Supporting Information for

Study on N^2-Indolyl-1,2,3-triazole's Fluorescent Activity

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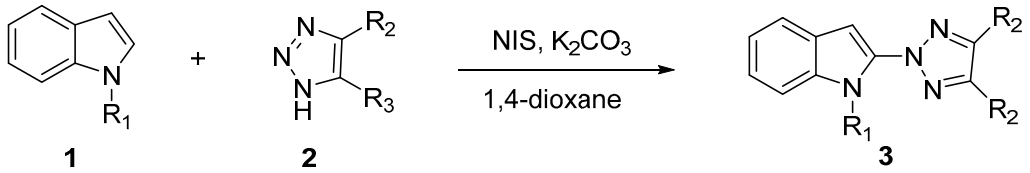
Contents

General Conditions

All reactions were run under an inert atmosphere (Ar) with flame-dried glassware using standard techniques for manipulating air-sensitive compounds. All solvents were dried and purified before use by standard procedures. Commercial reagents were used as supplied or purified by standard techniques where necessary. Column chromatography was performed using 200-300 mesh silica with the proper solvent system according to TLC analysis using $KMnO_4$ stain and UV light to visualize the reaction components. Unless otherwise noted, nuclear magnetic resonance spectra were recorded on 400 MHz spectrometer. NMR data were reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet and bs = broad singlet), coupling constant in Hz and integration. Chemical shifts for ^{13}C NMR spectra were recorded in parts per million from tetramethylsilane using the central peak of deuterochloroform (77.05 ppm) as the internal standard. IR spectra were recorded on an FTIR spectrometer (KBr) and reported in reciprocal centimeters (cm^{-1}). HRMS data were obtained using ESI ionization. Mp data were measured with micro melting point apparatus. Electronic absorption spectra were obtained on a CARY50 PROBE UV-visible spectrometer; Photoluminescent spectra were recorded with a LS55 luminescence spectrometer with the excitation and emission slit widths at 2.5 nm.[1] The indoles **1c**,**1d**,**1e**,**1s-1u**,**1w**,**1x**, tryptophan **1y**, triazoles were prepared according to the reported procedures,[2-7] and 2,4-diphenyl-2H-1,2,3-triazole was prepared according to the reported procedures.[8] The indoles 1a,1b were bought from commercial source.

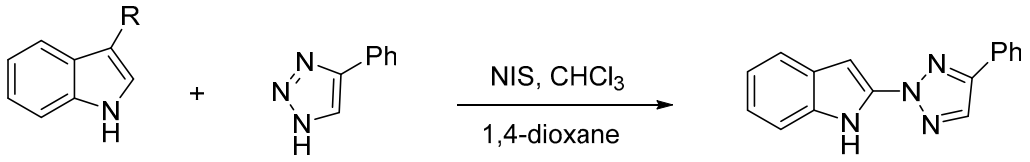
General procedure for coupling reaction, condition 1 for the synthesis of 3a-3u:



1 **2** **3**

To a suspension of N-iodosuccinimide (0.3 mmol) and K_2CO_3 (0.5 mmol) in dry dioxane (1 mL), was added dropwise a solution of 1 (0.2 mmol) and 2 (0.1 mmol) in dioxane (1 mL) in 5 min. 30 min later, the reaction mixture was diluted with 20 mL EtOAc, and was then washed with saturated aqueous $Na_2S_2O_3$ (5 mL), brine (10 mL) and water (10 mL). The organic phase was dried over anhydrous sodium sulfate, filtered and concentrated in vacuo. Purification of the crude product through flash chromatography (petroleum/EtOAc=50/1 as the eluent) afforded **3**.

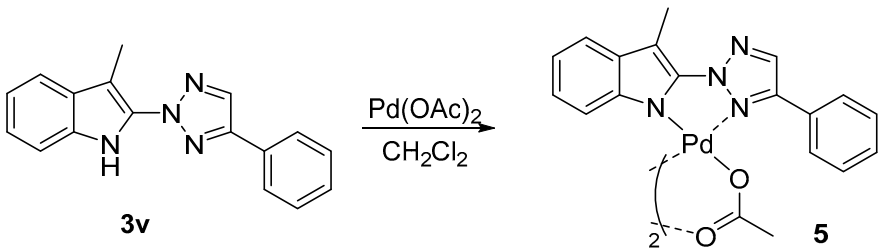
General procedure for coupling reaction, condition 2 for the synthesis of 3v-3y:



1 2a 3

To a suspension of 1 (0.1 mmol), 2a (0.2 mmol) in dry dioxane (1 mL), was added 0.1 mL $CHCl_3$, and then added dropwise a solution of N-iodosuccinimide (0.3 mmol) in dioxane (1 mL) in 5 min. 30 min later, the reaction mixture was diluted with 20 mL EtOAc, and was then washed with saturated aqueous $Na_2S_2O_3$ (5 mL), brine (10 mL) and water (10 mL). The organic phase was dried over anhydrous sodium sulfate, filtered and concentrated in vacuo. Purification of the crude product through flash chromatography (petroleum/EtOAc=50/1 as the eluent) afforded 3.

Synthetic procedure for compound 5:



3v 5

To a suspension of 3v (0.05 mmol) and $Pd(OAc)_2$ (0.05 mmol) in dry CH_2Cl_2 (1 mL) at rt gave a white solid 5 in 45% yield.

The absorption and emission spectra of products[1]

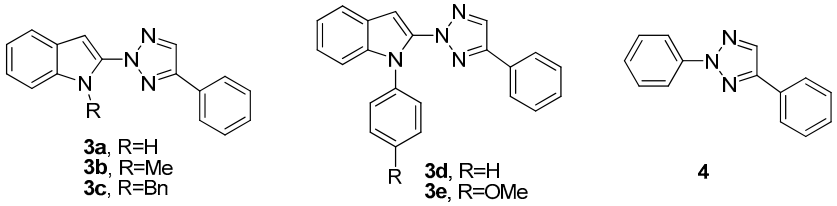
For the method to determine the fluorescence quantum yield:

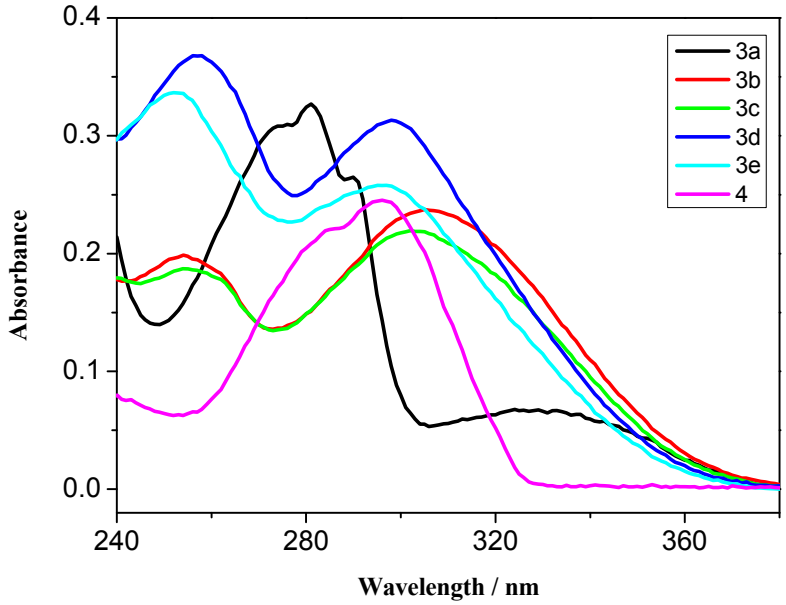
Fluorescence quantum yield was determined in DCM using optically matching solutions of 9,10-Diphenylanthracene (Φ_f = 0.95 in cyclohexane) as standard at an excitation wavelength of 320 nm and the quantum yield was calculated using the following equation:

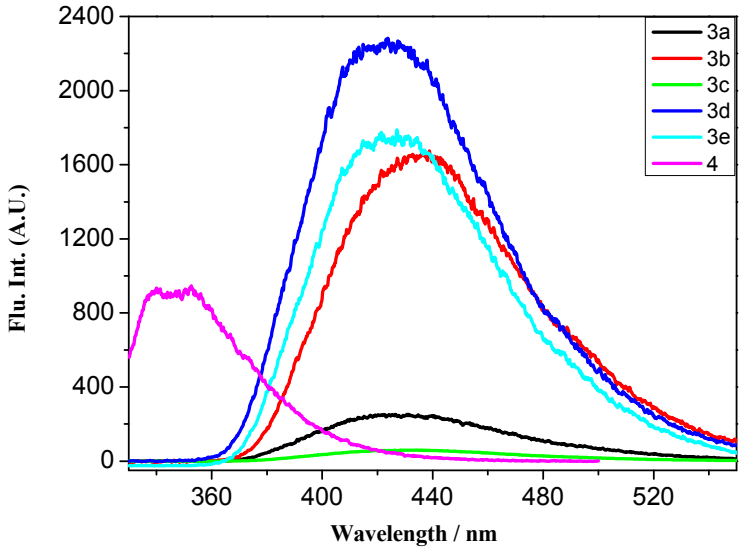
$$\Phi_f = \Phi_r (A_r F_s / A_s F_r) (n_s^2 / n_r^2)$$

where, As and Ar are the absorbance of the sample and the reference, respectively, at the same excitation wavelength, Fs and Fr are the corresponding relative integrated fluorescence intensities, and n is the refractive index of the solvent.

The absorption and emission spectra of products **3(a-e),4**:

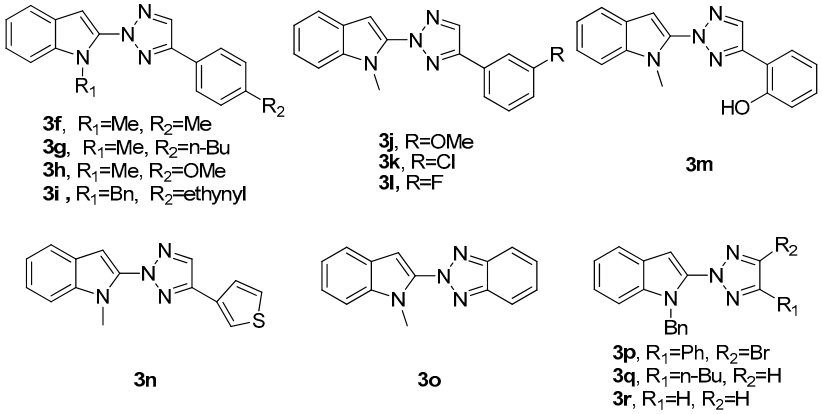


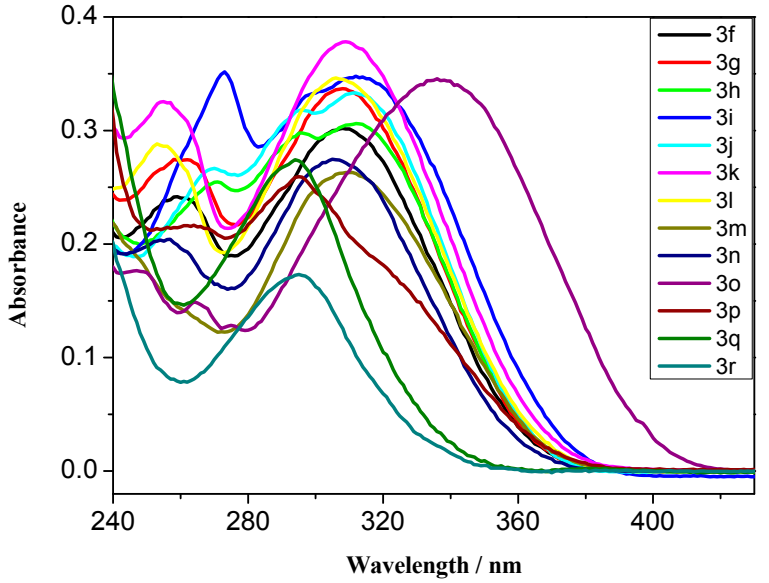


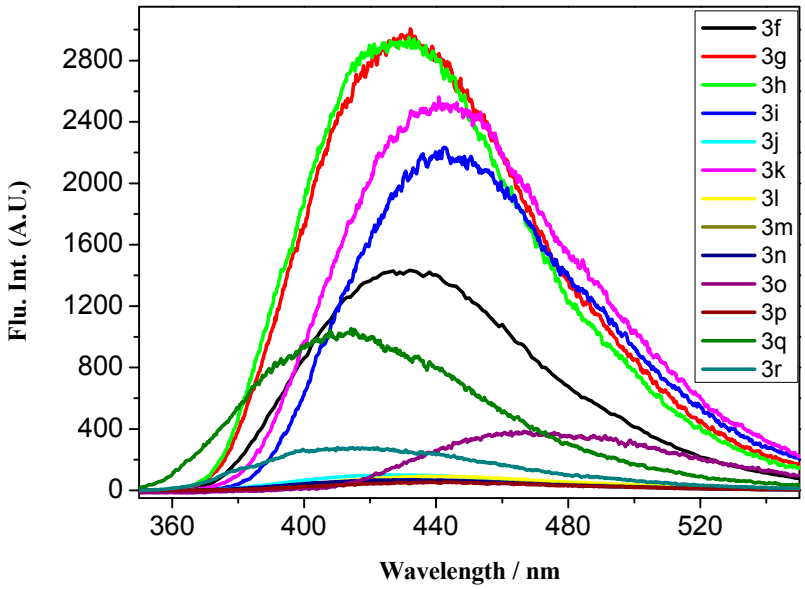


Sample preparation: 1.0 x 10^{-5} mol/L in CH_2Cl_2, with 2.5 nm slit.

The absorption and emission spectra of products **3(f-r)**:

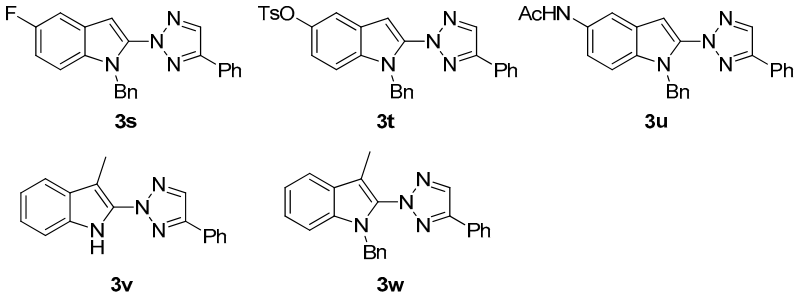


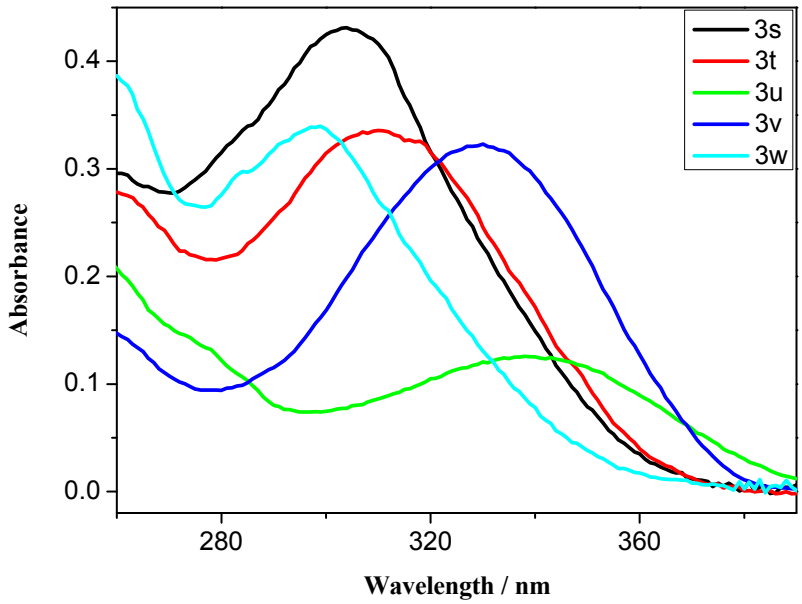


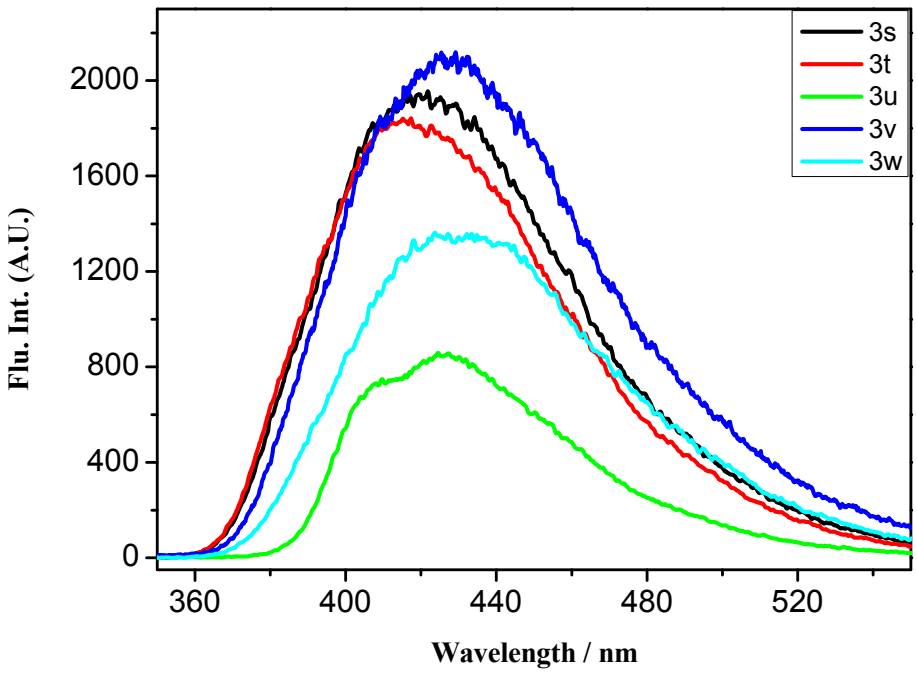


Sample preparation: 1.0 x 10^{-5} mol/L in CH_2Cl_2, with 2.5 nm slit.

The absorption and emission spectra of products **3(s-w)**:

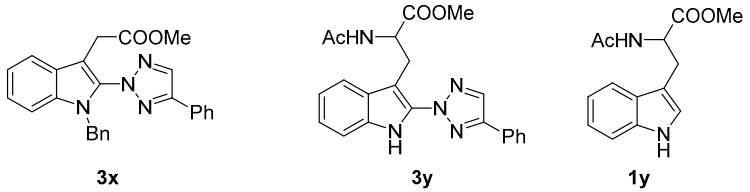


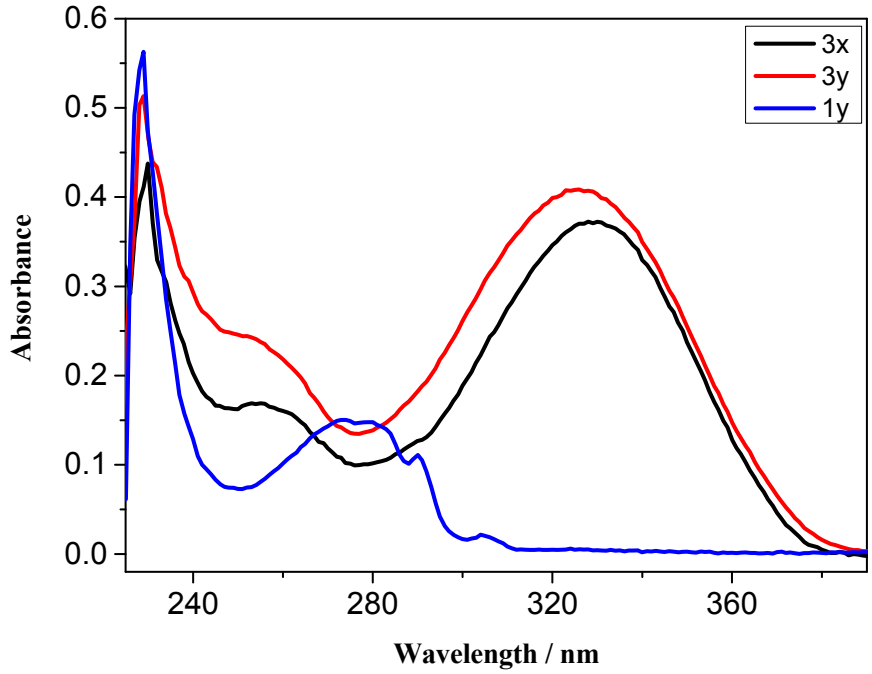


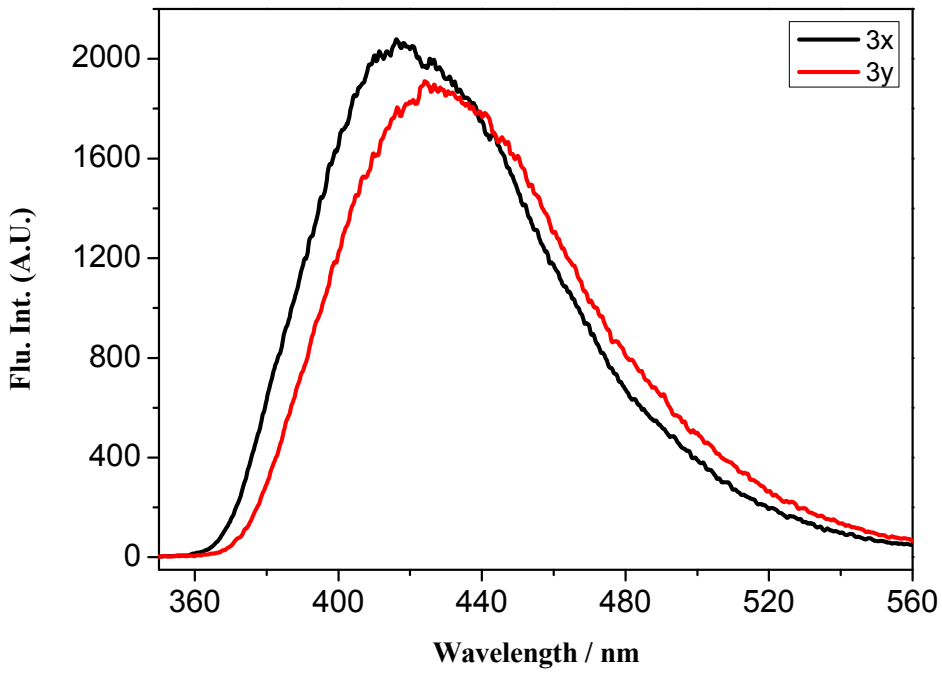


Sample preparation: 1.0 x 10^{-5} mol/L in CH_2Cl_2, with 2.5 nm slit.

The absorption and emission spectra of products **3(x-y)**

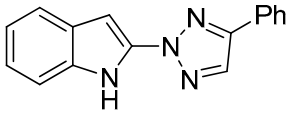






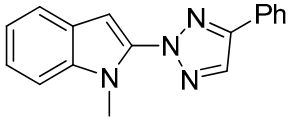
Sample preparation: 1.0 x 10^{-5} mol/L in CH_2Cl_2, with 2.5 nm slit.

Characterization Data:



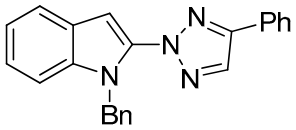
2-(4-phenyl-2H-1,2,3-triazol-2-yl)-1H-indole 3a :

Obtained as a white solid in 60.2% yield; M.p. 128 – 130 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.07 (br, 1H), 8.07 (s, 1H), 7.89 (d, J = 7.1 Hz, 2H), 7.66 (d, J = 7.8 Hz, 1H), 7.49 (t, J = 7.4 Hz, 2H), 7.42 (dd, J = 7.7, 2.8 Hz, 2H), 7.28 – 7.22 (m, 1H), 7.21 – 7.15 (m, 1H), 6.90 (d, J = 1.4 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.05, 134.80, 133.54, 132.82, 129.44, 129.16, 129.06, 127.89, 126.22, 122.86, 121.04, 120.98, 111.20, 90.31; IR (neat) 3119, 3036, 2928, 1564, 1495, 1336, 1091, 956, 858, 767, 732, 686cm^{-1}; HRMS(ESI) m/z calcd for $C_{16}H_{12}N_4$, $[M+H]^+$ 261.1135, found 261.1126



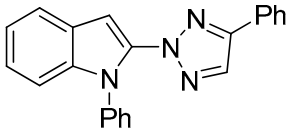
1-methyl-2-(4-phenyl-2H-1,2,3-triazol-2-yl)-1H-indole 3b

Obtained as a white solid in 63.8% yield; M.p. 90 – 91 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (s, 1H), 7.88 (d, J = 7.1 Hz, 2H), 7.66 (d, J = 7.9 Hz, 1H), 7.46 (t, J = 7.4 Hz, 2H), 7.38 (dd, J = 12.9, 7.8 Hz, 2H), 7.30 (t, J = 7.1 Hz, 1H), 7.18 (t, J = 6.9 Hz, 1H), 6.84 (s, 1H), 3.83 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.08, 135.92, 135.44, 133.02, 129.61, 129.17, 129.10, 126.27, 122.96, 121.41, 120.71, 120.30, 109.83, 96.27, 30.56; IR (neat) 3061, 3035, 1587, 1457, 1326, 968, 832, 767, 701, 502cm^{-1}; HRMS(ESI) m/z calcd for $C_{17}H_{14}N_4$, $[M+H]^+$ 275.1291, found 275.1283



1-Benzyl-2-(4-phenyl-2*H*-1,2,3-triazol-2-yl)-1*H*-indole 3c :

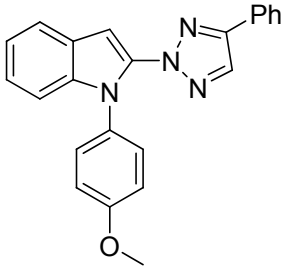
Obtained as a white solid in 71.6% yield; M.p. 91 – 92 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.77 (d, J = 7.2 Hz, 2H), 7.67 (d, J = 7.6 Hz, 1H), 7.39 (t, J = 7.3 Hz, 2H), 7.34 (d, J = 7.1 Hz, 1H), 7.28 (d, J = 8.1 Hz, 1H), 7.22 (d, J = 6.9 Hz, 1H), 7.20 – 7.11 (m, 4H), 7.04 (d, J = 7.0 Hz, 2H), 6.92 (s, 1H), 5.57 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.31, 137.45, 135.77, 135.39, 133.09, 129.60, 129.18, 129.10, 128.70, 127.44, 126.60, 126.44, 126.29, 123.30, 121.57, 121.06, 110.62, 96.96, 47.71; IR (neat) 3059, 3032, 1564, 1454, 1346, 956, 767, 727, 692cm^{-1};HRMS (ESI) Calcd for $C_{23}H_{19}N_4$ $[M+H]^+$: 351.1604; Found: 351.1594.



1-phenyl-2-(4-phenyl-2H-1,2,3-triazol-2-yl)-1H-indole 3d:

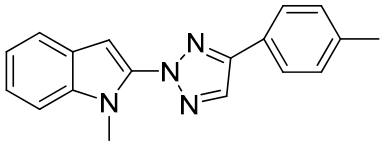
Obtained as a white solid in 56.8% yield; M.p. 91 – 93 ºC; ^{1}H NMR (400 MHz,

$CDCl_3$) δ 8.02 (s, 1H), 7.92 – 7.78 (m, 3H), 7.43 (t, J = 20.5 Hz, 11H), 7.15 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.06, 136.91, 136.60, 135.28, 133.03, 129.70, 129.39, 129.08, 128.07, 127.56, 126.27, 123.87, 121.67, 121.63, 111.11, 98.86; IR (neat) 3061, 3028, 1607, 1534, 1461, 1356, 1055, 946, 768, 723, 692, 483cm^{-1}; HRMS(ESI) m/z calcd for $C_{22}H_{16}N_4$, $[M+H]^+$ 337.1448, found 337.1444



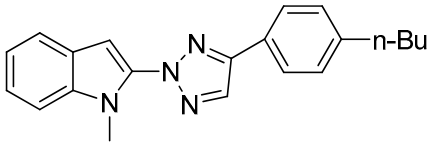
1-(4-methoxyphenyl)-2-(4-phenyl-2H-1,2,3-triazol-2-yl)-1H-indole 3e :

Obtained as a white solid in 51.2% yield; M.p. 94 – 96 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.94 (s, 1H), 7.76 – 7.71 (m, 3H), 7.45 – 7.39 (m, 2H), 7.37 (d, J = 7.2 Hz, 1H), 7.27 – 7.22 (m, 5H), 6.97 (s, 1H), 6.91 (d, J = 8.9 Hz, 2H), 3.81 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.12, 148.87, 136.81, 135.28, 132.84, 129.51, 129.22, 128.95, 128.79, 126.15, 125.94, 123.56, 121.45, 121.25, 114.38, 110.97, 98.30, 55.56; IR (neat): 3118, 3035, 2924, 1589, 1496, 1454, 1328, 1091, 975, 858, 767, 688, 505cm^{-1}; HRMS (ESI) Calcd for $C_{23}H_{18}N_4O$ [M+H]+: 367.1553; Found: 367.1541



1-methyl-2-(4-p-tolyl-2H-1,2,3-triazol-2-yl)-1H-indole 3f :

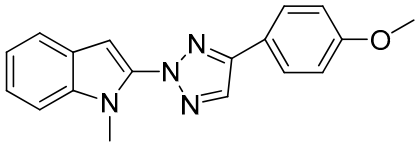
Obtained as a white solid in 58.6% yield; M.p. 94 – 96 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 8.09 (s, 1H), 7.78 (d, J = 8.1 Hz, 2H), 7.66 (d, J = 7.9 Hz, 1H), 7.38 (d, J = 8.2 Hz, 1H), 7.34 – 7.25 (m, 3H), 7.19 (t, J = 7.0 Hz, 1H), 6.83 (s, 1H), 3.87 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.21, 139.17, 135.89, 135.48, 132.85, 129.76, 126.76, 126.15, 122.88, 121.36, 120.65, 109.79, 96.18, 30.87, 21.44; IR (neat) 3056, 3032, 2931, 1559, 1467, 1331, 1145, 966, 772, 701, 536, 458cm^{-1}; HRMS(ESI) m/z calcd for $C_{18}H_{16}N_4$, $[M+H]^+$ 289.1448, found 289.1439



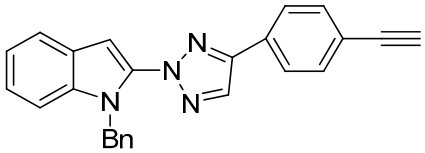
2-(4-(4-butylphenyl)-2H-1,2,3-triazol-2-yl)-1-methyl-1H-indole 3g :

Obtained as a white solid in 51.9% yield; M.p. 87 – 89 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.78 (d, J = 8.1 Hz, 2H), 7.65 (d, J = 7.9 Hz, 1H), 7.35 (d, J = 8.1 Hz, 1H), 7.27 (t, J = 7.8 Hz, 3H), 7.17 (t, J = 7.4 Hz, 1H), 6.83 (s, 1H), 3.85 (s, 3H), 2.69 – 2.60 (m, 2H), 1.69 – 1.56 (m, 2H), 1.43 – 1.30 (m, 2H), 0.93 (t, J = 7.3 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.48, 144.22, 135.94, 135.54, 132.88, 129.15, 127.13, 126.20, 122.91, 121.38, 120.68, 109.81, 96.18, 35.58, 33.59, 30.89, 22.42, 14.06; IR (neat) 3059, 3028, 1594, 1523, 1336, 988, 956, 845, 747, 526, 412cm^{-1};

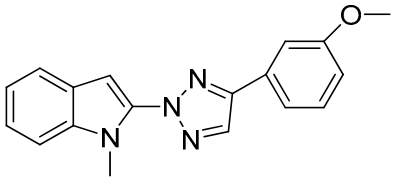
HRMS(ESI) m/z calcd for $C_{21}H_{22}N_4$, $[M+H]^+$ 331.1917, found 331.1909



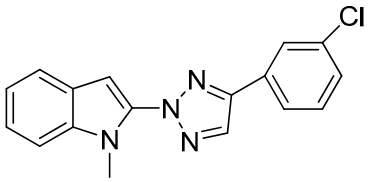
2-(4-(4-methoxyphenyl)-2H-1,2,3-triazol-2-yl)-1-methyl-1H-indole 3h :
Obtained as a white solid in 59.6% yield; M.p. 92 – 93 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.82 (d, J = 8.8 Hz, 2H), 7.66 (d, J = 7.9 Hz, 1H), 7.38 (d, J = 8.2 Hz, 1H), 7.31 (t, J = 7.6 Hz, 1H), 7.18 (t, J = 7.4 Hz, 1H), 6.99 (d, J = 8.8 Hz, 2H), 6.83 (s, 1H), 3.87 (s, 3H), 3.84 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.26, 149.09, 135.86, 135.49, 132.51, 127.57, 126.12, 122.82, 122.18, 121.30, 120.60, 114.44, 109.50, 95.96, 55.37, 30.82; IR (neat) 3061, 2986, 1628, 1495, 1441, 1276, 1063, 987, 823, 715, 681, 512cm^{-1}; HRMS(ESI) m/z calcd for $C_{18}H_{16}N_4O$, $[M+H]^+$ 305.1397, found 305.1387



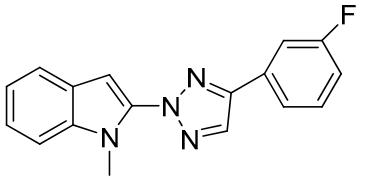
1-benzyl-2-(4-(4-ethynylphenyl)-2H-1,2,3-triazol-2-yl)-1H-indole 3i :
Obtained as a white solid in 52.5% yield; M.p. 108 – 110 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.75 (d, J = 8.0 Hz, 2H), 7.69 (d, J = 7.7 Hz, 1H), 7.55 (d, J = 8.0 Hz, 2H), 7.32 (d, J = 8.1 Hz, 1H), 7.26 – 7.15 (m, 5H), 7.05 (d, J = 7.2 Hz, 2H), 6.93 (s, 1H), 5.60 (s, 2H), 3.15 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.36, 137.30, 135.74, 135.14, 133.11, 132.76, 129.83, 128.62, 127.38, 126.45, 126.30, 126.02, 123.31, 122.74, 121.51, 121.01, 110.51, 97.00, 83.26, 78.53, 47.67; IR (neat) 3356, 3069, 3027, 2109, 1612, 1574, 1452, 1326, 956, 811, 707, 652, 485cm^{-1}; HRMS(ESI) m/z calcd for $C_{25}H_{18}N_4$, $[M+H]^+$ 375.1604, found 375.1593



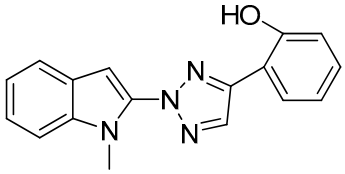
2-(4-(3-methoxyphenyl)-2H-1,2,3-triazol-2-yl)-1-methyl-1H-indole 3j :
Obtained as a white solid in 57.7% yield; M.p. 102 – 104 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.82 (d, J = 8.3 Hz, 2H), 7.66 (d, J = 7.8 Hz, 1H), 7.37 (d, J = 8.1 Hz, 1H), 7.30 (t, J = 7.5 Hz, 1H), 7.18 (t, J = 7.3 Hz, 1H), 6.99 (d, J = 8.3 Hz, 2H), 6.83 (s, 1H), 3.87 (s, 3H), 3.84 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.33, 149.09, 135.85, 135.48, 132.51, 127.56, 126.11, 122.82, 122.18, 121.30, 120.60, 114.20, 109.73, 96.08, 55.37, 30.70; IR (neat) 3059, 2923, 1619, 1486, 1442, 1253, 1072, 986, 836, 727, 692, 518cm^{-1}; HRMS(ESI) m/z calcd for $C_{18}H_{16}N_4O$, $[M+H]^+$ 305.1397, found 305.1390



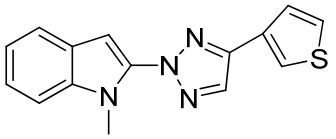
2-(4-(3-chlorophenyl)-2H-1,2,3-triazol-2-yl)-1-methyl-1H-indole 3k :
Obtained as a white solid in 64.9% yield; M.p. 88 – 90 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (s, 1H), 7.86 (s, 1H), 7.69 (td, J = 4.0, 1.5 Hz, 1H), 7.64 (d, J = 7.9 Hz, 1H), 7.36 – 7.26 (m, 4H), 7.17 (t, J = 6.7 Hz, 1H), 6.82 (s, 1H), 3.82 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.79, 135.83, 135.11, 134.93, 132.89, 131.24, 130.21, 128.96, 126.14, 125.93, 124.17, 122.94, 121.30, 120.66, 109.73, 96.19, 30.81; IR (neat) 3062, 3016, 1703, 1561, 1467, 1352, 1266, 1056, 956, 796, 737, 628, 491cm^{-1}; HRMS(ESI) m/z calcd for $C_{17}H_{13}ClN_4$, $[M+H]^+$ 309.0902, found 309.0893



2-(4-(3-fluorophenyl)-2H-1,2,3-triazol-2-yl)-1-methyl-1H-indole 3l :
Obtained as a white solid in 62.1% yield; M.p. 80 – 82 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (s, 1H), 7.66 (t, J = 7.7 Hz, 2H), 7.61 (dd, J = 9.6, 2.0 Hz, 1H), 7.46 – 7.36 (m, 2H), 7.32 (t, J = 7.6 Hz, 1H), 7.19 (t, J = 7.4 Hz, 1H), 7.09 (td, J = 8.4, 2.5 Hz, 1H), 6.85 (s, 1H), 3.88 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.45, 162.00, 148.14, 135.92, 135.21, 133.03, 131.70 (d, J = 8.4 Hz), 130.67 (d, J = 8.3 Hz), 126.03, 123.03, 121.85 (d, J = 2.4 Hz), 121.40, 120.73, 116.96 (d, J = 21.3 Hz), 113.16 (d, J = 23.0 Hz), 109.79, 96.35, 30.87; IR (neat) 3059, 3036, 1601, 1553, 1492, 1352, 1231, 1142, 956, 843, 737, 628, 503, 492cm^{-1}; HRMS(ESI) m/z calcd for $C_{17}H_{13}FN_4$, $[M+H]^+$ 293.1197, found 293.1191

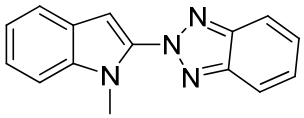


2-(2-(1-methyl-1H-indol-2-yl)-2H-1,2,3-triazol-4-yl)phenol 3m :
Obtained as a white solid in 46.6% yield; M.p. 132 – 135 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.46 (s, 1H), 8.25 (s, 1H), 7.69 (d, J = 7.6 Hz, 2H), 7.41 (d, J = 8.2 Hz, 1H), 7.38 – 7.30 (m, 2H), 7.22 (t, J = 7.4 Hz, 1H), 7.11 (d, J = 8.2 Hz, 1H), 7.02 (t, J = 7.5 Hz, 1H), 6.85 (s, 1H), 3.86 (s, 3H).^{1}H NMR (400 MHz, $CDCl_3$): δ 9.47 (s, 1H), 8.26 (s, 1H), 7.69 (d, J = 8.0Hz, 2H), 7.42 (d, J = 8.2Hz, 1H), 7.38-7.33 (m, 2H), 7.23 (t, J = 7.4Hz, 1H), 7.11 (d, J = 8.3Hz, 1H), 7.03 (t, J = 7.4Hz, 1H) 6.85 (s, 1H), 3.87 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.42, 154.18, 135.86, 132.78, 130.95, 126.66, 123.34, 121.43, 120.92, 120.08, 117.63, 109.86, 96.80, 88.55, 86.71, 30.82; IR (neat) 3108, 3049, 2986, 1663, 1564, 1474, 1366, 996, 757, 727, 691, 479cm^{-1}; HRMS(ESI) m/z calcd for $C_{17}H_{14}N_4O$, $[M+H]^+$ 291.1240, found 291.1236



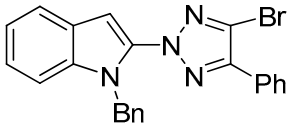
1-methyl-2-(4-(thiophen-3-yl)-2H-1,2,3-triazol-2-yl)-1H-indole 3n :

Obtained as a white solid in 50.6% yield; M.p. 92 – 94 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (s, 1H), 7.70 (d, J = 2.0 Hz, 1H), 7.64 (d, J = 7.9 Hz, 1H), 7.51 (d, J = 4.8 Hz, 1H), 7.39 – 7.36 (m, 1H), 7.34 (d, J = 8.2 Hz, 1H), 7.28 (t, J = 7.5 Hz, 1H), 7.17 (t, J = 7.3 Hz, 1H), 6.82 (s, 1H), 3.82 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.31, 135.82, 135.26, 133.09, 130.85, 126.73, 126.03, 125.91, 122.87, 122.61, 121.30, 120.61, 109.72, 96.24, 30.44; IR (neat) 3033, 2932, 1586, 1454, 1336, 1189, 965, 873, 769, 715, 473cm^{-1}; HRMS(ESI) m/z calcd for $C_{15}H_{12}N_4S$, $[M+H]^+$ 281.0855, found 281.0847



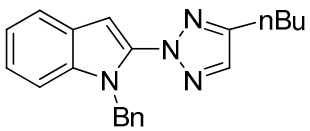
2-(1-methyl-1H-indol-2-yl)-2H-benzo[d][1,2,3]triazole 3o :

Obtained as a white solid in 53.5% yield; M.p. 137 – 139 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (dd, J = 6.6, 3.1 Hz, 2H), 7.70 (d, J = 7.9 Hz, 1H), 7.50 – 7.38 (m, 3H), 7.34 (t, J = 7.5 Hz, 1H), 7.21 (t, J = 7.1 Hz, 1H), 7.06 (s, 1H), 4.00 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.93, 136.51, 135.80, 127.48, 126.06, 123.41, 121.59, 120.89, 118.31, 109.79, 97.65, 31.44; IR (neat) 3052, 3028, 1568, 1452, 1346, 1271, 1059, 956, 771, 732, 692, 433cm^{-1}; HRMS(ESI) m/z calcd for $C_{15}H_{12}N_4$, $[M+H]^+$ 249.1135, found 249.1124



1-benzyl-2-(4-bromo-5-phenyl-2H-1,2,3-triazol-2-yl)-1H-indole 3p

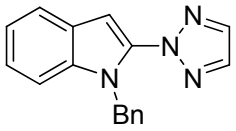
Obtained as a white solid in 53% yield; M.p. 90 – 91 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, J = 6.5 Hz, 2H), 7.70 (d, J = 7.8 Hz, 1H), 7.50 – 7.40 (m, 3H), 7.34 (d, J = 8.1 Hz, 1H), 7.28 (d, J = 7.0 Hz, 1H), 7.24 – 7.17 (m, 4H), 7.05 (d, J = 6.6 Hz, 2H), 6.93 (s, 1H), 5.61 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.99, 137.07, 135.75, 134.54, 129.39, 128.71, 128.64, 128.32, 127.50, 127.45, 126.77, 126.51, 126.11, 123.52, 121.62, 121.08, 110.51, 97.33, 47.65; IR (neat) 3059, 3030, 2924, 1558, 1454, 1328, 1161, 1010, 956, 727, 694cm^{-1}; HRMS (ESI) Calcd for $C_{23}H_{18}BrN_4$ $[M+H]^+$: 429.07094; Found: 429.06996.



1-Benzyl-2-(4-butyl-2H-1,2,3-triazol-2-yl)-1H-indole 3q

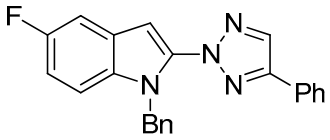
Obtained as a colorless oil in 60% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, J = 7.7 Hz, 1H), 7.51 (s, 1H), 7.22 (d, J = 8.0 Hz, 1H), 7.18 – 7.05 (m, 5H), 6.94 (d, J =

6.9 Hz, 2H), 6.74 (s, 1H), 5.46 (s, 2H), 2.66 (t, J = 7.7 Hz, 2H), 1.83 – 1.46 (m, 2H), 1.36 – 1.20 (m, 2H), 0.85 (t, J = 7.3 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.56, 137.32, 135.46, 134.87, 128.54, 127.28, 126.49, 126.38, 122.96, 121.37, 120.77, 110.44, 96.66, 47.42, 31.09, 25.14, 22.15, 13.75; IR (neat) 3059, 3030, 2929, 1566, 1456, 1346, 1161, 1029, 954, 748, 727, 694cm^{-1}; HRMS (ESI) Calcd for $C_{21}H_{23}N_4$ $[M+H]^+$: 331.1923; Found: 331.1910.



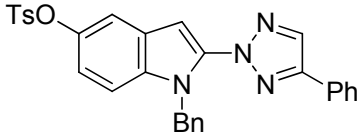
1-Benzyl-2-(2H-1,2,3-triazol-2-yl)-1H-indole 3r

Obtained as a white solid in 95% yield; M.p. 95 – 98 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (s, 2H), 7.61 (d, J = 7.7 Hz, 1H), 7.22 (d, J = 8.2 Hz, 1H), 7.17 – 7.07 (m, 5H), 6.94 (d, J = 6.7 Hz, 2H), 6.80 (s, 1H), 5.45 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.16, 135.97, 135.51, 135.14, 128.69, 127.37, 126.43, 126.25, 123.24, 121.58, 120.92, 110.43, 97.20, 47.57; IR (neat) 3059, 3032, 2360, 1566, 1454, 1163, 945, 748, 727, 455cm^{-1}; HRMS (ESI) Calcd for C17H15N4 $[M+H]^+$: 275.1297; Found: 275.1285.



5-Fluoro-2-(4-phenyl-2H-1,2,3-triazol-2-yl)-1H-indole 3s

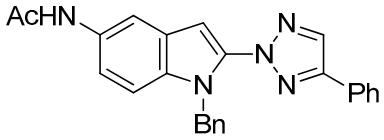
Obtained as a white solid in 78% yield; M.p. 116 – 119 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (s, 1H), 7.81 (d, J = 7.0 Hz, 2H), 7.48 – 7.38 (m, 3H), 7.33 (dd, J = 9.2, 2.4 Hz, 1H), 7.26 – 7.18 (m, 4H), 7.06 (d, J = 6.6 Hz, 2H), 6.98 (td, J = 9.1, 2.5 Hz, 1H), 6.89 (s, 1H), 5.61 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.46(d, *J* =235.9Hz), 149.40, 137.06, 136.43, 133.17, 132.19, 129.38, 129.19, 129.04, 128.69, 127.50, 126.70, 126.59, 126.45, 126.22, 111.84, 111.53(d, *J* =9.5Hz), 111.39, 106.24(d, *J* =23.6Hz), 96.72(d, *J* =4.5Hz), 96.69, 47.85; IR (neat) 3064, 3034, 1722, 1585, 1454, 1342, 1122, 950, 767, 690, 520cm^{-1}; HRMS (ESI) Calcd for $C_{23}H_{18}FN_4$ $[M+H]^+$: 369.1515; Found: 369.1502.



1-Benzyl-2-(4-phenyl-2H-1,2,3-triazol-2-yl)-1H-indol-5-yl-4-methylbenzenesulfonate 3t

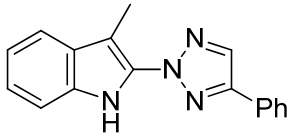
Obtained as a white solid in 83% yield; M.p. 169 – 171 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.80 (d, J = 6.9 Hz, 2H), 7.70 (d, J = 8.3 Hz, 2H), 7.48 – 7.36 (m, 3H), 7.28 (d, J = 8.1 Hz, 2H), 7.25-7.18 (m, 5H), 7.04 (d, J = 6.3 Hz, 2H), 6.89 (dd, J = 8.9, 2.3 Hz, 1H), 6.84 (s, 1H), 5.58 (s, 2H), 2.43 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.50, 145.15, 144.25, 136.78, 136.42, 133.98, 133.28, 132.48, 129.71, 129.26, 129.06, 128.70, 128.64, 127.58, 126.50, 126.22, 123.62, 118.06, 114.65,

111.24, 97.07, 47.96, 21.76; IR (neat) 3064, 3034, 1732, 1581, 1477, 1454, 1176, 1091, 948, 854, 692, 551cm^{-1}; HRMS (ESI) Calcd for C30H25N4O3S [M+H]$^{+}$: 521.1647; Found: 521.1646.



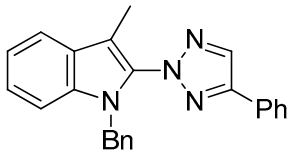
N-(1-Benzyl-2-(4-phenyl-2H-1,2,3,-triazol-2-yl)-1H-indol-5-yl)acetamide 3u

Obtained as a white solid in 60% yield; M.p. 128 – 131 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.87 (br, 1H), 7.80 (d, J = 7.2 Hz, 2H), 7.51 – 7.36 (m, 4H), 7.30 – 7.15 (m, 5H), 7.04 (d, J = 6.8 Hz, 2H), 6.87 (s, 1H), 5.58 (s, 2H), 2.17 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.44, 149.27, 137.20, 135.88, 133.04, 131.50, 129.43, 129.13, 129.02, 128.63, 127.40, 126.46, 126.21, 117.51, 113.23, 110.78, 96.88, 47.77, 24.49; IR (neat) 3062, 3032, 1658, 1550, 1485, 1452, 1276, 956, 767, 692cm^{-1}; HRMS (ESI) Calcd for C25H22N5O [M+H]$^{+}$: 408.1824; Found: 408.1818.



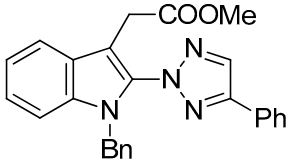
3-Methyl-2-(4-phenyl-2H-1,2,3,-triazol-2-yl)-1H-indole 3v

Obtained as a white solid in 55% yield; M.p. 132 – 134 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.88 (br, 1H), 8.03 (s, 1H), 7.86 (d, J = 5.3 Hz, 2H), 7.60 (d, J = 7.8 Hz, 1H), 7.45 (t, J = 7.4 Hz, 2H), 7.41 – 7.35 (m, 1H), 7.31 (d, J = 8.0 Hz, 1H), 7.23 (t, J = 7.0 Hz, 1H), 7.17 (t, J = 7.0 Hz, 1H), 2.66 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.41, 132.86, 132.15, 130.67, 129.67, 129.14, 129.05, 129.02, 126.17, 123.07, 120.22, 119.38, 110.88, 100.67, 9.02; IR (neat) 3118, 3035, 2924, 1589, 1496, 1454, 1328, 1091, 975, 858, 767, 688, 505cm^{-1}; HRMS (ESI) Calcd for C17H15N4 [M+H]$^{+}$: 275.1297; Found: 275.1286.



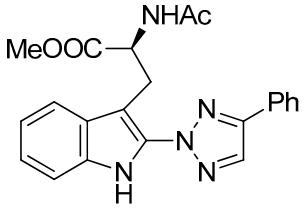
1-Benzyl-3-methyl-2-(4-phenyl-2H-1,2,3,-triazol-2-yl)-1H-indole 3w

Obtained as a white solid in 75% yield; M.p. 78 – 80 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (s, 1H), 7.81 (d, J = 7.0 Hz, 2H), 7.66 (d, J = 7.8 Hz, 1H), 7.43 (t, J = 7.3 Hz, 2H), 7.40 – 7.34 (m, 1H), 7.30 – 7.23 (m, 2H), 7.21 – 7.13 (m, 4H), 7.03 (d, J = 6.4 Hz, 2H), 5.26 (s, 2H), 2.36 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.24, 137.35, 134.70, 133.01, 131.66, 129.69, 129.09, 129.07, 128.60, 127.39, 126.90, 126.68, 126.26, 123.67, 120.17, 119.99, 110.33, 107.43, 47.18, 8.39; IR (neat) 3061, 3034, 1622, 1454, 1350, 1186, 1091, 956, 740, 692, 455cm^{-1}; HRMS (ESI) Calcd for C24H21N4 [M+H]$^{+}$: 365.1766; Found: 365.1756.



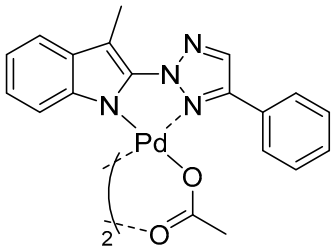
Methyl 2-(1-benzyl-2-(4-phenyl-2H-1,2,3,-triazol-2-yl)-1H-indol-3-yl)acetate 3x

Obtained as a white solid in 67% yield; M.p. 104 – 106 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (s, 1H), 7.82 (d, J = 7.0 Hz, 2H), 7.69 (d, J = 7.8 Hz, 1H), 7.45 (t, J = 7.3 Hz, 2H), 7.42 – 7.37 (m, 1H), 7.33 – 7.27 (m, 2H), 7.24 – 7.18 (m, 4H), 7.06 (d, J = 6.6 Hz, 2H), 5.42 (s, 2H), 3.91 (s, 2H), 3.63 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.49, 149.37, 137.06, 134.65, 133.19, 132.61, 129.49, 129.14, 129.03, 128.61, 127.41, 126.62, 126.23, 123.76, 120.82, 119.90, 110.55, 103.39, 52.09, 47.46, 29.79; IR (neat) 3061, 3034, 1737, 1456, 1348, 1192, 1166, 975, 744, 692, cm^{-1}; HRMS (ESI) Calcd for $C_{26}H_{23}N_4O_2$ $[M+H]^+$: 423.1821; Found: 423.1825.



(S)-Methyl 2-acetamido-3-(2-(4-phenyl-2H-1,2,3,-triazol-2-yl)-1H-indol-3-yl) propanoate 3y

Obtained as a yellow solid in 62% yield, $[\alpha]_D^{20}$ = + 15.1 (*c* = 1.00); M.p. 137 – 140 ^{o}C; ^{1}H NMR (400 MHz, DMSO) δ 12.10 (br, 1H), 8.74 (s, 1H) , 8.47 (d, *J* =7.6Hz, 1H), 8.06 (d, J = 7.2 Hz, 2H), 7.64 (d, J = 7.9 Hz, 1H), 7.56 (t, J = 7.5 Hz, 2H), 7.50 – 7.42 (m, 2H), 7.20 (t, J = 7.5 Hz, 1H), 7.11 (t, J = 7.4 Hz, 1H), 4.69 (q, J = 7.5 Hz, 1H), 3.64 (dd, J = 13.9, 7.4 Hz, 1H), 3.44 (s, 3H), 3.37 (dd, J = 13.9, 7.5 Hz, 1H), 1.77 (s, 3H); ^{13}C NMR (101 MHz, DMSO) δ 172.82, 169.65, 148.85, 133.76, 133.60, 131.78, 129.63, 129.58, 128.12, 126.49, 125.90, 122.93, 120.23, 119.27, 112.15, 100.02, 53.34, 52.10, 26.63, 22.76; IR (neat) 3062, 2254, 1739, 1666, 1456, 1373, 1286, 1026, 977, 769, 696, 507cm^{-1}; HRMS (ESI) Calcd for $C_{22}H_{22}N_5O_3$ $[M+H]^+$: 404.1723; Found: 404.1714.



Compound 5

Obtained as a yellow solid in 45% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.38 (m, 1H), 7.36 (dt, J = 7.8, 3.8 Hz, 1H), 7.01 – 6.94 (m, 1H), 6.72 (d, J = 8.0 Hz, 1H), 6.61 (ddd, J = 7.9, 5.2, 2.7 Hz, 1H), 6.57 (s, 1H), 2.38 (s, 1H), 2.30 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.64, 186.49, 180.98, 173.69, 161.51, 129.30, 128.48, 126.61, 126.02, 121.68, 119.74, 117.96, 111.80, 98.63, 23.79, 7.65.

References:

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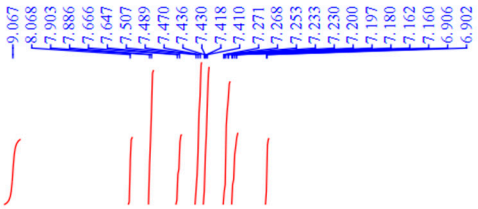
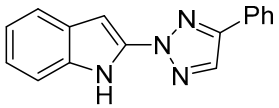
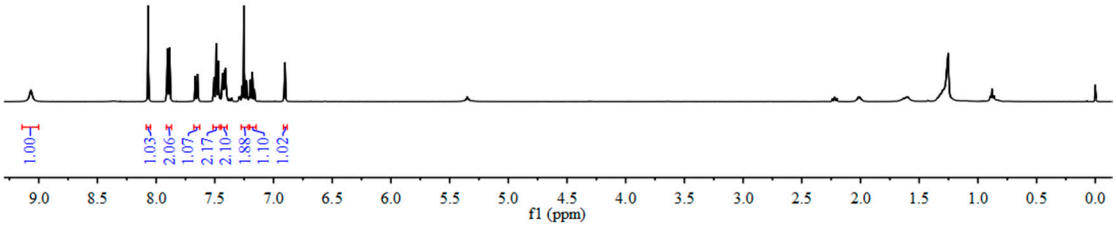
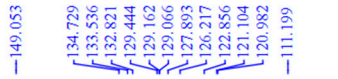
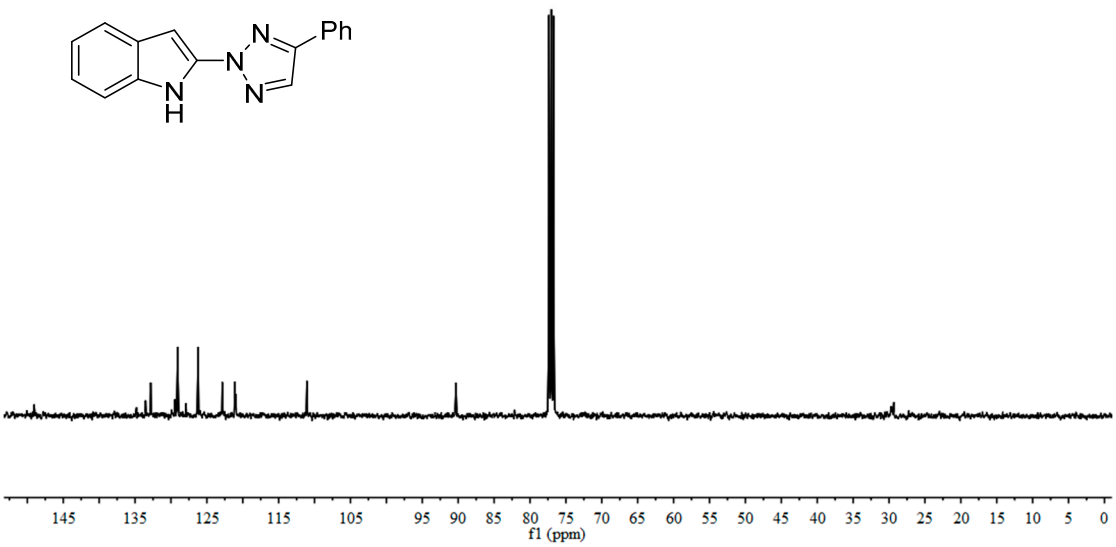
H^1 NMR and C^{13} NMR spectra

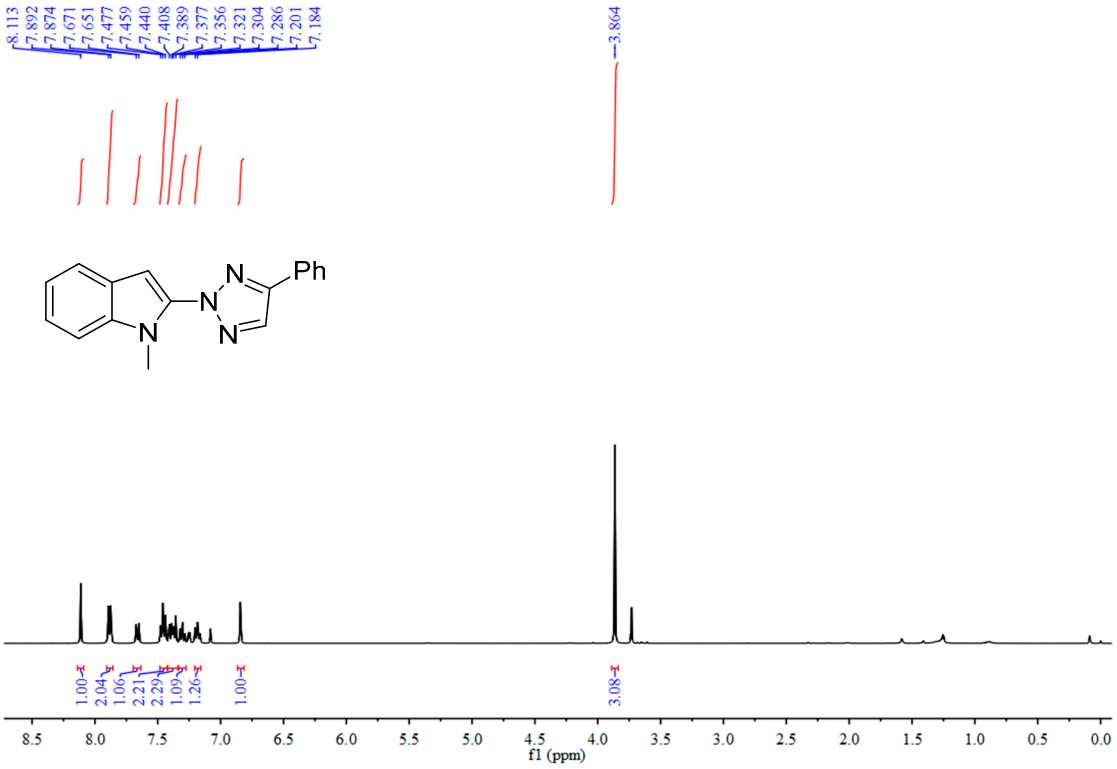








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7.440
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7.321
7.304
7.286
7.201
7.184
3.864
Ph
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N
N
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2.04
1.06
2.21
2.29
1.09
1.26
1.00
3.08
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
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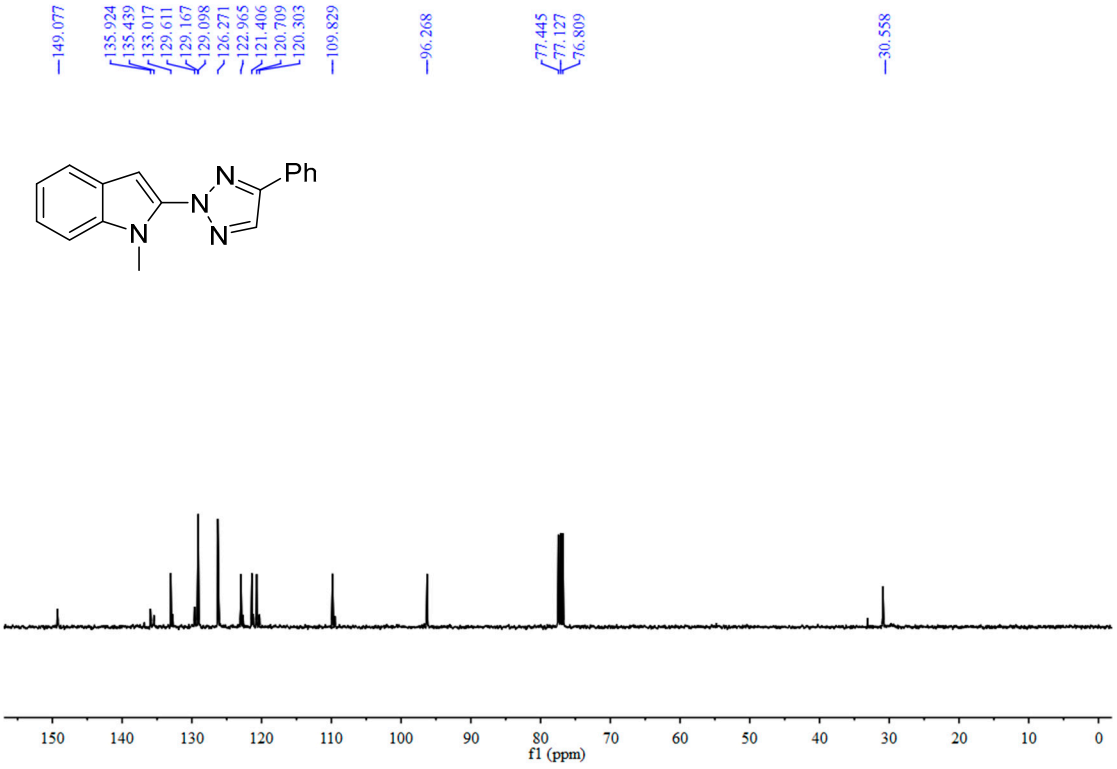
0.0
f1 (ppm)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129.098
126.271
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121.406
120.709
120.303
109.829
96.268
77.445
77.127
76.809
30.558
Ph
N
N
N
150
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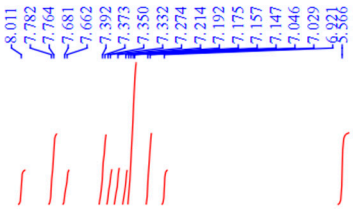
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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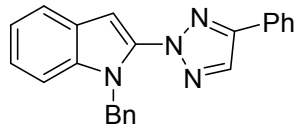
7.029
6.921
5.566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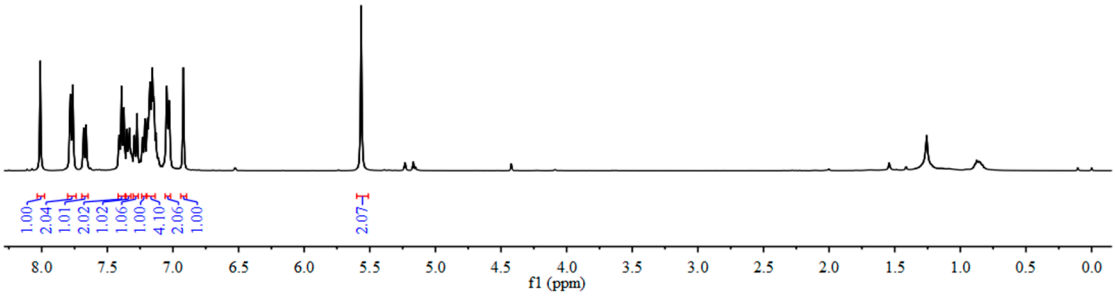
N
Ph
N
Bn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4.10
2.06
1.00
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6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


149.306
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127.445
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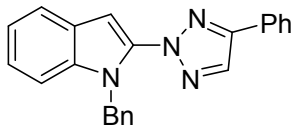
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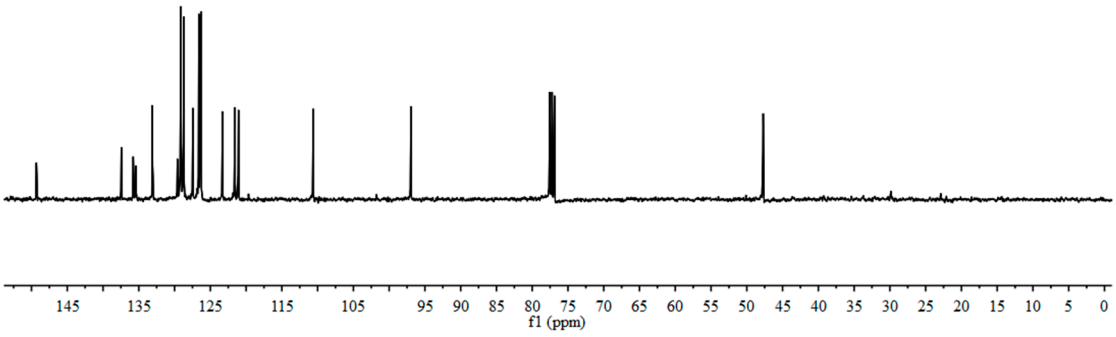
N
Ph
N
Bn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125
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105
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90
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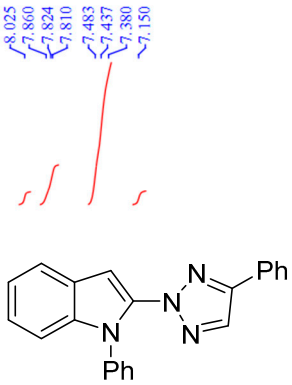
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
f1 (ppm)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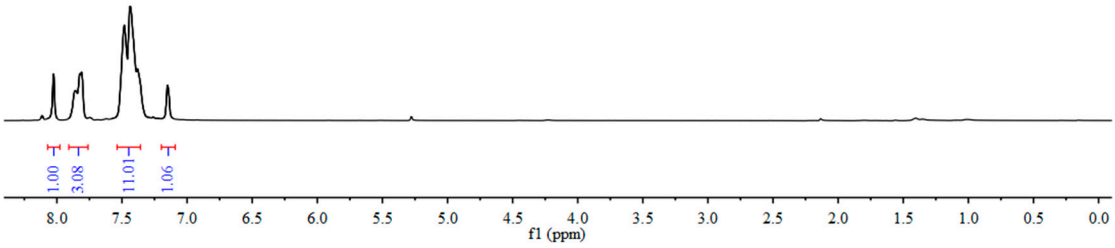
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2.5
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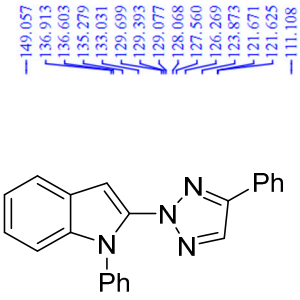
0.0
f1 (ppm)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N
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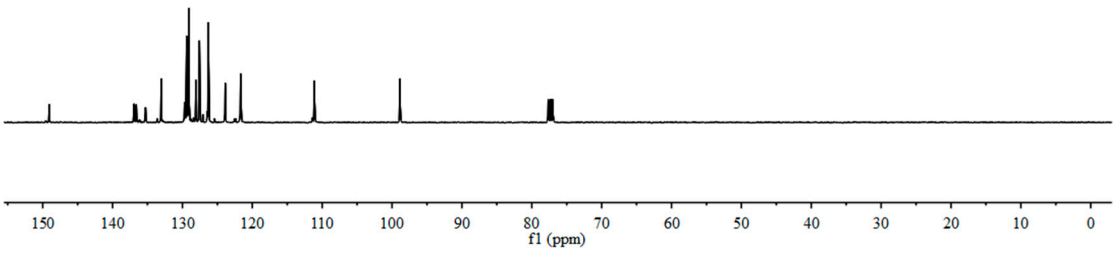
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50
40
30
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10
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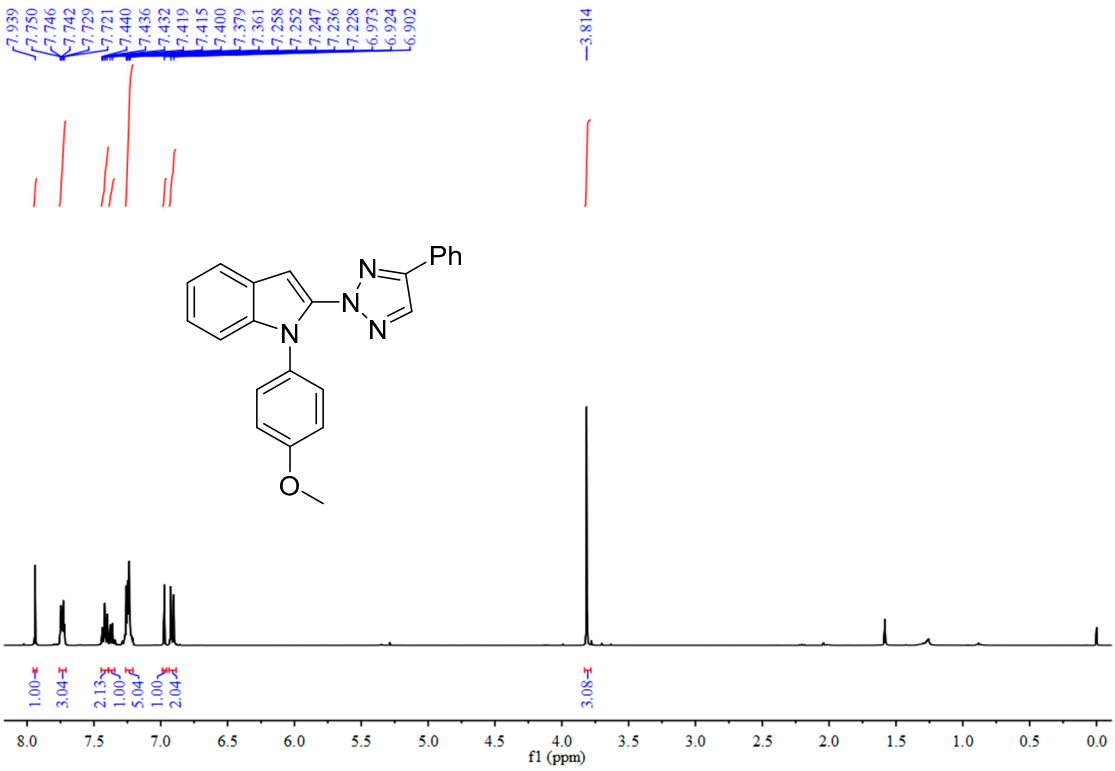
f1 (ppm)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7.432
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7.400
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7.236
7.228
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6.902
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N
N
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1.00
5.04
1.00
2.04
3.08
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
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2.5
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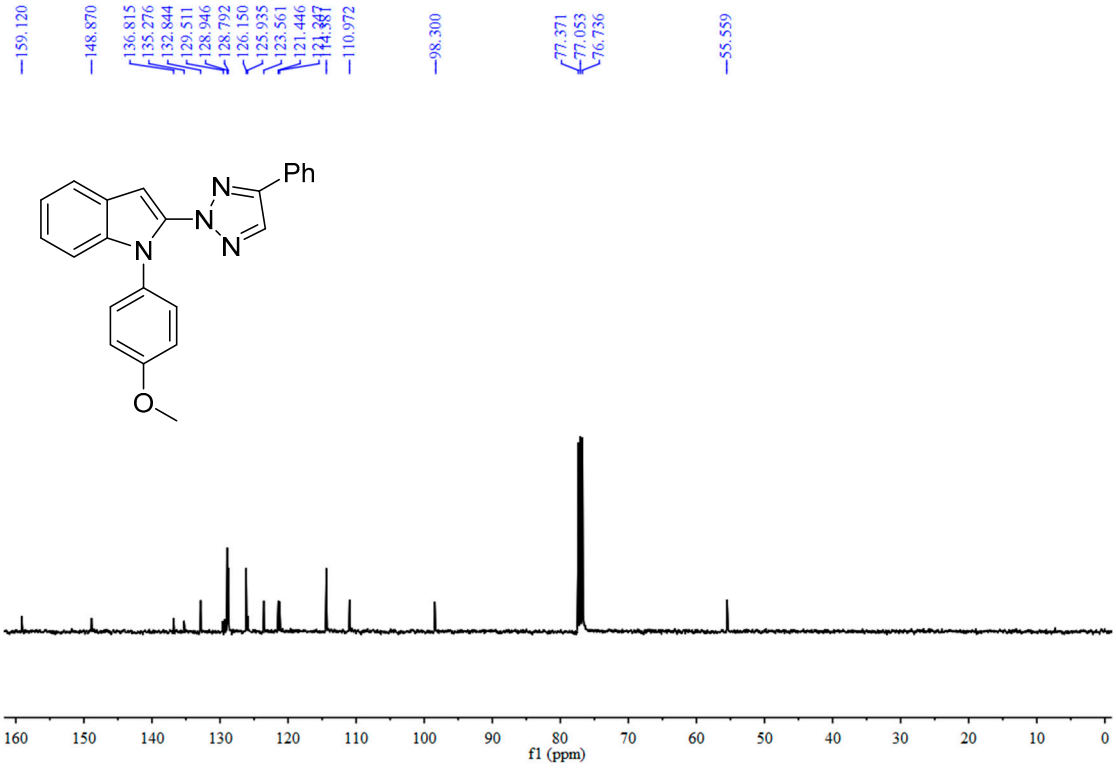
0.0
f1 (ppm)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76.736
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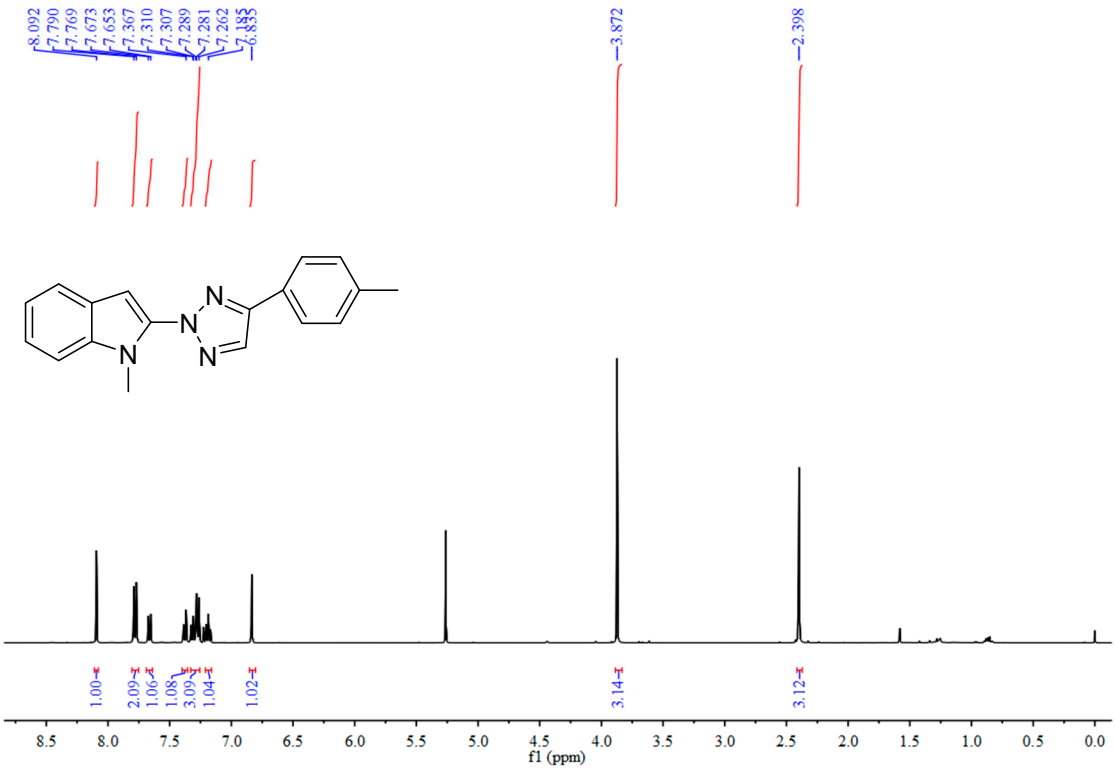
50
40
30
20
10
0
f1 (ppm)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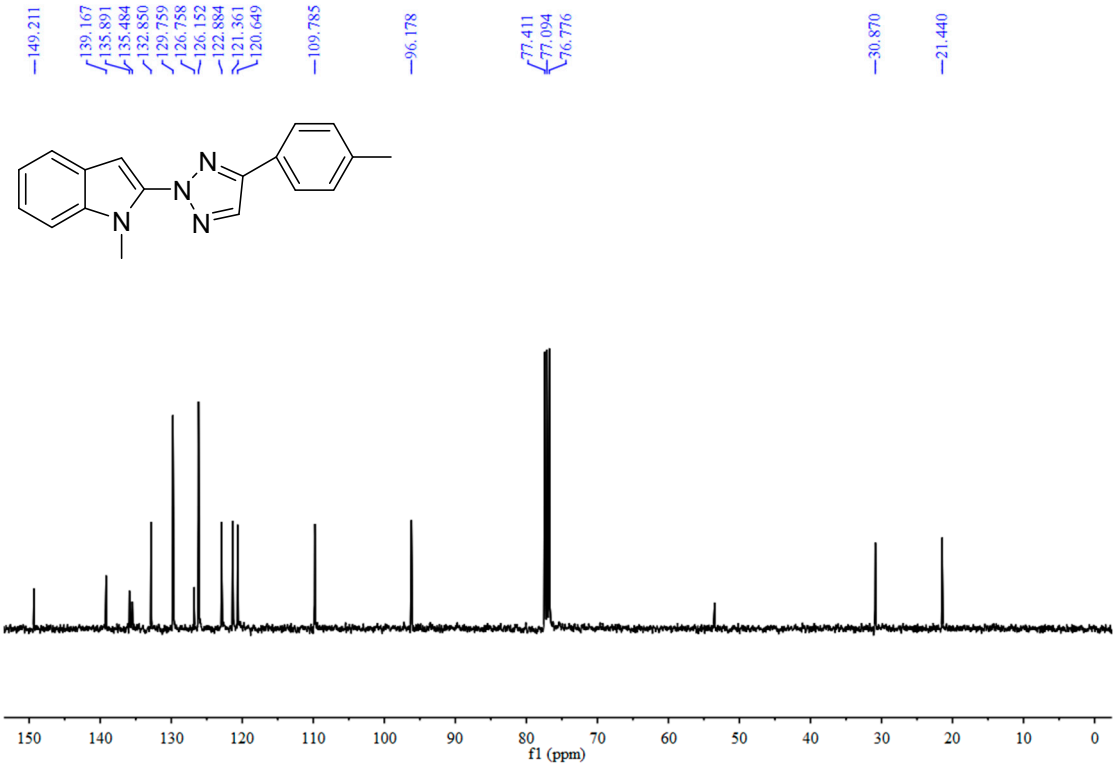
f1 (ppm)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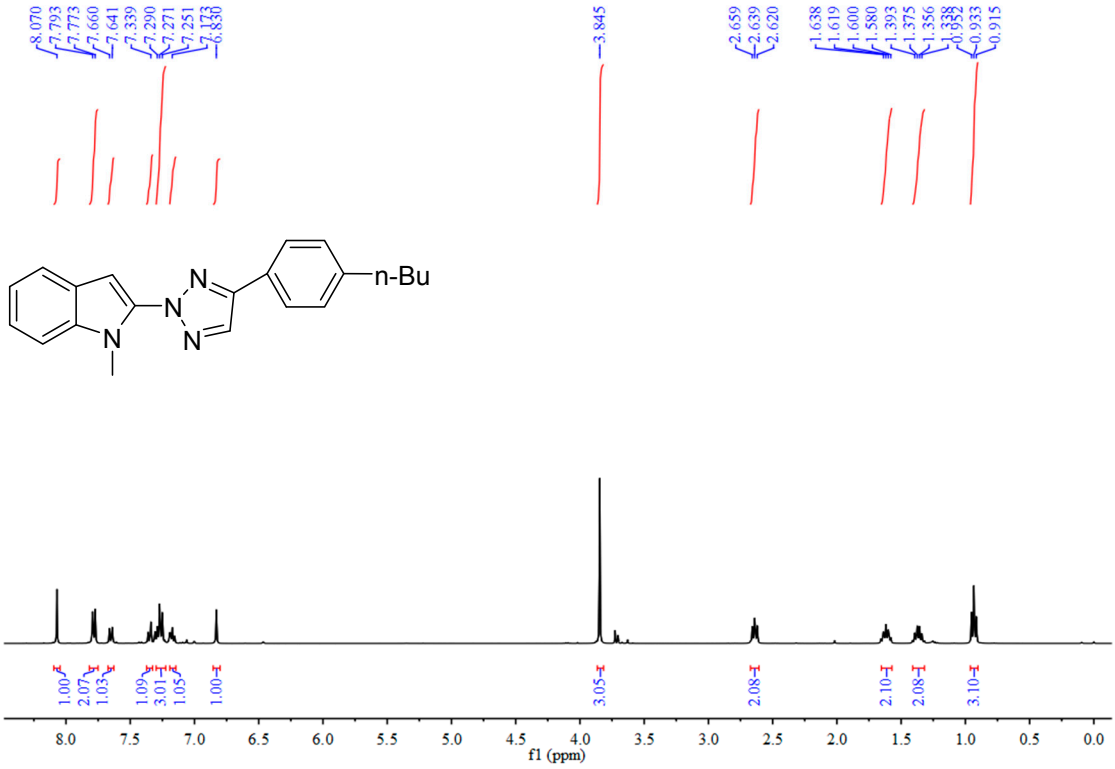
f1 (ppm)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2.639
2.620
1.638
1.619
1.600
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1.375
1.356
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0.952
0.933
0.915
n-Bu
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2.07
1.03
1.09
3.01
1.05
1.00
3.05
2.08
2.10
2.08
3.10
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7.0
6.5
6.0
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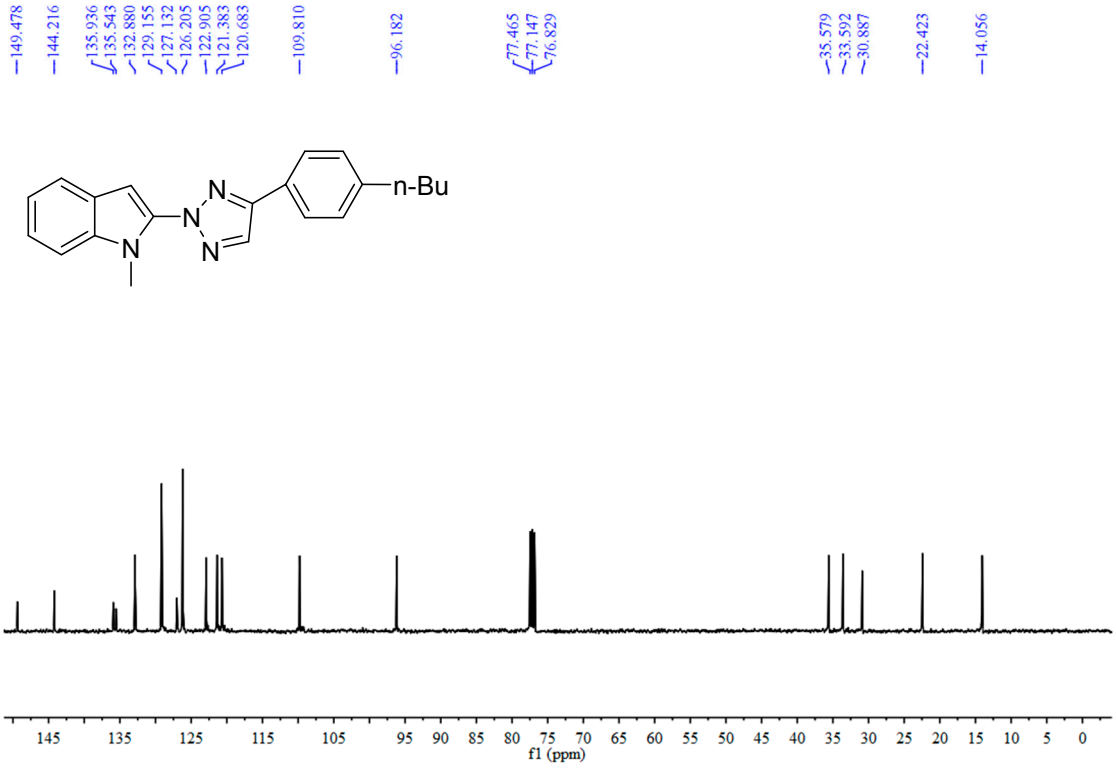
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96.182
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77.147
76.829
35.579
33.592
30.887
22.423
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n-Bu
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125
115
105
95
90
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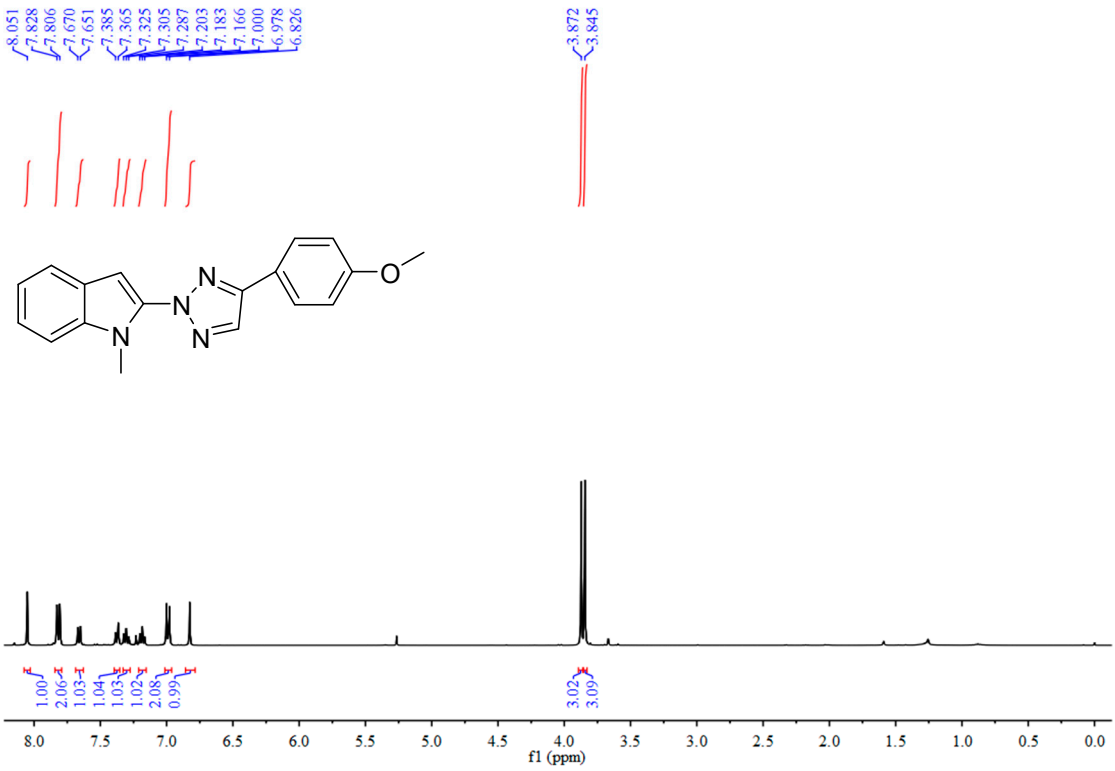
f1 (ppm)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7.000
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3.845
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N
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1.02
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0.99
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3.09
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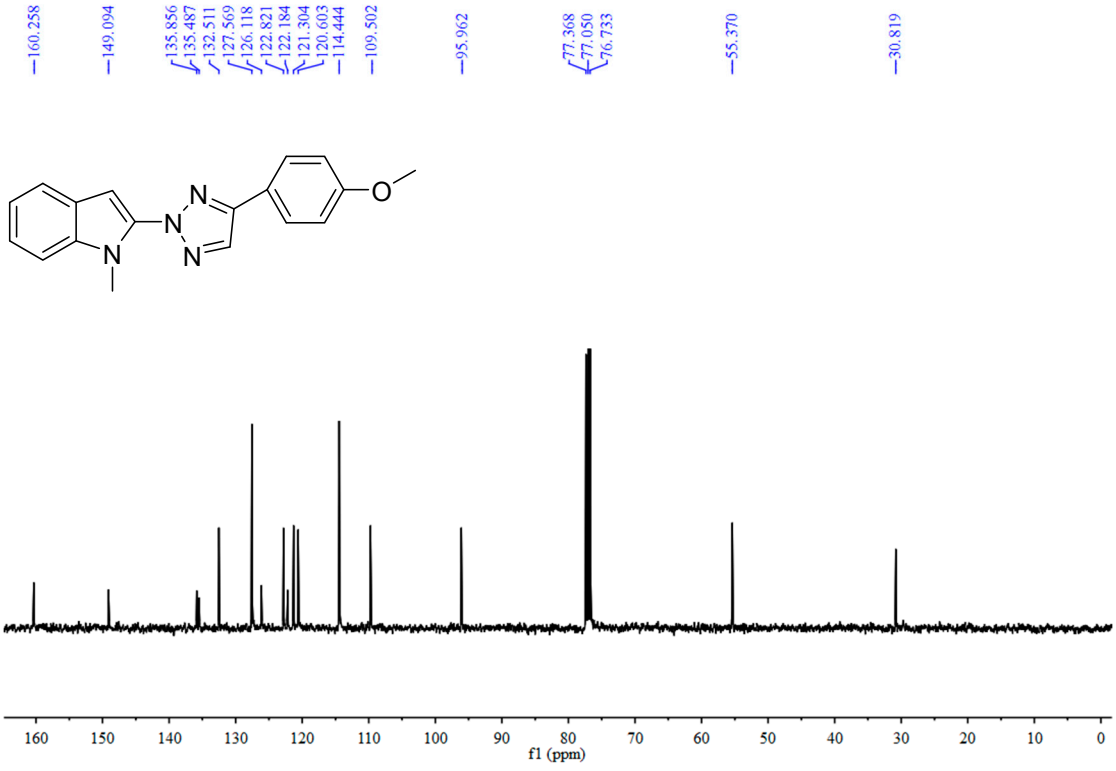
f1 (ppm)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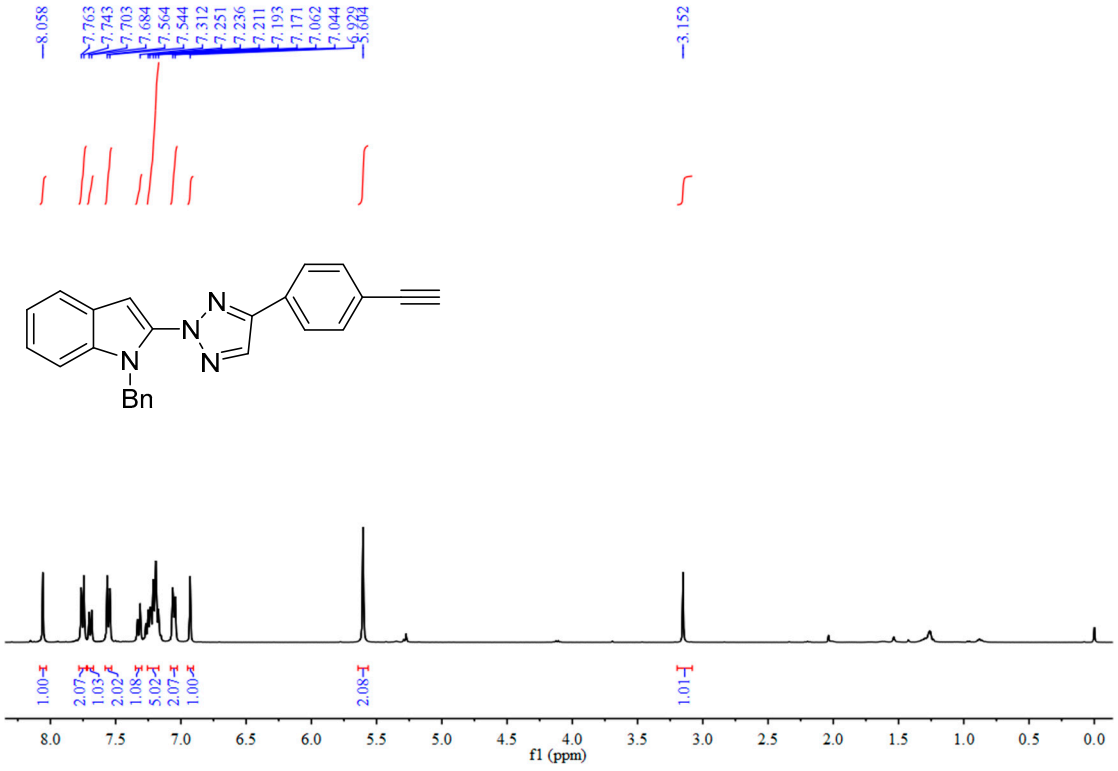
f1 (ppm)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2.02
1.08
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2.07
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5.5
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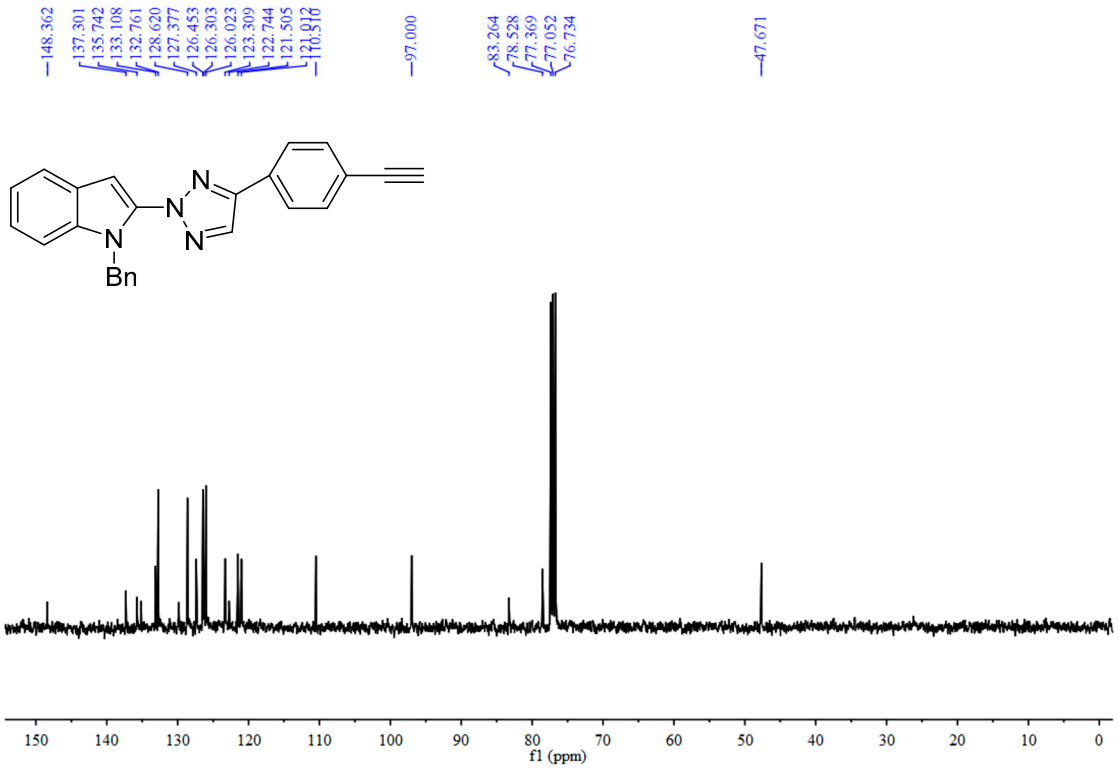
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78.528
77.369
77.052
76.734
47.671
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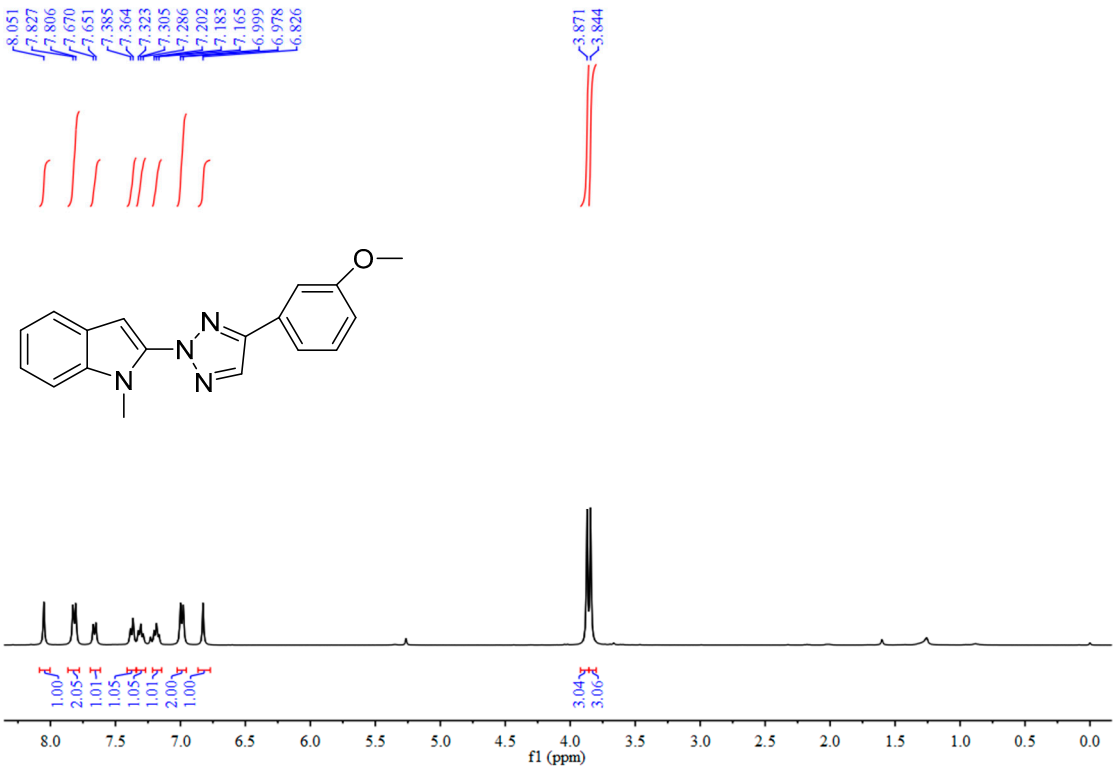
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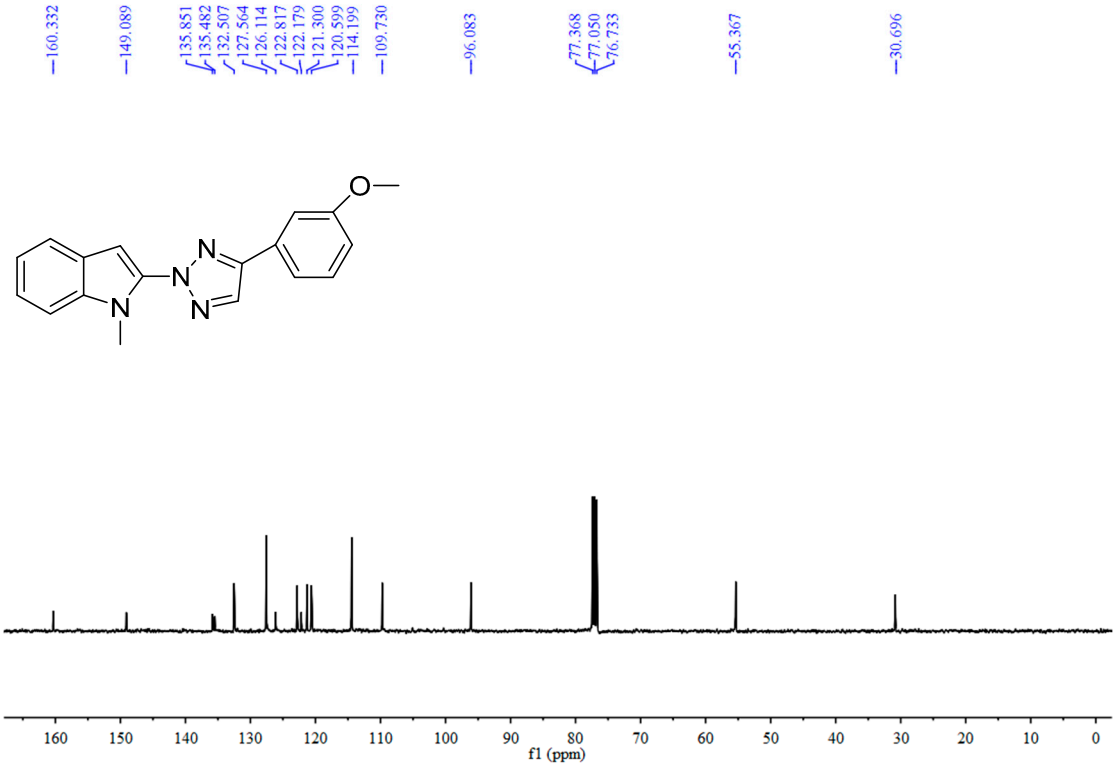
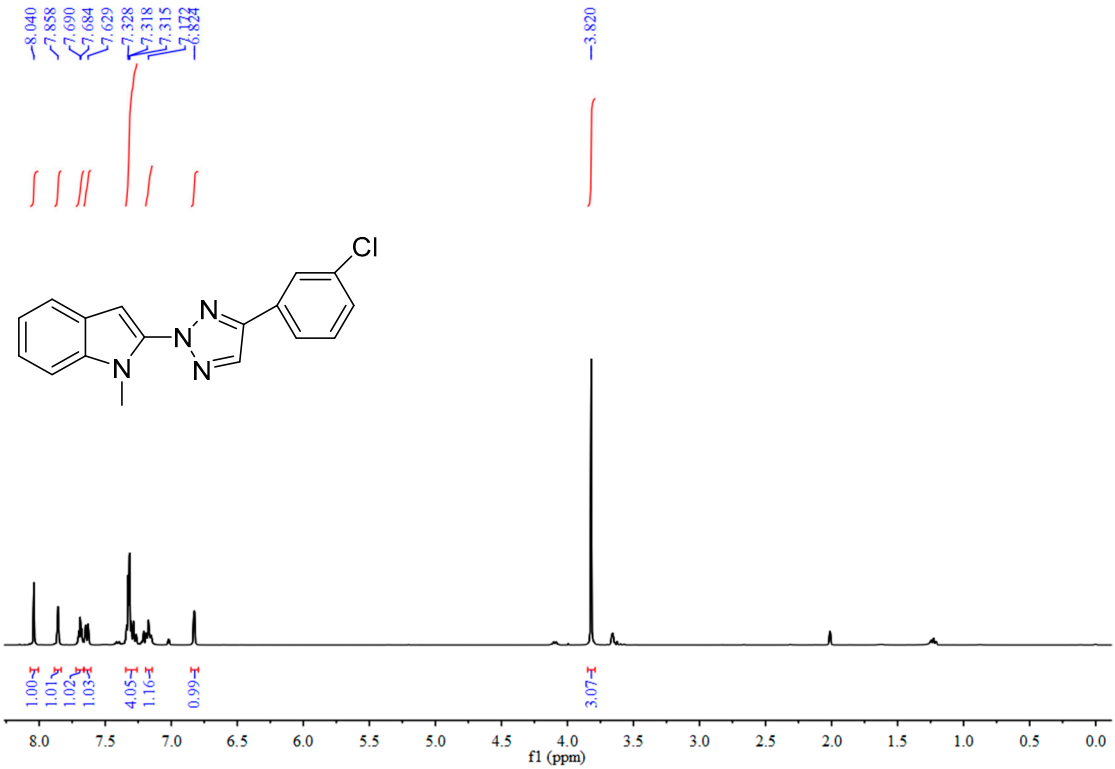
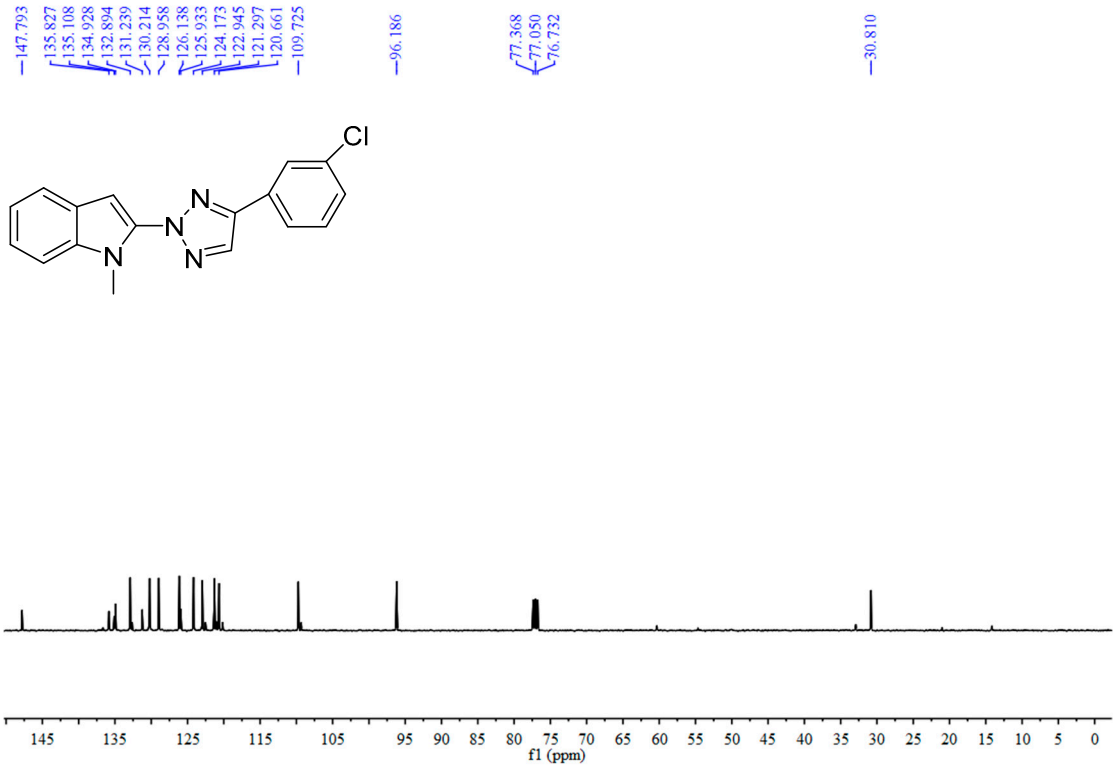
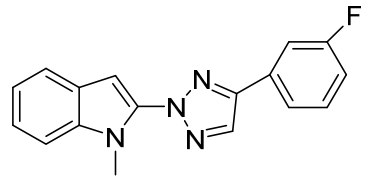
N
1.00
2.05
1.01
1.05
1.05
1.01
2.00
1.00
3.04
3.06
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

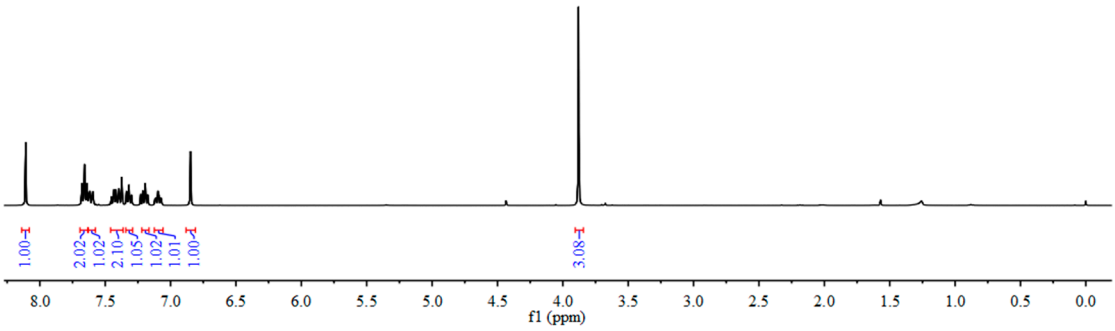

160.332
149.089
135.851
135.482
132.507
127.564
126.114
122.817
122.179
121.300
120.599
114.199
109.730
96.083
77.368
77.050
76.733
55.367
30.696
O
N
N
N
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.040
7.858
7.690
7.684
7.629
7.328
7.318
7.315
7.172
6.824
3.820
Cl
N
N
N
1.00
1.01
1.02
1.03
4.05
1.16
0.99
3.07
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

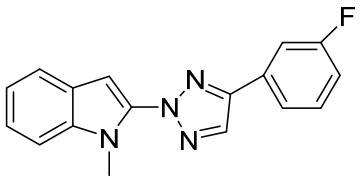

147.793
135.827
135.108
134.928
132.894
131.239
130.214
128.958
126.138
125.933
124.173
122.945
121.297
120.661
109.725
96.186
77.368
77.050
76.732
30.810
Cl
N
N
N
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
f1 (ppm)

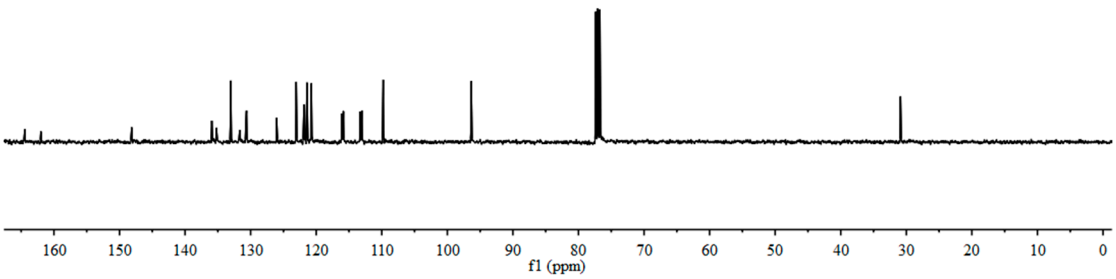

8.108
7.677
7.658
7.639
7.624
7.619
7.600
7.595
7.453
7.438
7.433
7.418
7.413
7.394
7.373
7.338
7.318
7.300
7.212
7.193
7.175
7.118
7.112
7.097
7.091
7.076
7.070
6.848
3.880

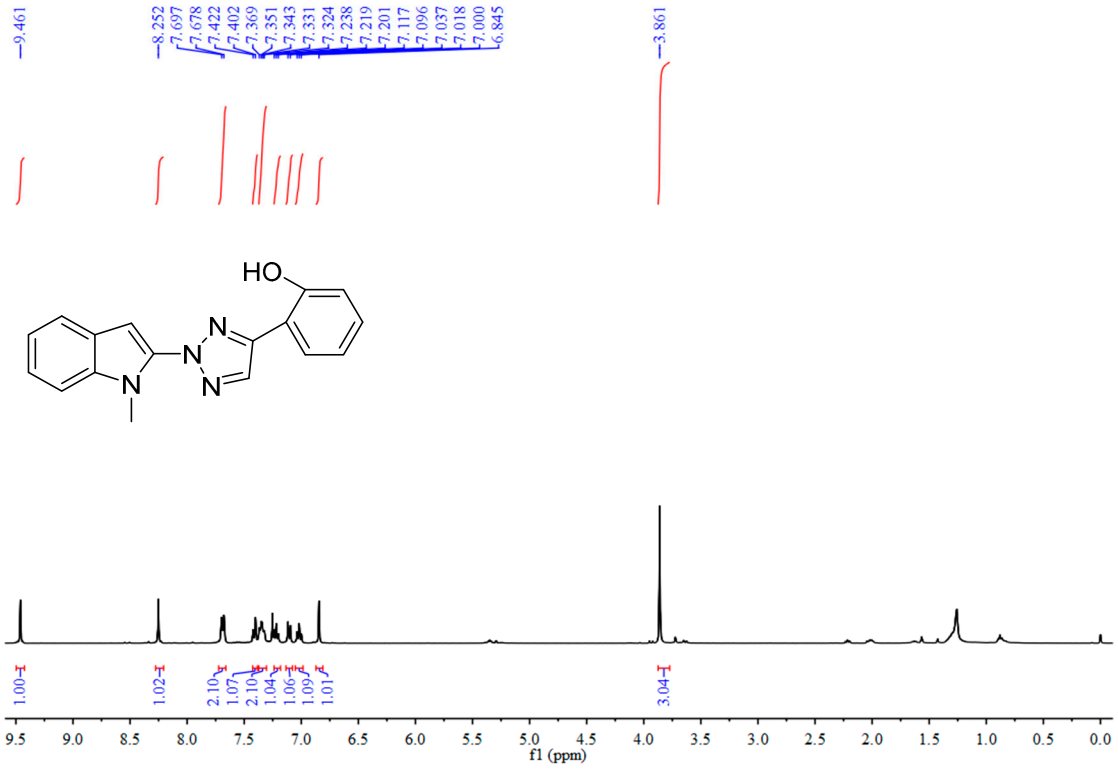

F
N
N
N
N

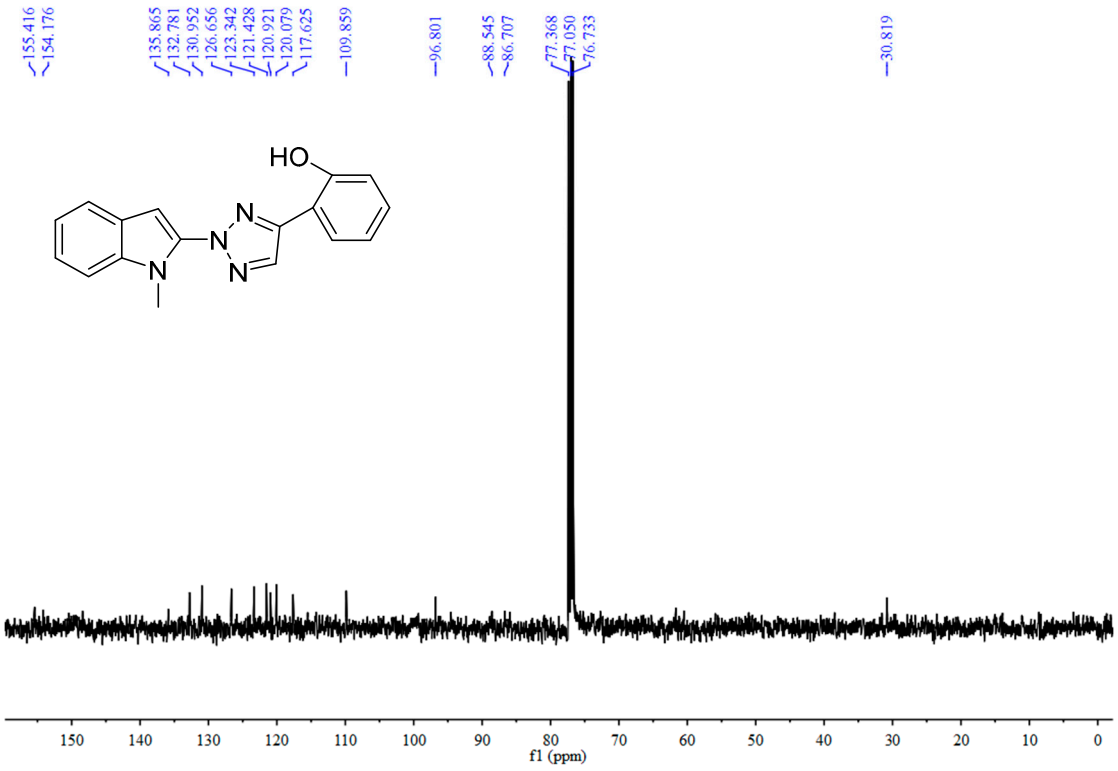

1.00
2.02
1.02
2.10
1.05
1.02
1.01
1.00
3.08
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

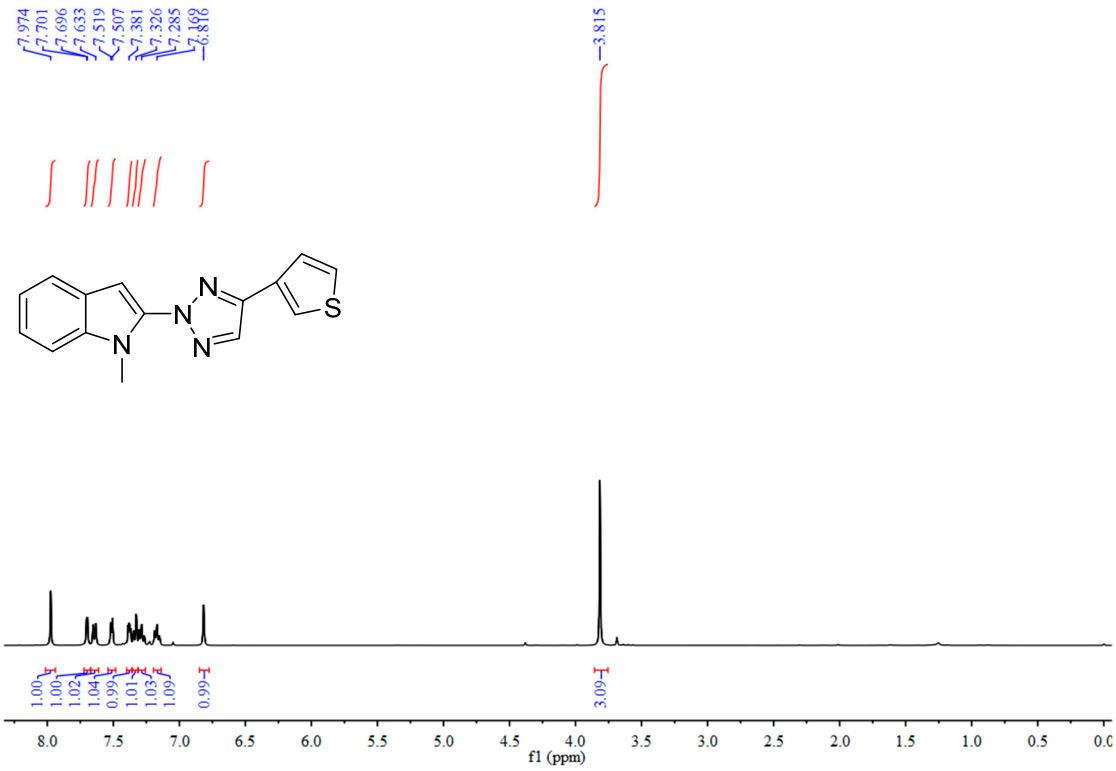

164.446
161.998
148.141
135.918
135.208
133.032
130.711
130.628
126.028
123.035
121.867
121.842
121.399
120.731
116.073
115.861
113.282
113.053
109.793
96.348
77.368
77.050
76.732
30.874

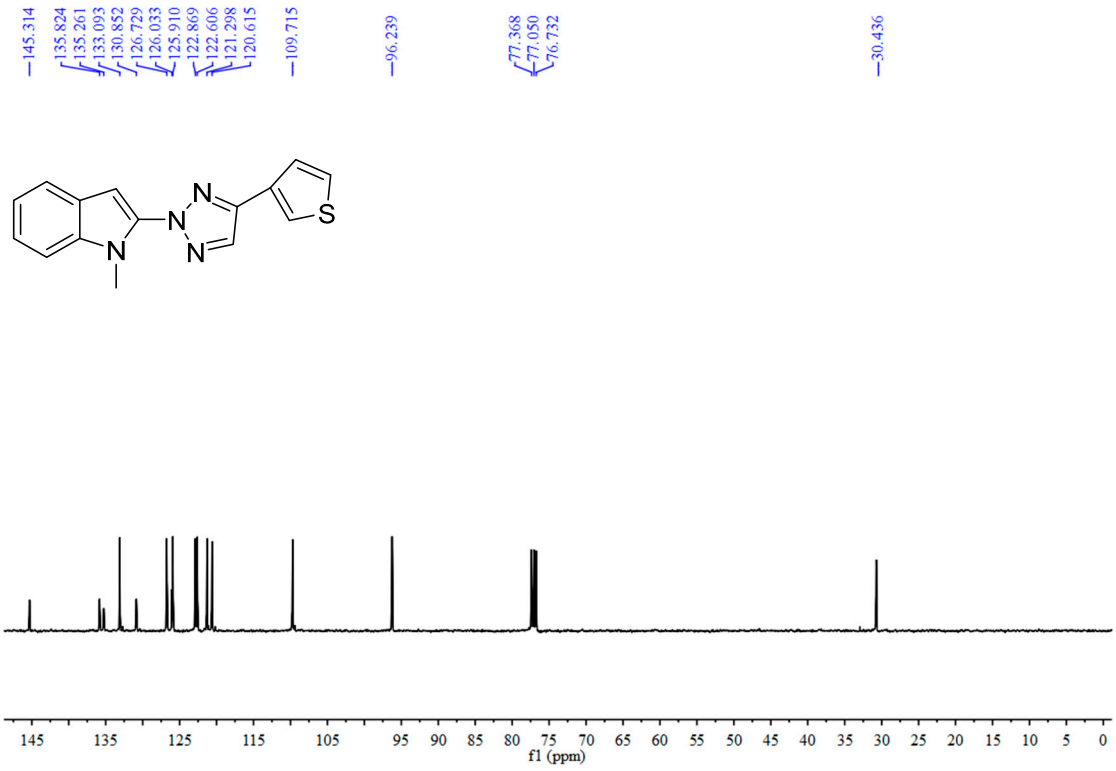

F
N
N
N
N

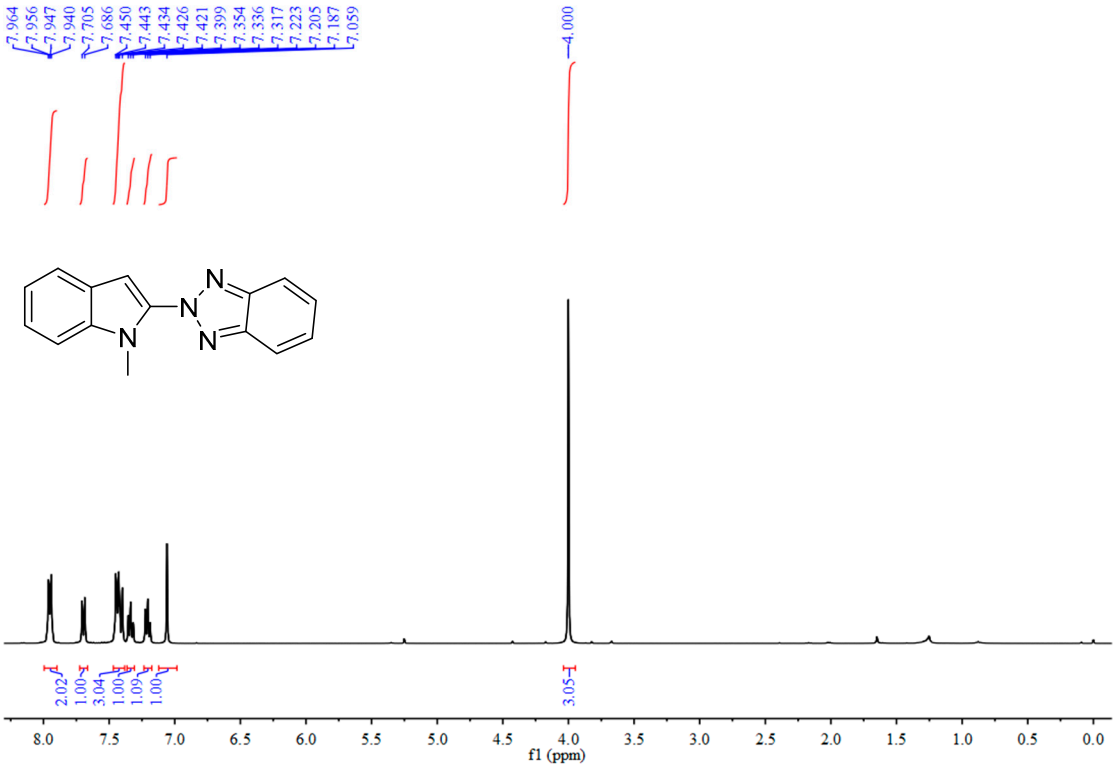

160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

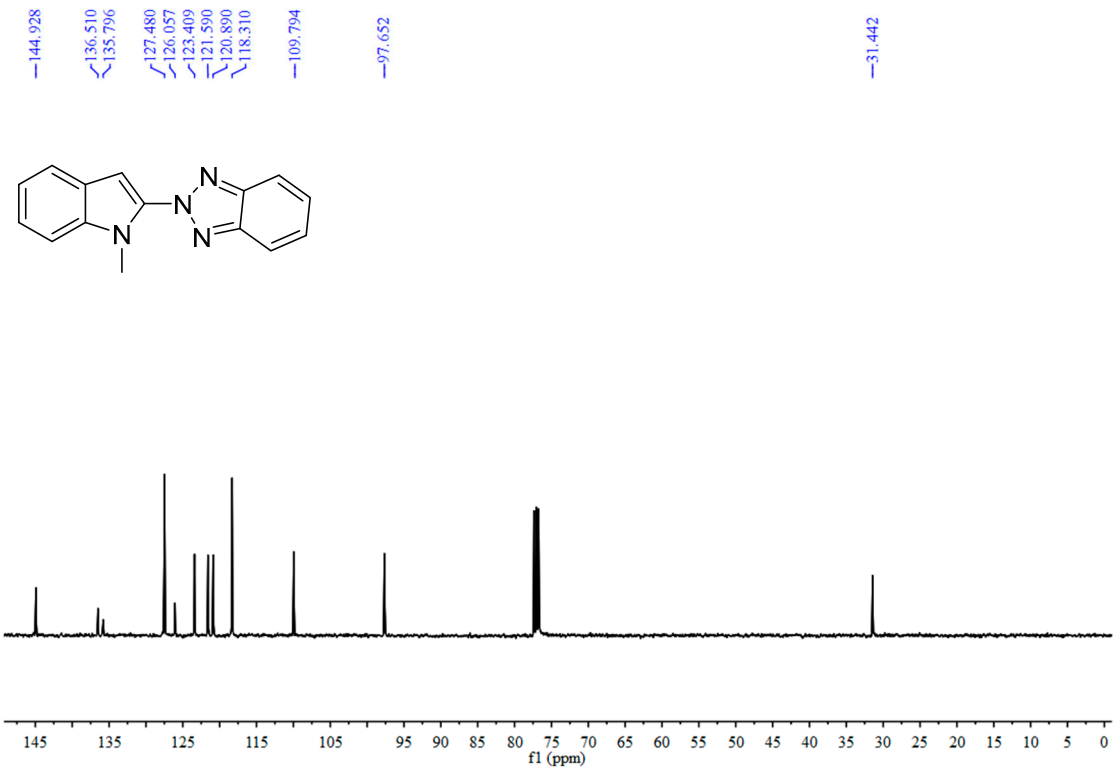

9.461
8.252
7.697
7.678
7.422
7.402
7.369
7.351
7.343
7.331
7.324
7.238
7.219
7.201
7.117
7.096
7.037
7.018
7.000
6.845
3.861
HO
N
N
N
1.00
1.02
2.10
1.07
2.10
1.04
1.06
1.09
1.01
3.04
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

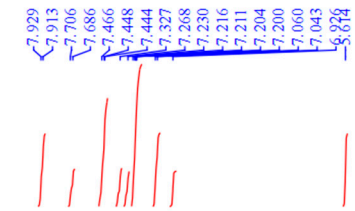

155.416
154.176
135.865
132.781
130.952
126.656
123.342
121.428
120.921
120.079
117.625
109.859
96.801
88.545
86.707
77.368
77.050
76.733
30.819
HO
N
N
N
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

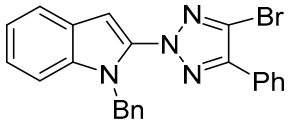

7.974
7.701
7.696
7.633
7.519
7.507
7.381
7.326
7.285
7.169
6.816
3.815
N
N
N
S
N
1.00
1.00
1.02
1.04
0.99
1.01
1.03
1.09
0.99
3.09
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

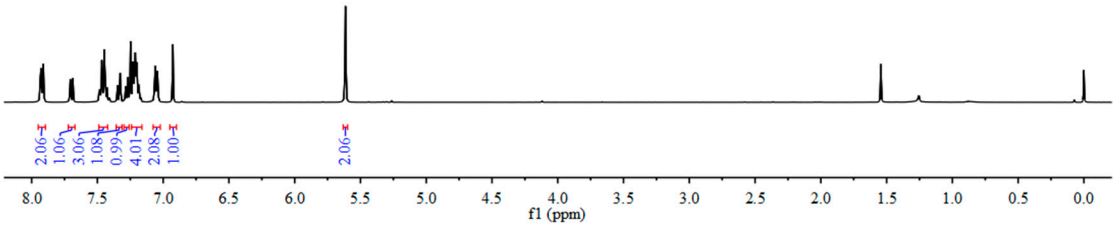

145.314
135.824
135.261
133.093
130.852
126.729
126.033
125.910
122.869
122.606
121.298
120.615
109.715
96.239
77.368
77.050
76.732
30.436
N
N
N
S
N
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
f1 (ppm)


7.964
7.956
7.947
7.940
7.705
7.686
7.450
7.443
7.434
7.426
7.421
7.399
7.354
7.336
7.317
7.223
7.205
7.187
7.059
4.000
2.02
1.00
3.04
1.00
1.09
1.00
3.05
f1 (ppm)

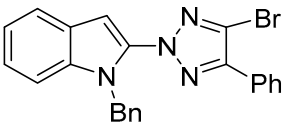

144.928
136.510
135.796
127.480
126.057
123.409
121.590
120.890
118.310
109.794
97.652
31.442
f1 (ppm)

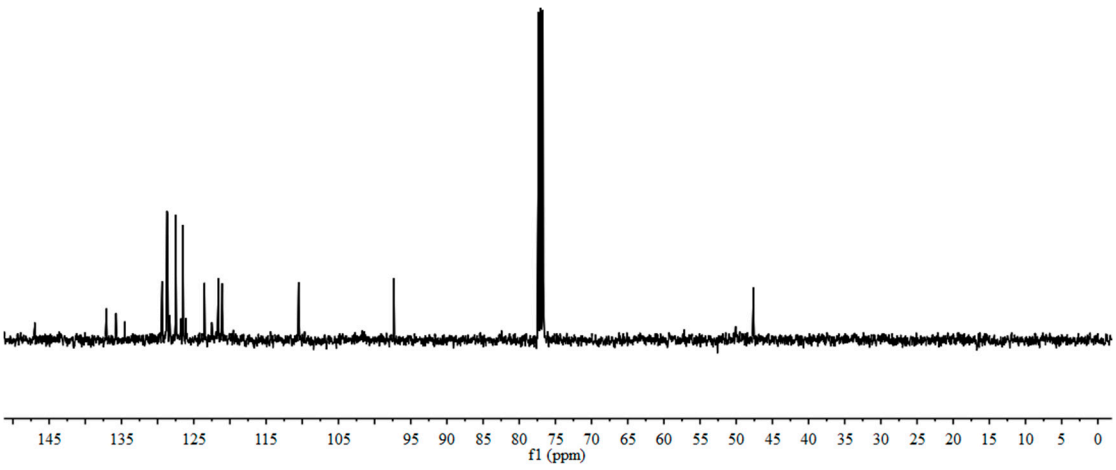

7.929
7.913
7.706
7.686
7.466
7.448
7.444
7.327
7.268
7.230
7.216
7.211
7.204
7.200
7.060
7.043
6.926
5.614


N
N
N
Br
Ph
N
Bn

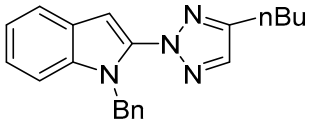

2.06
1.06
3.06
1.08
0.99
4.01
2.08
1.00
2.06
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

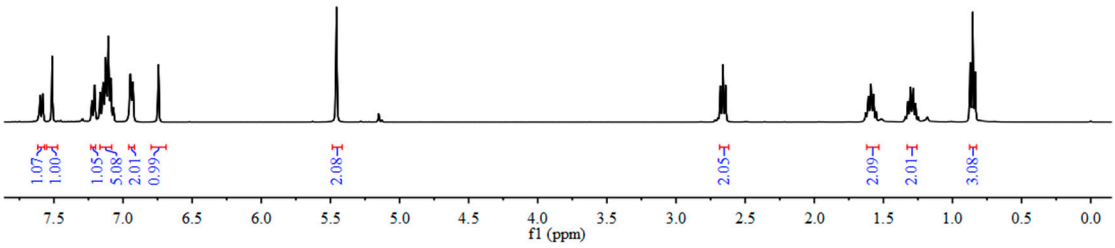

146.985
137.069
135.753
129.388
128.706
128.643
128.319
127.500
127.447
126.506
123.522
121.617
110.506
97.329
77.368
77.050
76.732
47.647


N
N
N
Br
Ph
N
Bn

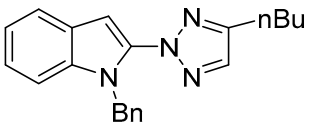

145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
f1 (ppm)

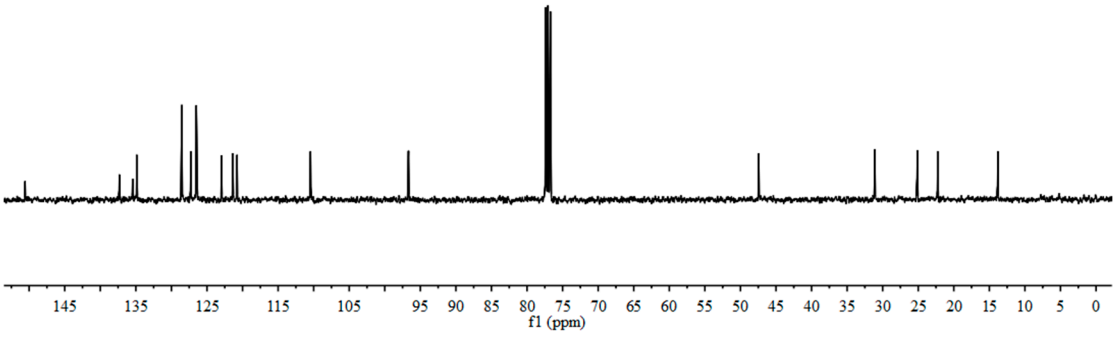

7.600
7.581
7.513
7.225
7.205
7.167
7.144
7.126
7.107
7.087
7.070
6.947
6.930
6.744
5.456
2.679
2.660
2.641
1.627
1.609
1.590
1.571
1.552
1.341
1.323
1.304
1.285
0.872
0.854
0.835

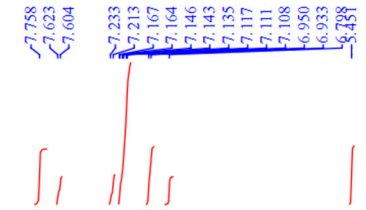

N
N
N
nBu
N
Bn

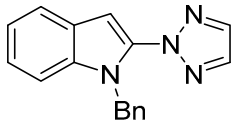

1.07
1.00
1.05
5.08
2.01
0.99
2.08
2.05
2.09
2.01
3.08
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

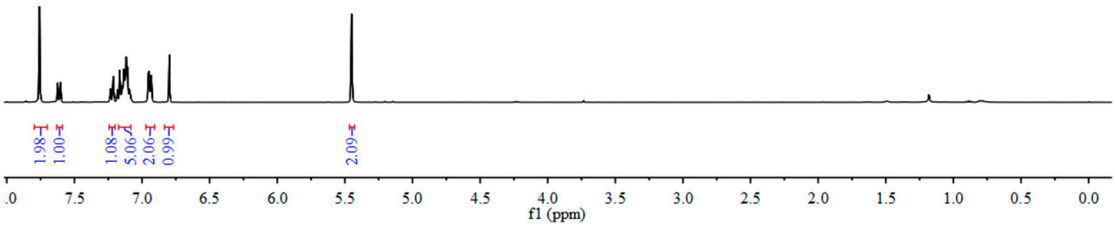

150.558
137.323
135.461
134.867
128.537
127.277
126.493
126.376
122.960
121.365
120.767
110.439
96.665
77.368
77.050
76.733
47.415
31.095
25.137
22.150
13.753


N
N
N
nBu
N
Bn

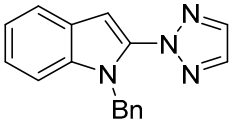

145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
f1 (ppm)

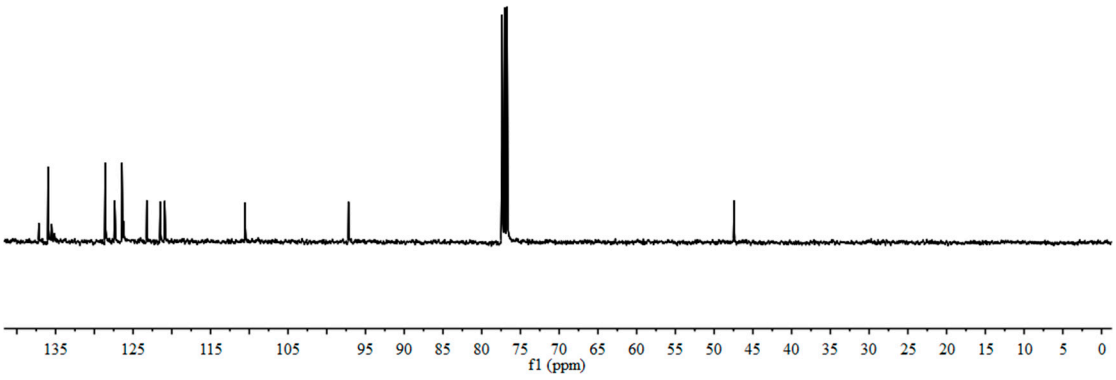

7.758
7.623
7.604
7.233
7.213
7.167
7.164
7.146
7.143
7.135
7.117
7.111
7.108
6.950
6.933
5.451

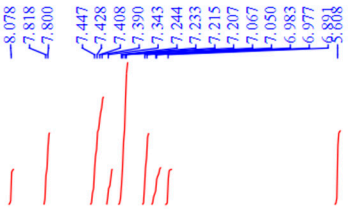

N
N
N
N
Bn

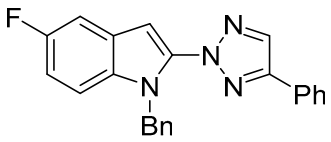

1.98
1.00
1.08
5.06
2.06
0.99
2.09
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

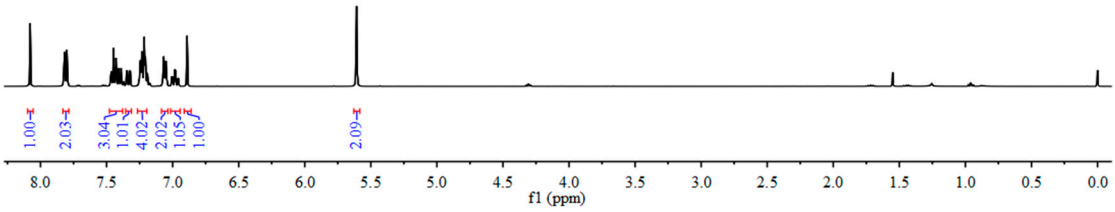

137.161
135.973
135.511
135.145
128.689
127.371
126.431
126.255
123.237
121.582
120.919
110.432
97.198
77.368
77.050
76.732
47.568


N
N
N
N
Bn


135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
f1 (ppm)


8.078
7.818
7.800
7.447
7.428
7.408
7.390
7.343
7.244
7.233
7.215
7.207
7.067
7.050
6.983
6.977
6.891
5.608


F
N
N
N
Ph
N
Bn


1.00
2.03
3.04
1.01
4.02
2.02
1.05
1.00
2.09
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


159.668
157.256
149.401
137.058
133.169
132.191
129.385
129.194
129.042
128.690
127.499
126.450
126.224
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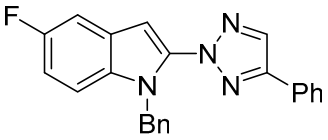
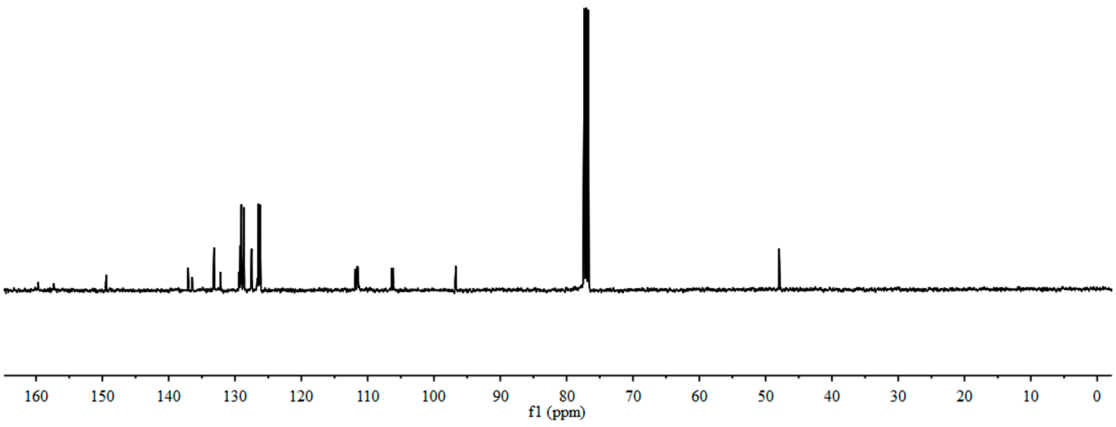
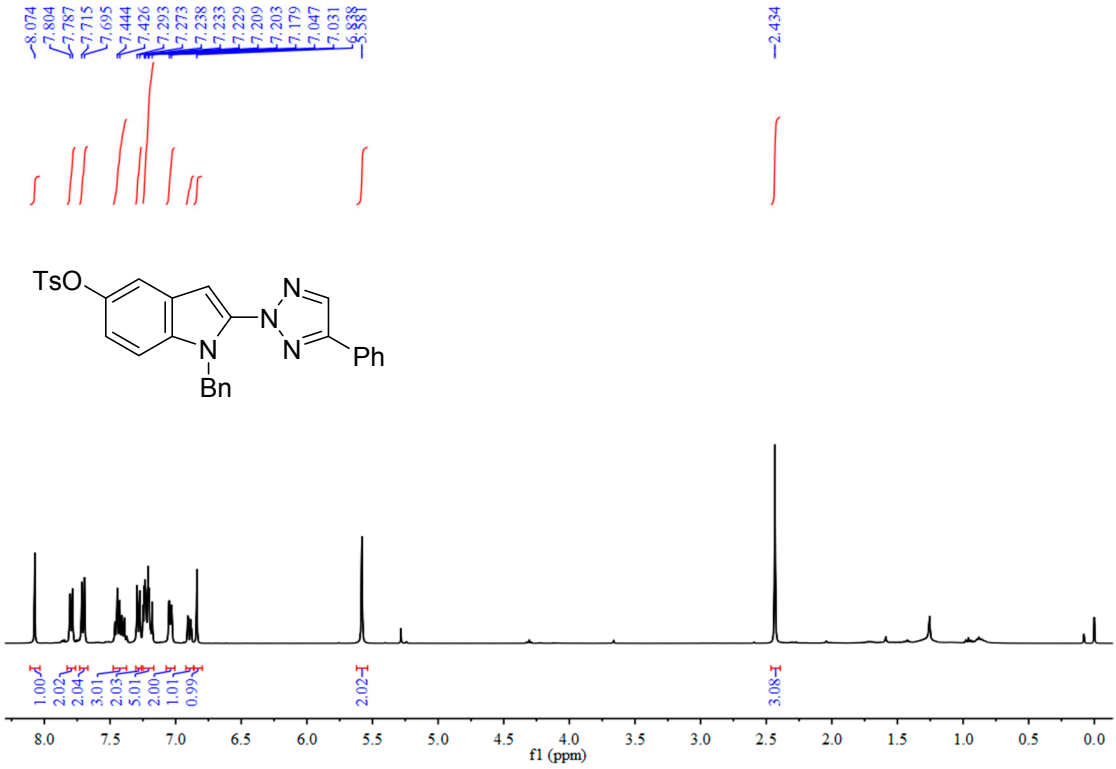
96.690
77.368
77.051
76.733
47.847


F
N
N
N
Ph
N
Bn


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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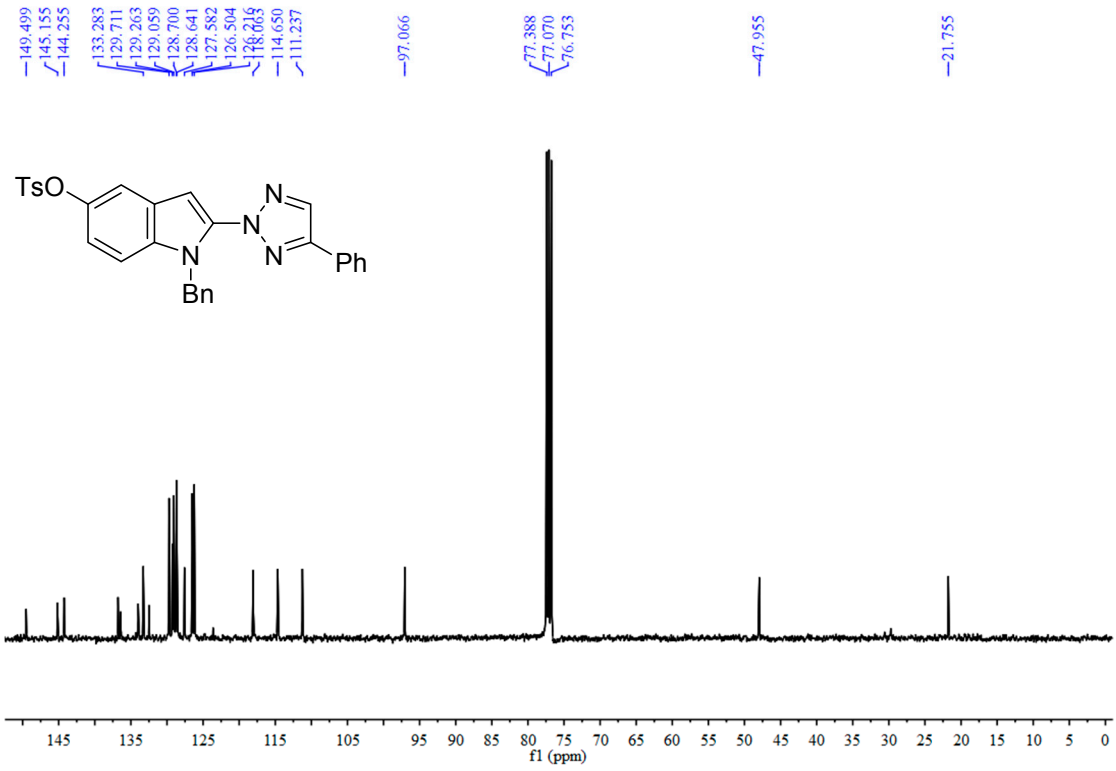
7.804
7.787
7.715
7.695
7.444
7.426
7.293
7.273
7.238
7.233
7.229
7.209
7.203
7.179
7.047
7.031
6.838
6.821
2.434
TsO
N
N
N
Ph
N
Bn
1.00
2.02
2.04
3.01
2.03
5.01
2.00
1.01
0.99
2.02
3.08
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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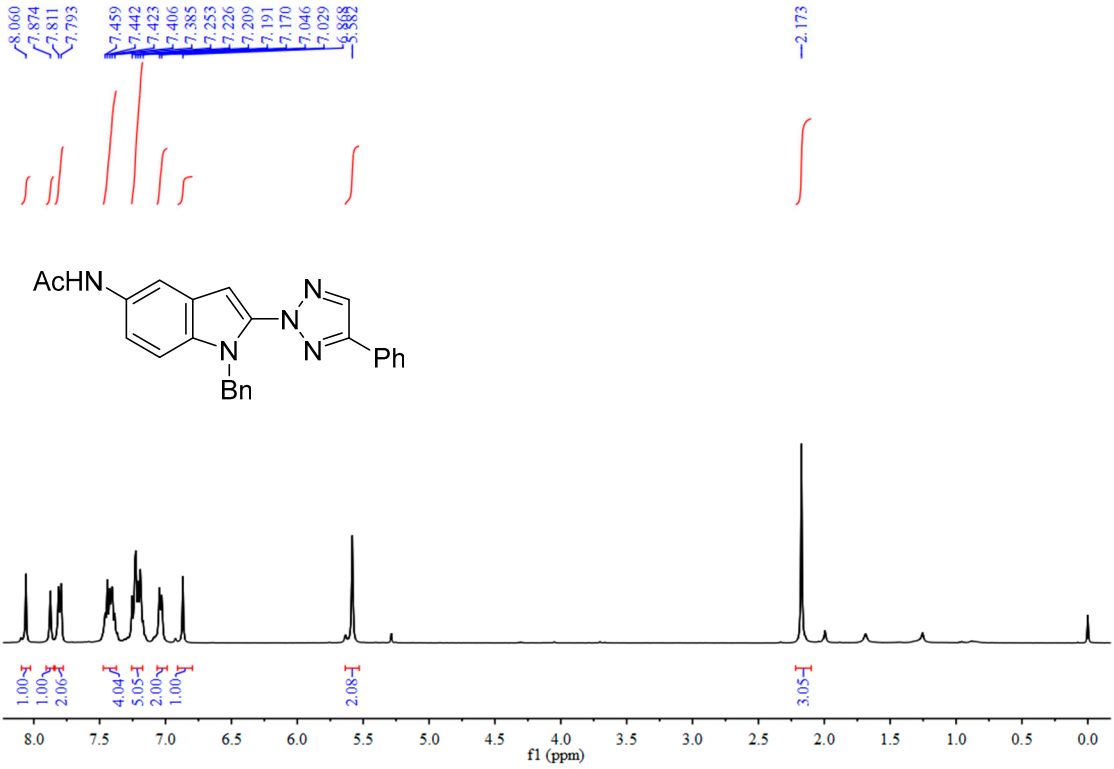
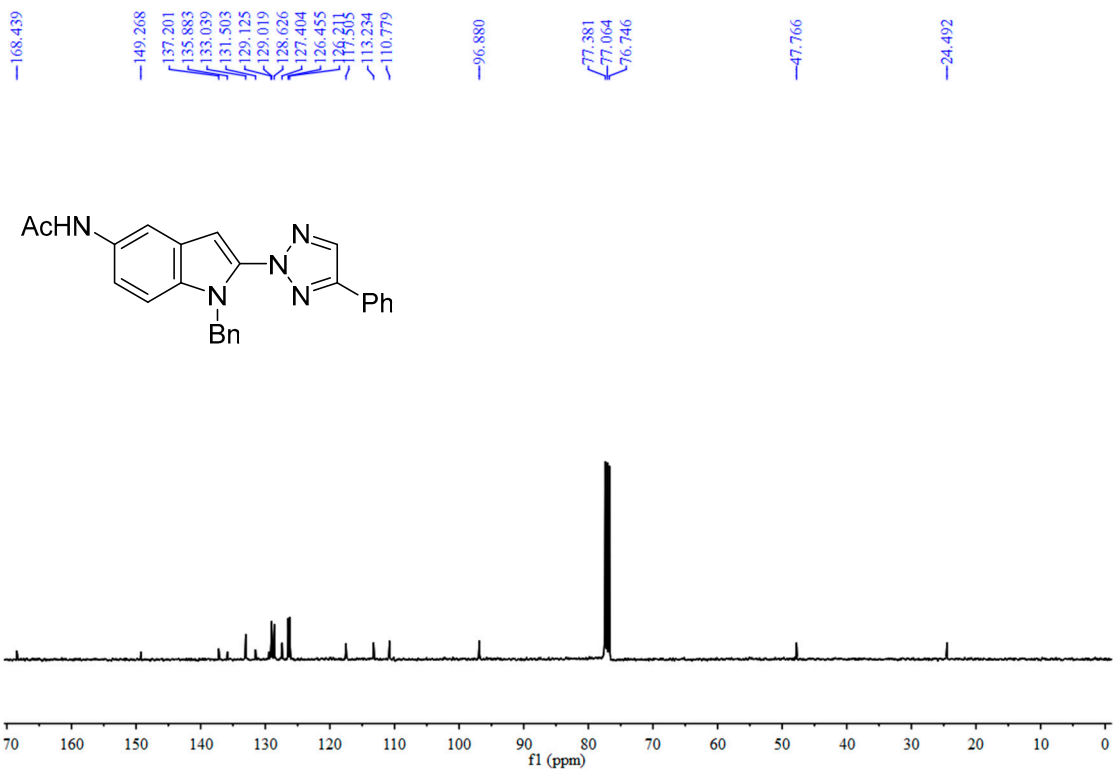
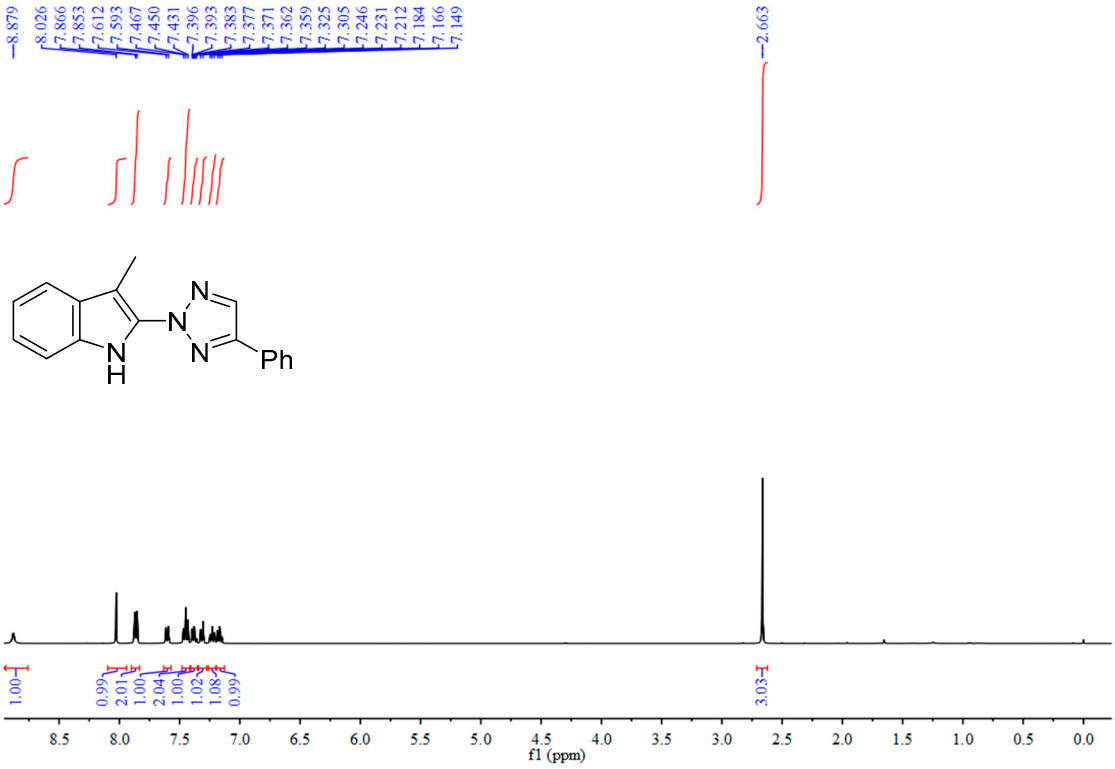
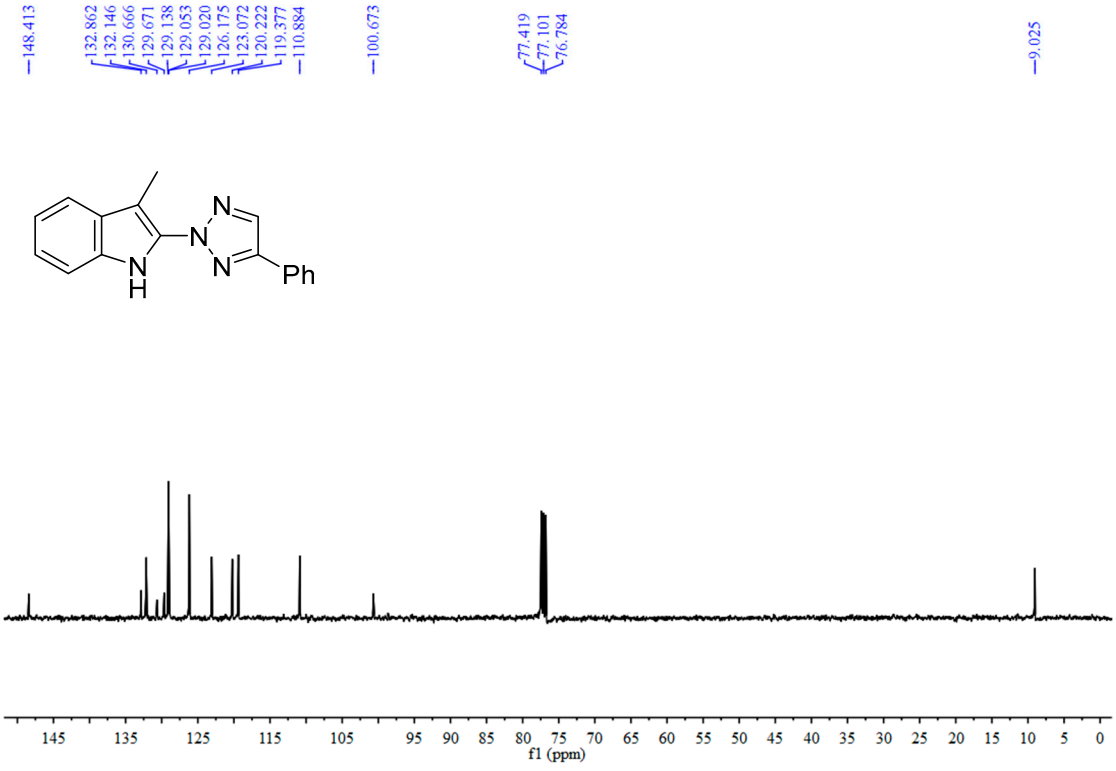
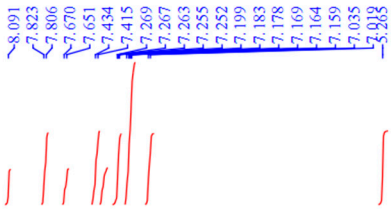
145.155
144.255
133.283
129.711
129.263
129.059
128.700
128.641
127.582
126.504
126.216
126.063
114.650
111.237
97.066
77.388
77.070
76.753
47.955
21.755
TsO
N
N
N
Ph
N
Bn
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
f1 (ppm)

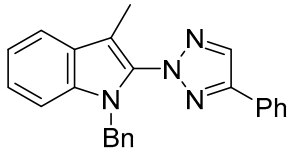

8.060
7.874
7.811
7.793
7.459
7.442
7.423
7.406
7.385
7.253
7.226
7.209
7.191
7.170
7.046
7.029
6.888
6.882
2.173
AcHN
N
N
N
N
Ph
Bn
1.00
1.00
2.06
4.04
5.05
2.00
1.00
2.08
3.05
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

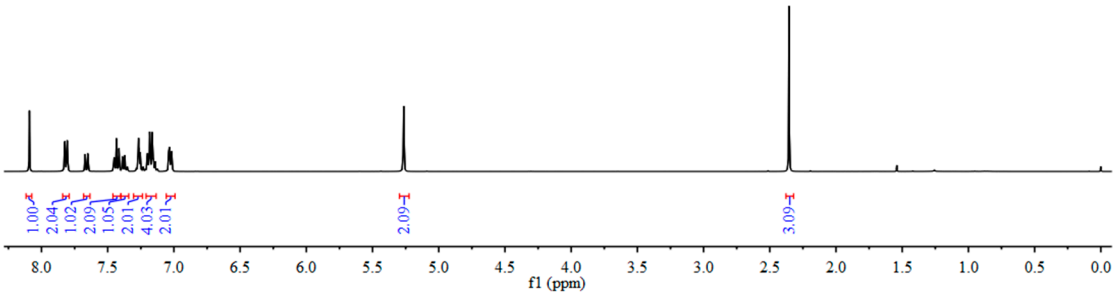

168.439
149.268
137.201
135.883
133.039
131.503
129.125
129.019
128.626
127.404
126.455
113.234
110.779
96.880
77.381
77.064
76.746
47.766
24.492
AcHN
N
N
N
N
Ph
Bn
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.879
8.026
7.866
7.853
7.612
7.593
7.467
7.450
7.431
7.396
7.393
7.383
7.377
7.371
7.362
7.359
7.325
7.305
7.246
7.231
7.212
7.184
7.166
7.149
2.663
N
N
N
H
Ph
1.00
0.99
2.01
1.00
2.04
1.00
1.02
1.08
0.99
3.03
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

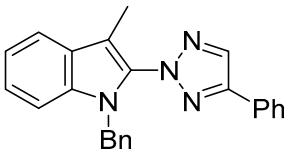

148.413
132.862
132.146
130.666
129.671
129.138
129.053
129.020
126.175
123.072
120.222
119.377
110.884
100.673
77.419
77.101
76.784
9.025
N
N
N
H
Ph
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
f1 (ppm)

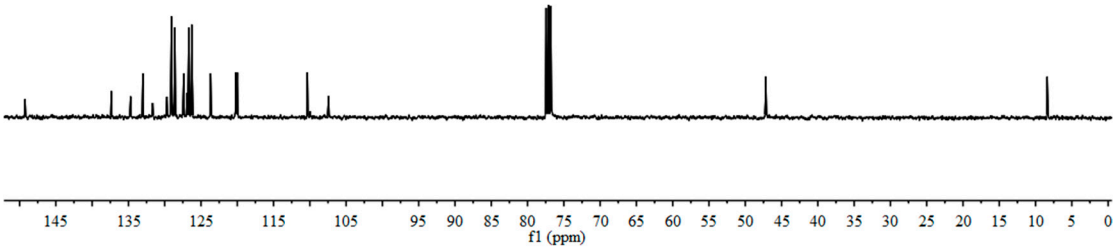

8.091
7.823
7.806
7.670
7.651
7.434
7.415
7.269
7.267
7.263
7.255
7.252
7.199
7.183
7.178
7.169
7.164
7.159
7.035
5.019
5.003
2.355

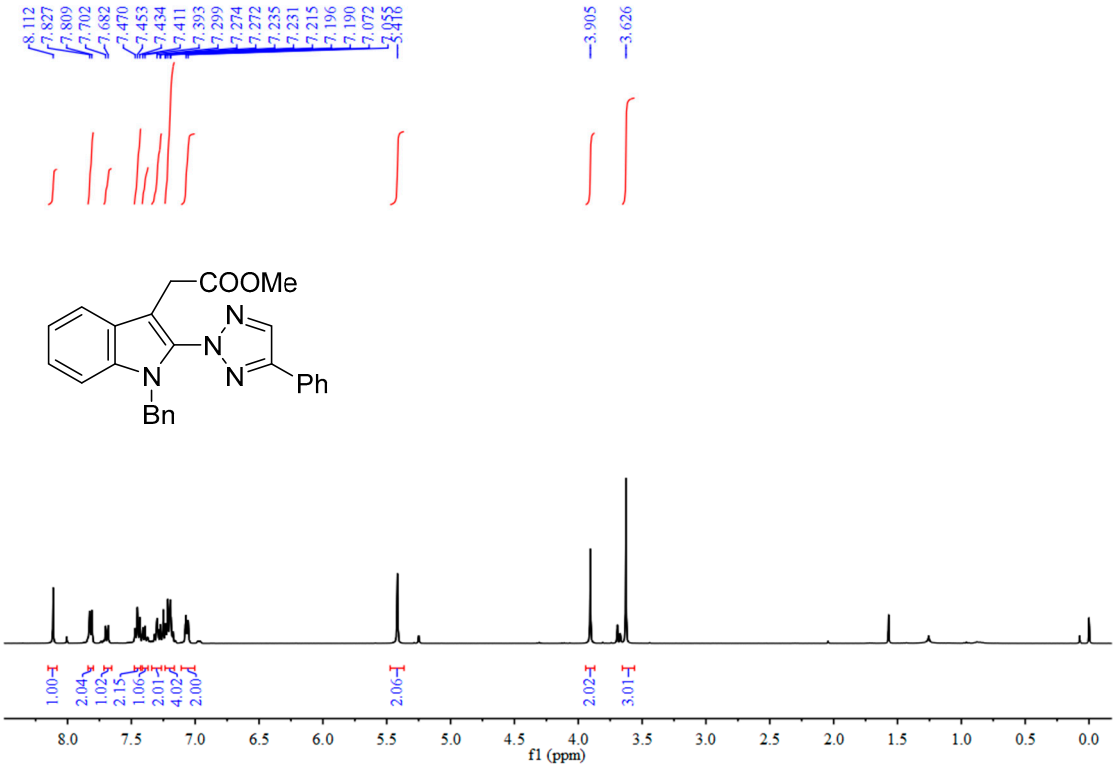

N
N
N
Ph
Bn

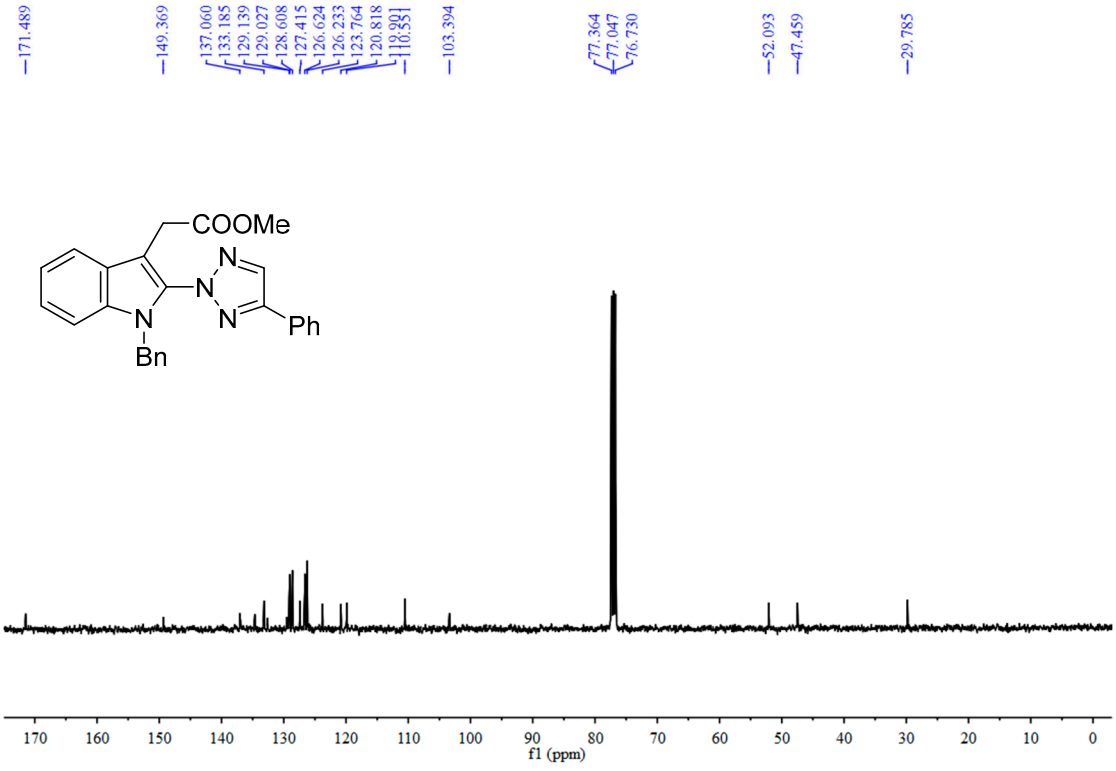

1.00
2.04
1.02
2.09
1.05
2.01
4.03
2.01
2.09
3.09
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

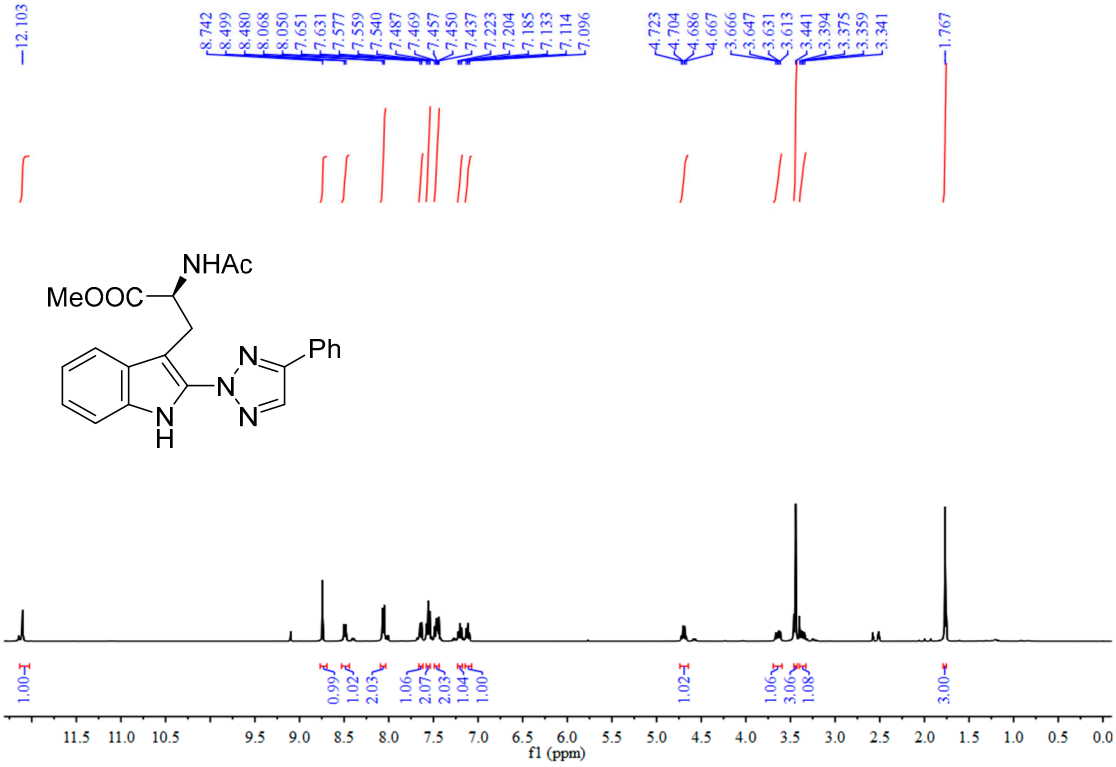

149.245
137.348
134.702
133.010
129.689
129.095
129.067
128.605
127.387
126.901
126.676
126.257
123.666
120.169
110.332
107.427
77.444
77.126
76.809
47.181
8.388

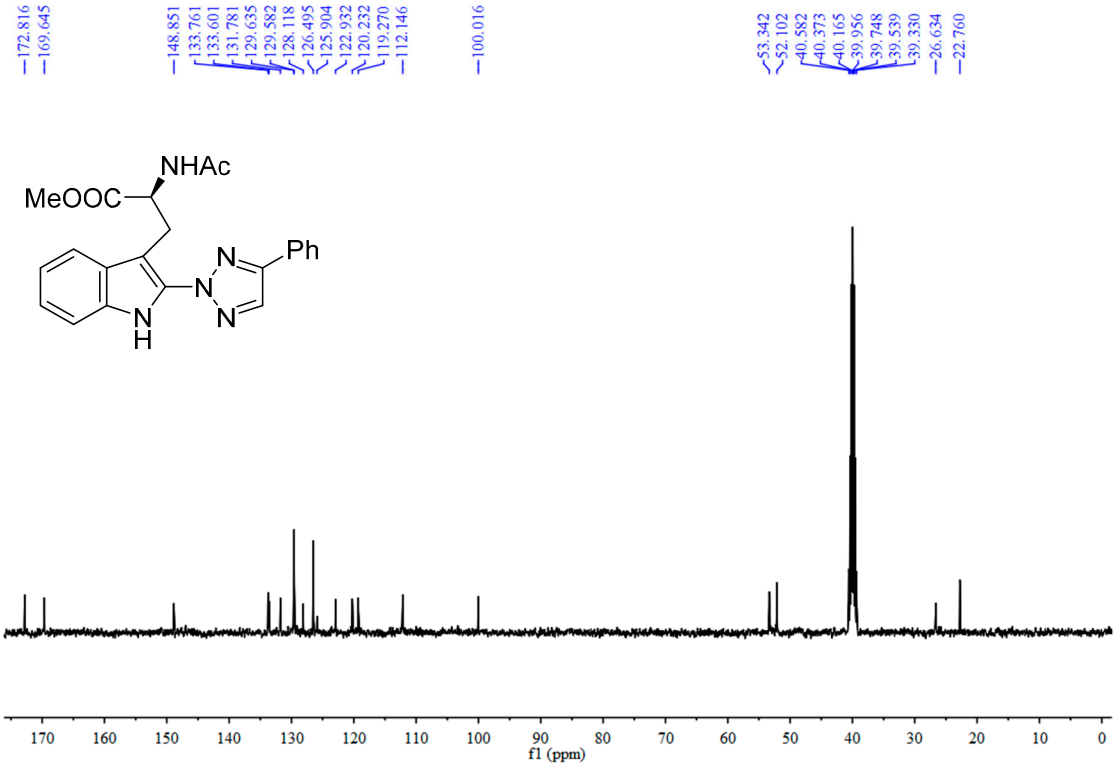

N
N
N
Ph
Bn

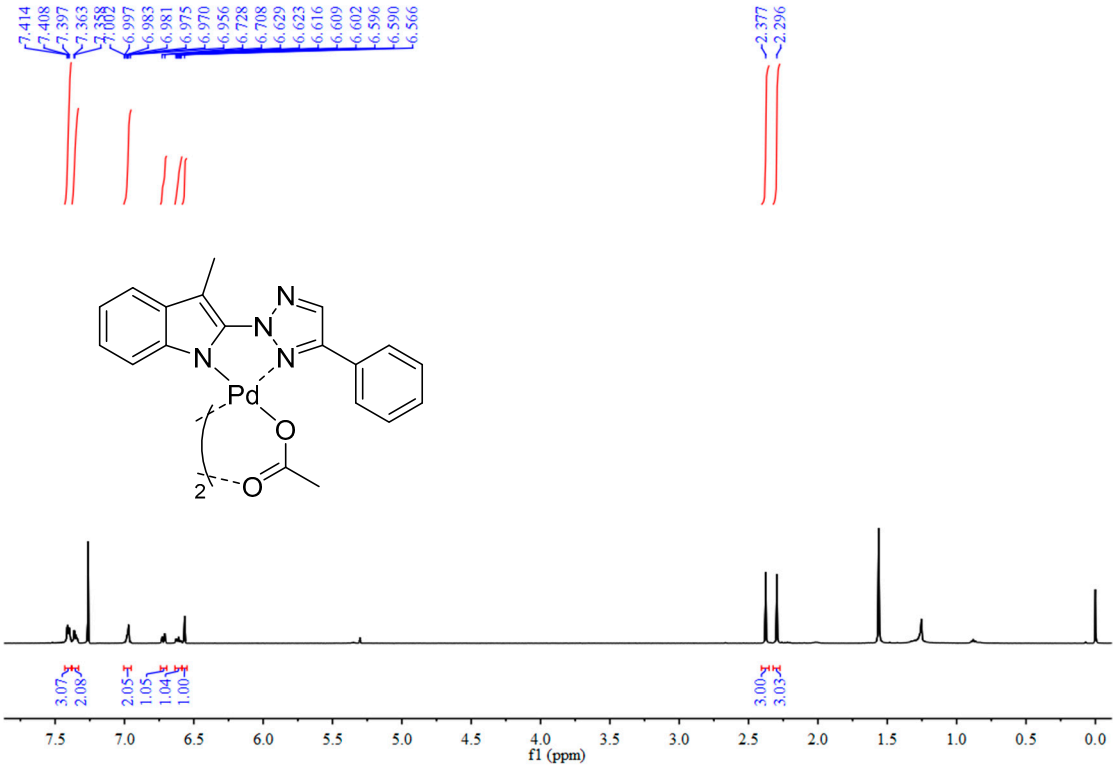

145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
f1 (ppm)

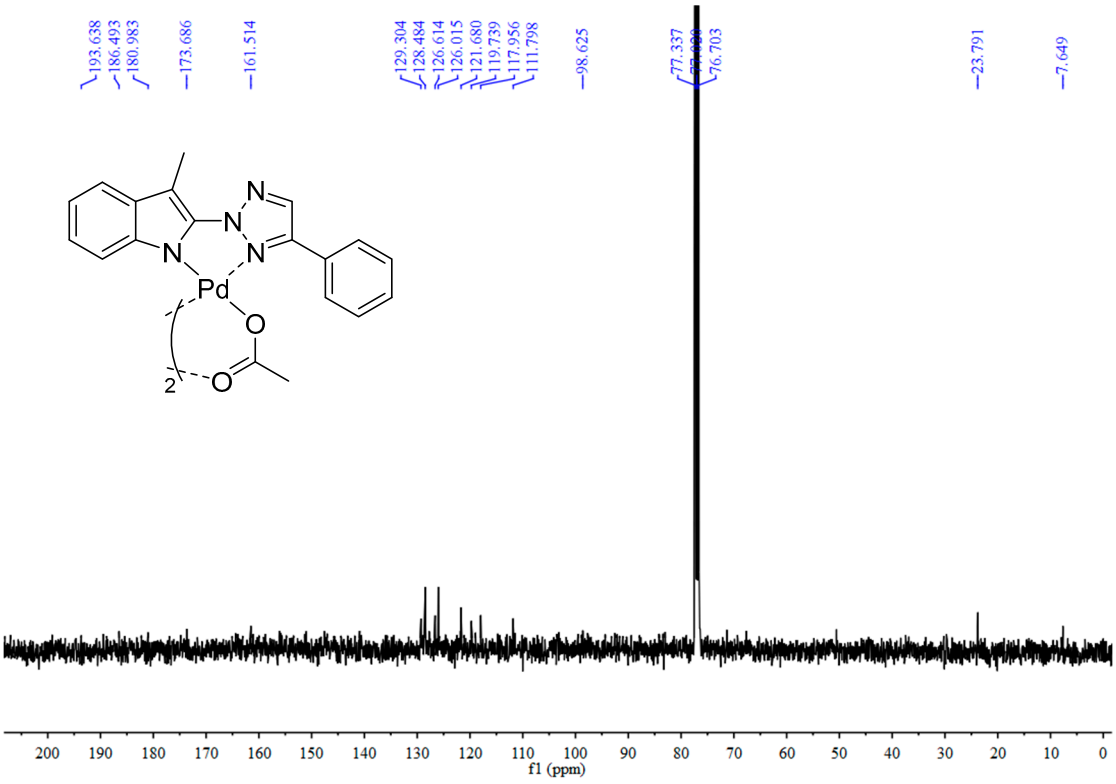

8.112
7.827
7.809
7.702
7.682
7.470
7.453
7.434
7.411
7.393
7.299
7.274
7.272
7.235
7.231
7.215
7.196
7.190
7.072
5.416
3.905
3.626
COOMe
N
N
N
Ph
N
Bn
1.00
2.04
1.02
2.15
1.06
2.01
4.02
2.00
2.06
2.02
3.01
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


171.489
149.369
137.060
133.185
129.139
129.027
128.608
127.415
126.624
126.233
123.764
120.818
110.581
103.394
77.364
77.047
76.730
52.093
47.459
29.785
COOMe
N
N
N
Ph
N
Bn
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


12.103
8.742
8.499
8.480
8.068
8.050
7.651
7.631
7.577
7.559
7.540
7.487
7.469
7.457
7.450
7.437
7.223
7.204
7.185
7.133
7.114
7.096
4.723
4.704
4.686
4.667
3.666
3.647
3.631
3.613
3.441
3.394
3.375
3.359
3.341
1.767
NHAc
MeOOC
Ph
N
N
N
H
1.00
0.99
1.02
2.03
1.06
2.07
2.03
1.04
1.00
1.02
1.06
3.06
1.08
3.00
11.5 11.0 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


172.816
169.645
148.851
133.761
133.601
131.781
129.635
129.582
128.118
126.495
125.904
122.932
120.232
119.270
112.146
100.016
53.342
52.102
40.582
40.373
40.165
39.956
39.748
39.539
39.330
26.634
22.760
NHAc
MeOOC
Ph
N
N
N
H
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.414
7.408
7.397
7.363
7.358
6.997
6.983
6.981
6.975
6.970
6.956
6.728
6.708
6.629
6.623
6.616
6.609
6.602
6.596
6.590
6.566
2.377
2.296
N
N
N
N
Pd
O
O
2
3.07
2.08
2.05
1.05
1.04
1.00
3.00
3.03
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


193.638
186.493
180.983
173.686
161.514
129.304
128.484
126.614
126.015
121.680
119.739
117.956
111.798
98.625
77.337
76.703
23.791
7.649
N
N
N
N
Pd
O
O
2
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)