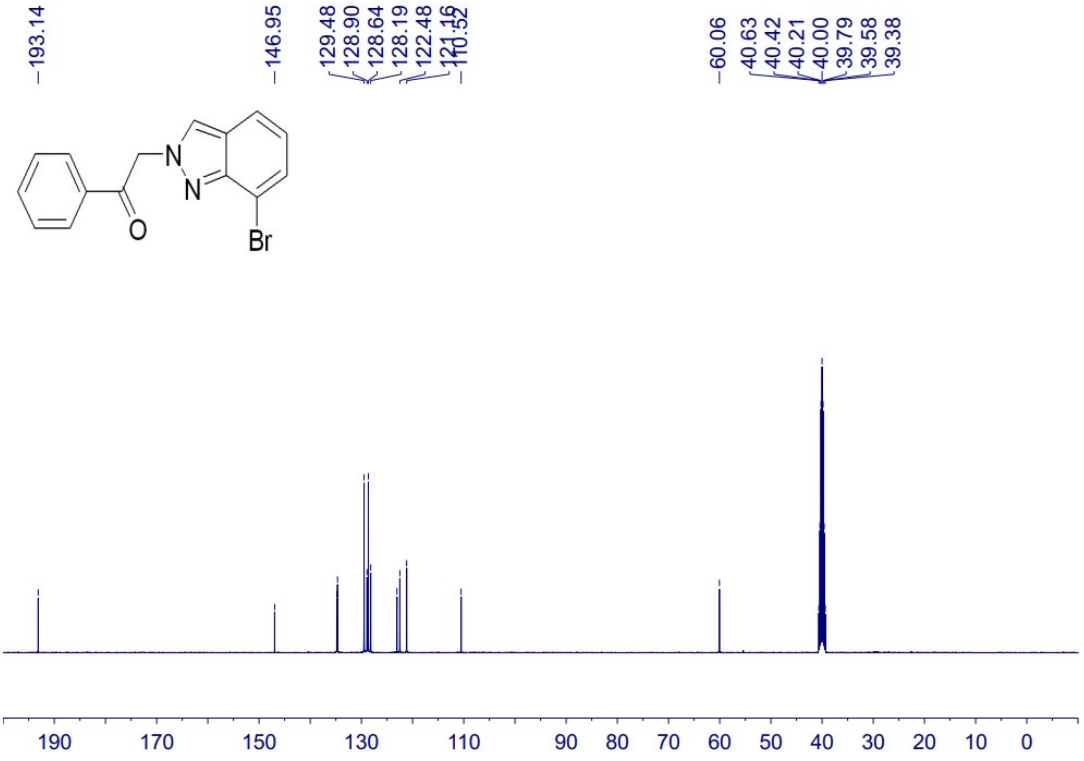
^{1}H NMR Spectrum of Compound **3ar** (400 MHz, DMSO-d_6)



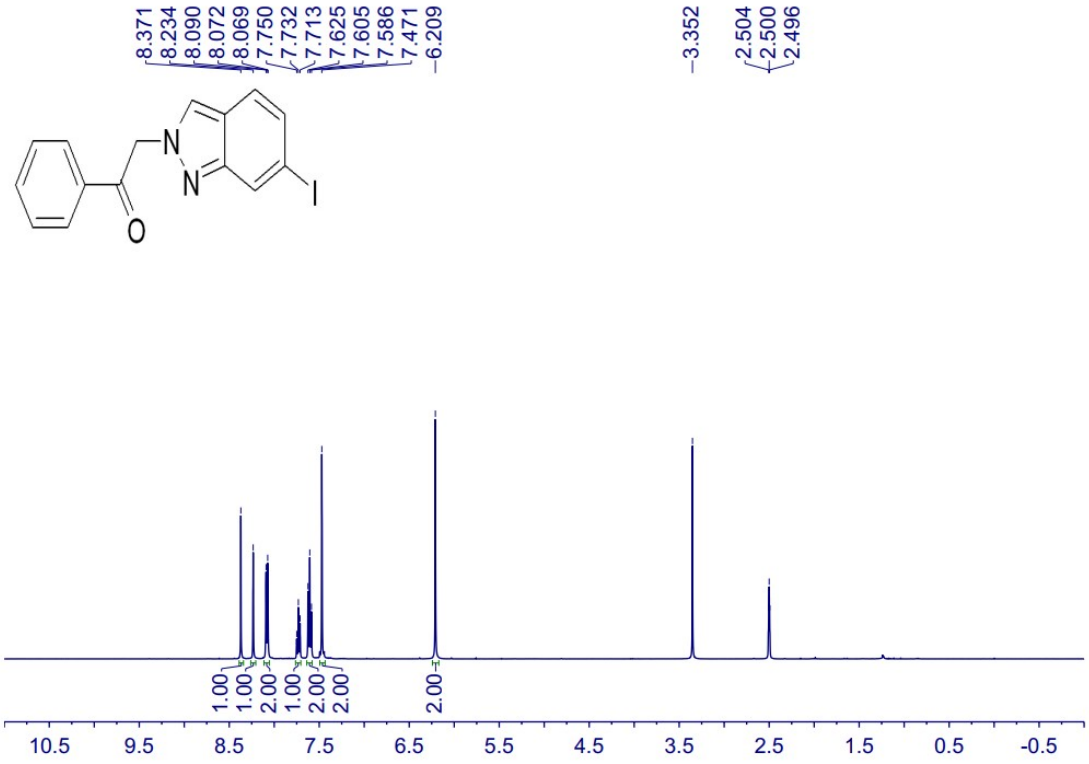
^{13}C NMR Spectrum of Compound **3ar** (100 MHz, DMSO-d_6)



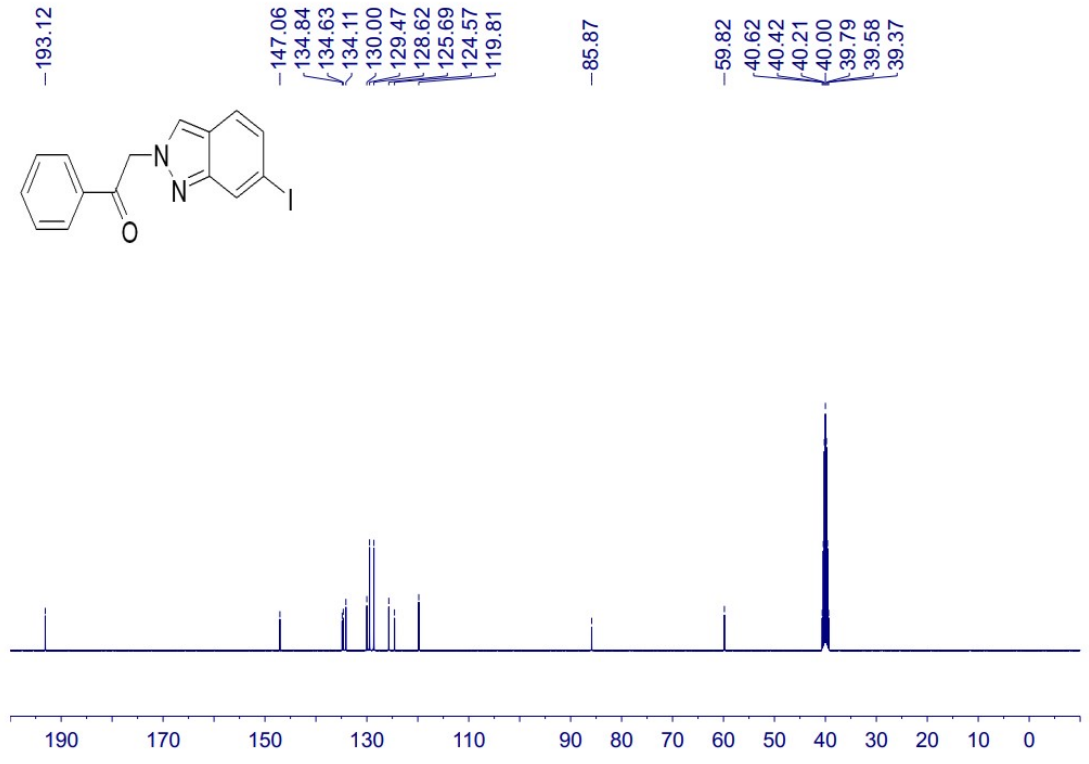
^{1}H NMR Spectrum of Compound **3as** (400 MHz, DMSO-d_6)



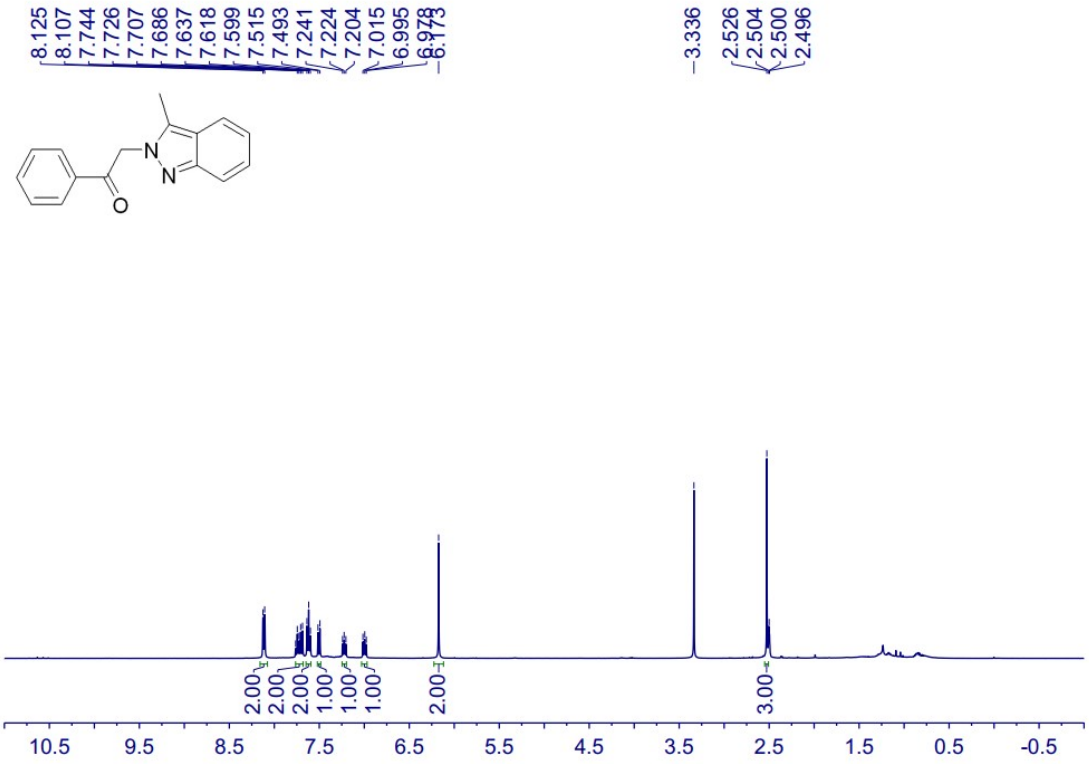
^{13}C NMR Spectrum of Compound **3as** (100 MHz, DMSO-d_6)



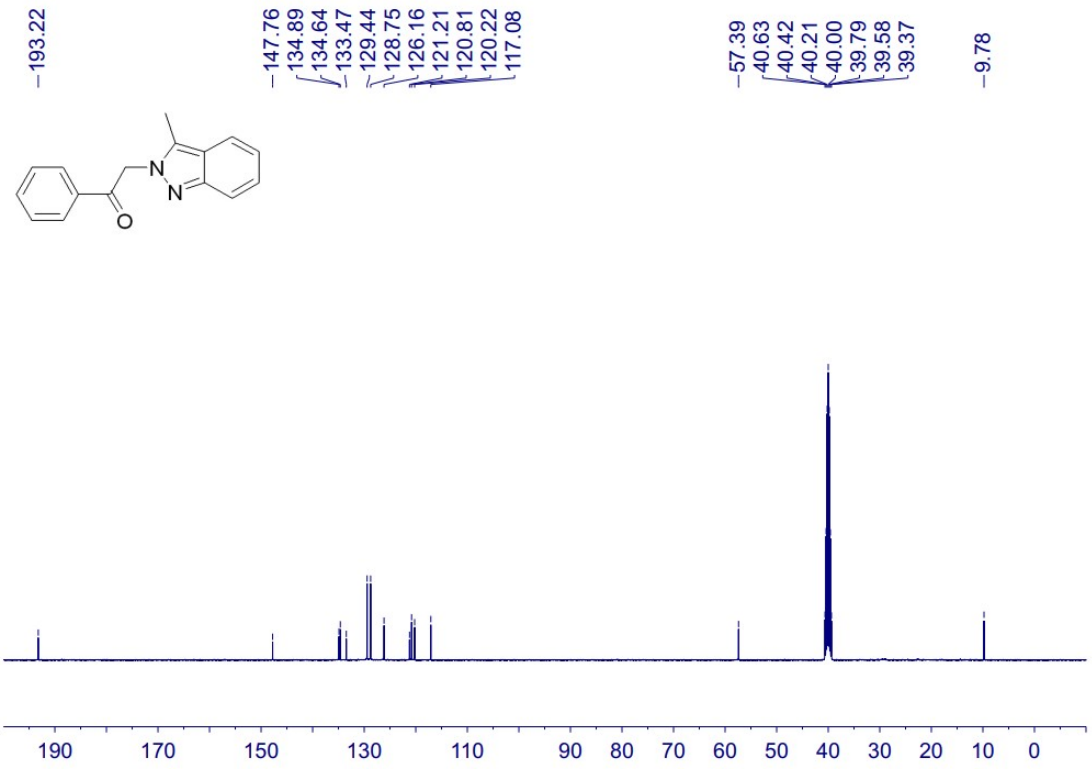
^{1}H NMR Spectrum of Compound **3at** (400 MHz, DMSO-d_6)



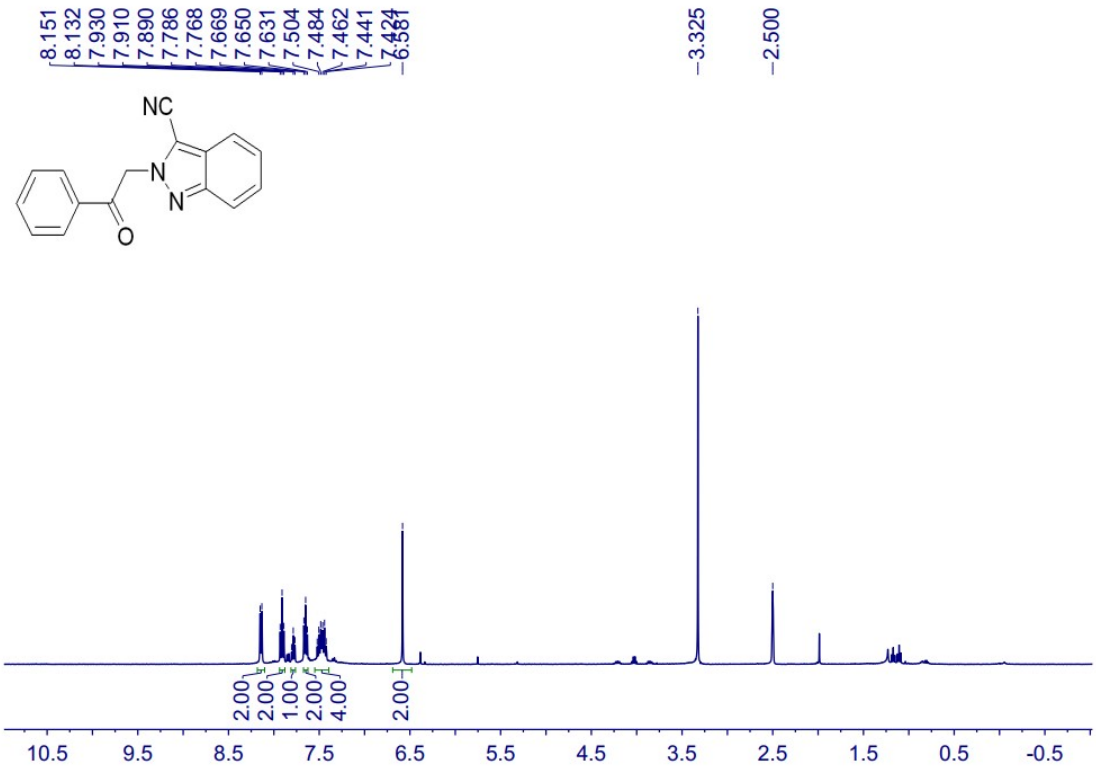
^{13}C NMR Spectrum of Compound **3at** (100 MHz, DMSO-d_6)



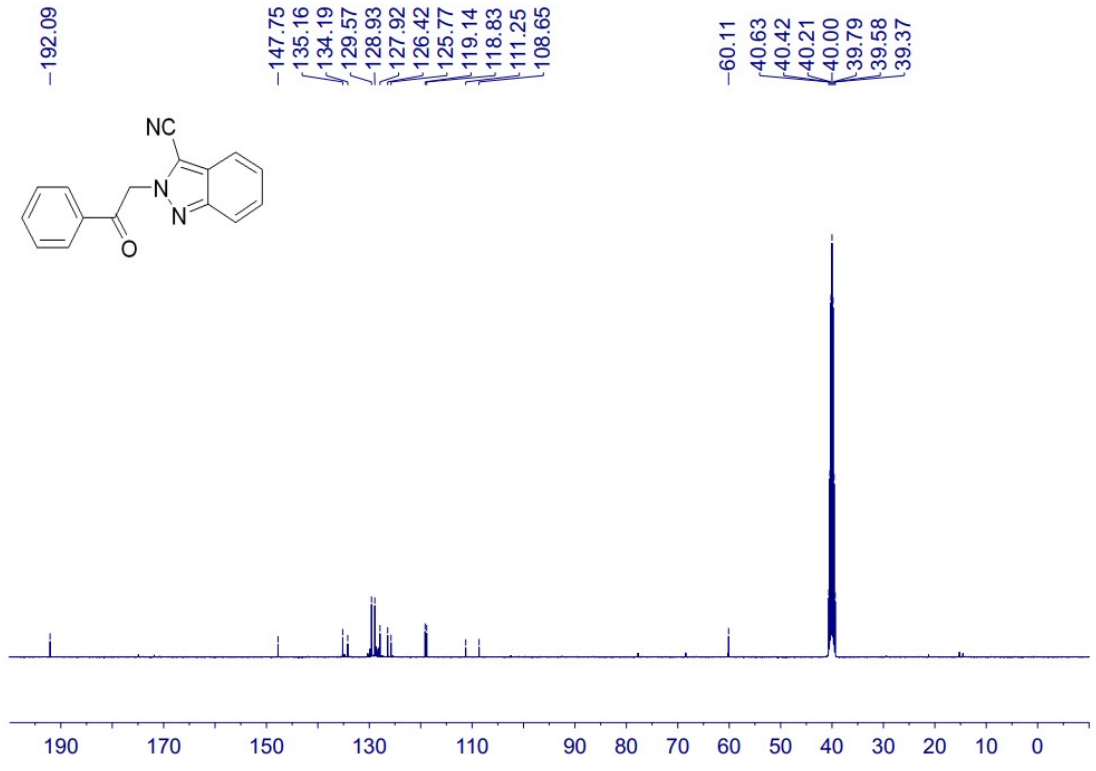
^{1}H NMR Spectrum of Compound **3au** (400 MHz, DMSO-d_6)



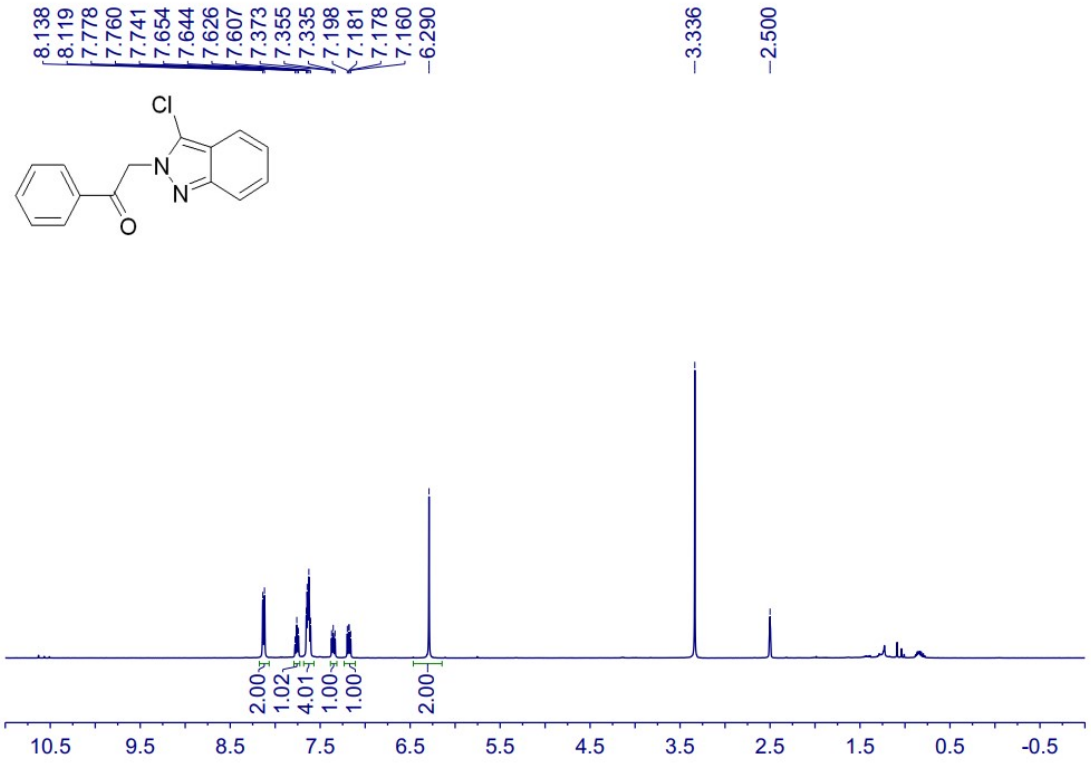
^{13}C NMR Spectrum of Compound **3au** (100 MHz, DMSO-d_6)



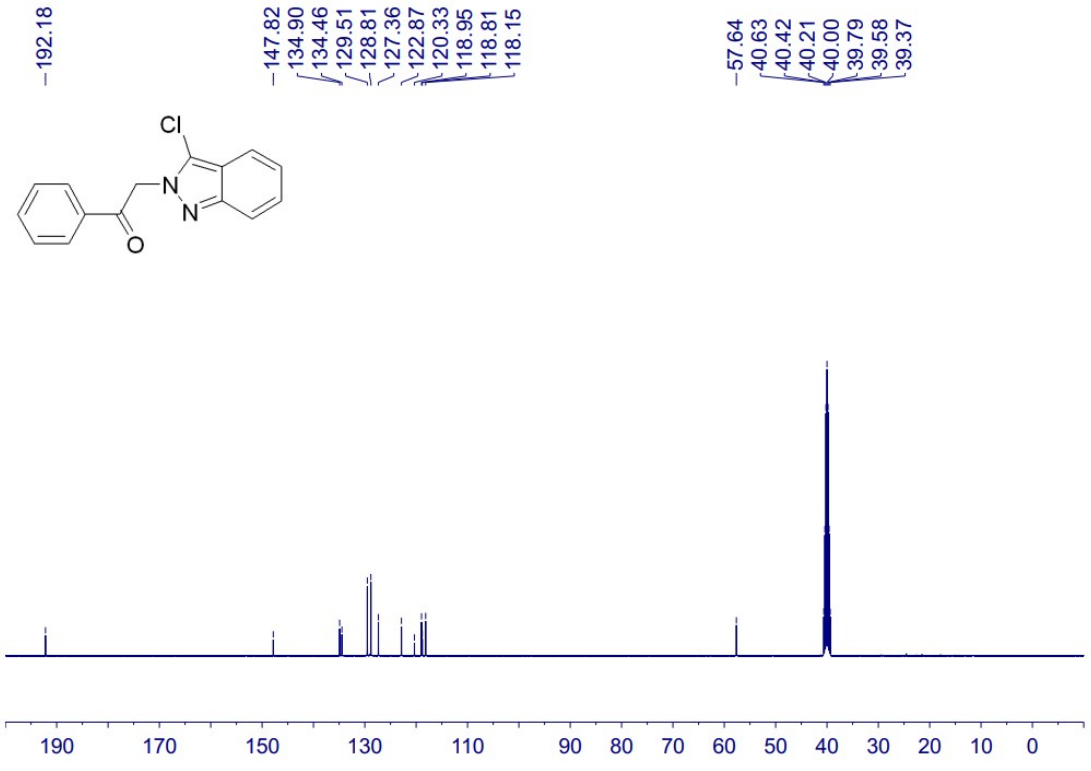
^{1}H NMR Spectrum of Compound **3av** (400 MHz, DMSO-d_6)



^{13}C NMR Spectrum of Compound **3av** (100 MHz, DMSO-d_6)

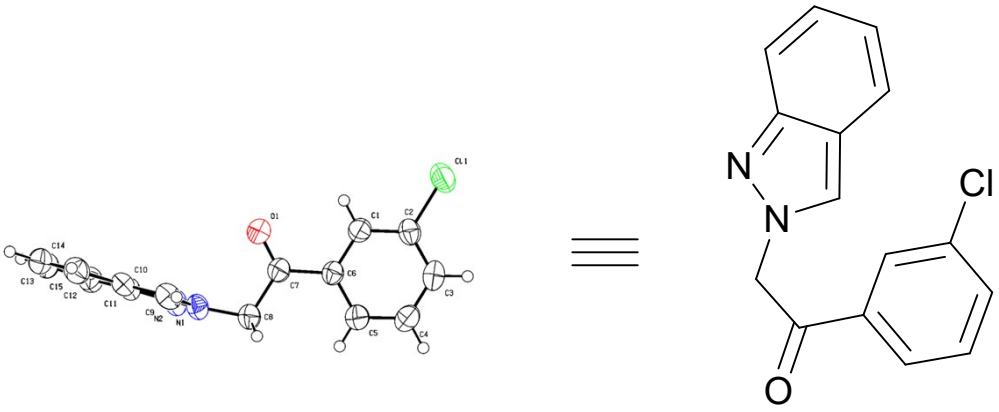


^{1}H NMR Spectrum of Compound **3aw** (400 MHz, DMSO-d_6)



^{13}C NMR Spectrum of Compound **3aw** (100 MHz, DMSO-d_6)

6. X-ray Diffraction Parameters and Data of 3p



Bond precision: C-C = 0.0041 A Wavelength=0.71073

Cell: a=8.134(3) b=8.219(3) c=19.460(8)
alpha=90 beta=101.500(9) gamma=90
Temperature: 296 K

	Calculated	Reported
Volume	1274.9(8)	1274.8(9)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C15 H11 Cl N2 O	?
Sum formula	C15 H11 Cl N2 O	C15 H11 Cl N2 O
Mr	270.71	270.71
Dx,g cm-3	1.410	1.410
Z	4	4
Mu (mm-1)	0.291	0.292
F000	560.0	560.0
F000'	560.79	
h,k,lmax	9,9,23	9,9,23
Nref	2275	2272
Tmin,Tmax	0.943,0.943	0.864,0.864
Tmin'	0.943	

Correction method= # Reported T Limits: Tmin=0.864 Tmax=0.864
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 25.104

R(reflections)= 0.0459(1395) wR2(reflections)= 0.1084(2272)

S = 1.042 Npar= 172

```
The following ALERTS were generated. Each ALERT has the format
      test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

 Alert level C
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00413 Ang.

 Alert level G
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check

   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   1 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   2 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   1 ALERT type 2 Indicator that the structure model may be wrong or deficient
   1 ALERT type 3 Indicator that the structure quality may be low
   0 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

Table 1. Crystal data and structure refinement for 1_a.

Identification code	1_a	
Empirical formula	C15 H11 Cl N2 O	
Formula weight	270.71	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 8.134(3) Å	α= 90°.
	b = 8.219(3) Å	β= 101.500(9)°.
	c = 19.460(8) Å	γ = 90°.
Volume	1274.8(9) $Å^3$	
Z	4	
Density (calculated)	1.410 Mg/m^3	
Absorption coefficient	0.292 mm^{-1}	
F(000)	560	
Crystal size	0.200 x 0.200 x 0.200 mm^3	
Theta range for data collection	2.699 to 25.104°.	
Index ranges	-9<=h<=9, -9<=k<=9, -23<=l<=23	
Reflections collected	34632	
Independent reflections	2272 [R(int) = 0.1018]	
Completeness to theta = 25.104°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2272 / 0 / 172	

Goodness-of-fit on F^2	1.042
Final R indices [I>2sigma(I)]	R1 = 0.0459, wR2 = 0.0852
R indices (all data)	R1 = 0.1031, wR2 = 0.1084
Extinction coefficient	n/a
Largest diff. peak and hole	0.210 and -0.196 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 1_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4542(3)	3369(3)	4407(1)	45(1)
C(2)	3347(3)	3011(3)	4793(1)	45(1)
C(3)	1790(4)	3732(4)	4647(2)	54(1)
C(4)	1428(4)	4832(4)	4102(2)	59(1)
C(5)	2608(3)	5205(4)	3708(1)	52(1)
C(6)	4187(3)	4483(3)	3859(1)	41(1)
C(7)	5518(4)	4862(3)	3457(1)	49(1)
C(8)	5102(3)	6017(3)	2838(1)	49(1)
C(9)	7856(3)	6891(3)	2575(1)	48(1)
C(10)	8802(3)	6383(3)	2095(1)	43(1)
C(11)	7789(3)	5190(3)	1687(1)	40(1)
C(12)	8347(4)	4401(3)	1131(1)	50(1)
C(13)	9888(4)	4799(4)	1013(2)	54(1)
C(14)	10901(4)	5986(4)	1415(2)	57(1)
C(15)	10389(3)	6789(4)	1945(2)	54(1)
Cl(1)	3824(1)	1637(1)	5486(1)	63(1)
N(1)	6420(3)	6042(3)	2438(1)	44(1)
N(2)	6322(3)	4966(3)	1900(1)	46(1)
O(1)	6913(3)	4285(3)	3624(1)	82(1)

Table 3. Bond lengths [Å] and angles [°] for 1_a.

C(1)-C(2)	1.373(3)
C(1)-C(6)	1.391(3)
C(1)-H(1)	0.9300
C(2)-C(3)	1.375(4)
C(2)-Cl(1)	1.743(3)
C(3)-C(4)	1.381(4)
C(3)-H(3)	0.9300
C(4)-C(5)	1.377(4)
C(4)-H(4)	0.9300
C(5)-C(6)	1.392(3)
C(5)-H(5)	0.9300
C(6)-C(7)	1.489(4)
C(7)-O(1)	1.213(3)
C(7)-C(8)	1.519(4)
C(8)-N(1)	1.444(3)
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700
C(9)-N(1)	1.340(3)
C(9)-C(10)	1.388(3)
C(9)-H(9)	0.9300
C(10)-C(11)	1.418(3)
C(10)-C(15)	1.419(4)
C(11)-N(2)	1.351(3)
C(11)-C(12)	1.413(4)
C(12)-C(13)	1.358(4)
C(12)-H(12)	0.9300
C(13)-C(14)	1.409(4)
C(13)-H(13)	0.9300
C(14)-C(15)	1.358(4)
C(14)-H(14)	0.9300
C(15)-H(15)	0.9300
N(1)-N(2)	1.361(3)
C(2)-C(1)-C(6)	119.9(2)
C(2)-C(1)-H(1)	120.1
C(6)-C(1)-H(1)	120.1

C(1)-C(2)-C(3)	121.3(3)
C(1)-C(2)-Cl(1)	119.3(2)
C(3)-C(2)-Cl(1)	119.5(2)
C(2)-C(3)-C(4)	119.1(3)
C(2)-C(3)-H(3)	120.5
C(4)-C(3)-H(3)	120.5
C(5)-C(4)-C(3)	120.5(3)
C(5)-C(4)-H(4)	119.7
C(3)-C(4)-H(4)	119.7
C(4)-C(5)-C(6)	120.2(3)
C(4)-C(5)-H(5)	119.9
C(6)-C(5)-H(5)	119.9
C(1)-C(6)-C(5)	119.0(2)
C(1)-C(6)-C(7)	118.6(2)
C(5)-C(6)-C(7)	122.4(2)
O(1)-C(7)-C(6)	121.2(2)
O(1)-C(7)-C(8)	120.3(2)
C(6)-C(7)-C(8)	118.5(2)
N(1)-C(8)-C(7)	111.4(2)
N(1)-C(8)-H(8A)	109.3
C(7)-C(8)-H(8A)	109.3
N(1)-C(8)-H(8B)	109.3
C(7)-C(8)-H(8B)	109.3
H(8A)-C(8)-H(8B)	108.0
N(1)-C(9)-C(10)	106.7(2)
N(1)-C(9)-H(9)	126.6
C(10)-C(9)-H(9)	126.6
C(9)-C(10)-C(11)	104.2(2)
C(9)-C(10)-C(15)	135.9(3)
C(11)-C(10)-C(15)	119.9(2)
N(2)-C(11)-C(12)	127.7(2)
N(2)-C(11)-C(10)	111.9(2)
C(12)-C(11)-C(10)	120.5(2)
C(13)-C(12)-C(11)	117.8(3)
C(13)-C(12)-H(12)	121.1
C(11)-C(12)-H(12)	121.1
C(12)-C(13)-C(14)	122.1(3)
C(12)-C(13)-H(13)	119.0

C(14)-C(13)-H(13)	119.0
C(15)-C(14)-C(13)	121.6(3)
C(15)-C(14)-H(14)	119.2
C(13)-C(14)-H(14)	119.2
C(14)-C(15)-C(10)	118.1(3)
C(14)-C(15)-H(15)	120.9
C(10)-C(15)-H(15)	120.9
C(9)-N(1)-N(2)	114.0(2)
C(9)-N(1)-C(8)	127.7(2)
N(2)-N(1)-C(8)	117.9(2)
C(11)-N(2)-N(1)	103.2(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 1_a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	42(2)	50(2)	44(2)	0(1)	10(1)	2(1)
C(2)	48(2)	50(2)	37(2)	-3(1)	11(1)	-7(1)
C(3)	50(2)	64(2)	53(2)	-7(2)	22(2)	-7(2)
C(4)	46(2)	72(2)	62(2)	1(2)	16(2)	10(2)
C(5)	52(2)	59(2)	46(2)	3(1)	14(1)	6(2)
C(6)	43(2)	44(2)	39(2)	-3(1)	12(1)	1(1)
C(7)	53(2)	50(2)	47(2)	2(1)	20(1)	10(2)
C(8)	53(2)	53(2)	43(2)	1(1)	17(1)	6(1)
C(9)	57(2)	45(2)	40(2)	-3(1)	6(1)	-8(2)
C(10)	49(2)	42(2)	38(2)	6(1)	9(1)	-1(1)
C(11)	44(2)	41(2)	37(1)	4(1)	11(1)	-2(1)
C(12)	57(2)	49(2)	46(2)	1(1)	14(1)	1(1)
C(13)	57(2)	60(2)	50(2)	6(2)	21(2)	10(2)
C(14)	45(2)	68(2)	61(2)	15(2)	16(2)	1(2)
C(15)	48(2)	58(2)	53(2)	7(2)	5(1)	-11(2)
Cl(1)	67(1)	71(1)	54(1)	13(1)	18(1)	-7(1)
N(1)	53(1)	45(1)	38(1)	-1(1)	15(1)	-2(1)
N(2)	53(1)	47(1)	40(1)	-4(1)	14(1)	-7(1)
O(1)	65(2)	102(2)	89(2)	45(1)	41(1)	34(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 1_a.

	x	y	z	U(eq)
H(1)	5587	2867	4512	54
H(3)	992	3482	4913	65
H(4)	378	5325	3999	71
H(5)	2349	5941	3339	62
H(8A)	4060	5680	2536	58
H(8B)	4944	7105	3006	58
H(9)	8159	7669	2924	58
H(12)	7681	3634	854	60
H(13)	10287	4273	656	65
H(14)	11947	6224	1315	69
H(15)	11060	7583	2202	65

Table 6. Torsion angles [°] for 1_a.

C(6)-C(1)-C(2)-C(3)	0.2(4)
C(6)-C(1)-C(2)-Cl(1)	-179.02(19)
C(1)-C(2)-C(3)-C(4)	0.2(4)
Cl(1)-C(2)-C(3)-C(4)	179.4(2)
C(2)-C(3)-C(4)-C(5)	0.0(4)
C(3)-C(4)-C(5)-C(6)	-0.4(4)
C(2)-C(1)-C(6)-C(5)	-0.7(4)
C(2)-C(1)-C(6)-C(7)	179.2(2)
C(4)-C(5)-C(6)-C(1)	0.8(4)
C(4)-C(5)-C(6)-C(7)	-179.0(3)
C(1)-C(6)-C(7)-O(1)	-3.9(4)
C(5)-C(6)-C(7)-O(1)	175.9(3)
C(1)-C(6)-C(7)-C(8)	177.1(2)
C(5)-C(6)-C(7)-C(8)	-3.0(4)
O(1)-C(7)-C(8)-N(1)	10.6(4)
C(6)-C(7)-C(8)-N(1)	-170.4(2)
N(1)-C(9)-C(10)-C(11)	-0.3(3)
N(1)-C(9)-C(10)-C(15)	178.9(3)
C(9)-C(10)-C(11)-N(2)	-0.3(3)
C(15)-C(10)-C(11)-N(2)	-179.6(2)
C(9)-C(10)-C(11)-C(12)	179.3(2)
C(15)-C(10)-C(11)-C(12)	-0.1(4)
N(2)-C(11)-C(12)-C(13)	-179.1(2)
C(10)-C(11)-C(12)-C(13)	1.4(4)
C(11)-C(12)-C(13)-C(14)	-1.6(4)
C(12)-C(13)-C(14)-C(15)	0.3(4)
C(13)-C(14)-C(15)-C(10)	1.1(4)
C(9)-C(10)-C(15)-C(14)	179.7(3)
C(11)-C(10)-C(15)-C(14)	-1.2(4)
C(10)-C(9)-N(1)-N(2)	0.8(3)
C(10)-C(9)-N(1)-C(8)	173.2(2)
C(7)-C(8)-N(1)-C(9)	-82.0(3)
C(7)-C(8)-N(1)-N(2)	90.2(3)
C(12)-C(11)-N(2)-N(1)	-178.8(2)
C(10)-C(11)-N(2)-N(1)	0.7(3)
C(9)-N(1)-N(2)-C(11)	-0.9(3)

C(8)-N(1)-N(2)-C(11)	-174.2(2)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for 1_a [Å and °].

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