Supplementary Information

A Reusable Polymer supported catalyst for Copper-Azide-Alkyne Cycloaddition (CuAAC) Under Ambient Condition

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1. General Information

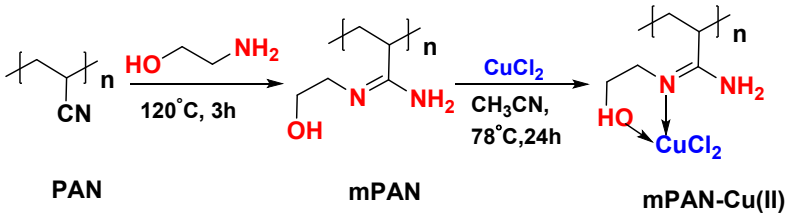
Reagents and solvents were purchased from commercial vendors, including Sigma Aldrich, Merck, Spectrochem, TCI and the solvents were distilled by standard procedures. All the experiments were conducted in oven dried glassware under atmospheric conditions. The samples were characterized by Fourier transform infrared spectroscopy (FTIR) recorded on a Perkin Elmer in the range of 4000-400 cm^{-1} under atmospheric conditions. Rigaku miniflex600 benchtop X-ray diffraction instrument was used to take the X-ray diffraction pattern (XRD) of catalysts, using Cu-Kα1 radiation. Perkin Elmer TGA 8000 analyzer was used to record the thermograms of catalysts with a heating rate of 20^0C/min from 30 to 700^0C in nitrogen atmosphere. ICP-MS analysis was conducted using Inductively Coupled Mass Spectrometer (ICP-MS) (Thermo Scientific).Thin layer chromatographic (TLC) techniques were used to monitor the progress of the reactions using silica gel 60 F254 plates (Merck) and fluorescence quenching was used to visualize reactions under UV light. The compounds were isolated and purified by column chromatography with silica gel (60–120 mesh) by using a mixture of ethyl acetate and hexane solvents as eluent. ^{1}H and ^{13}C NMR (400 MHz and 100 MHz respectively) spectra were recorded on a Bruker nuclear resonance spectrometer using $CDCl_3$ as the solvent and chemical shifts are expressed in parts per million (ppm) downfield from TMS (δ = 0.00). In assignment of the NMR spectra, multiplicities and abbreviations used are as follows: Ar = Aromatic, Ph = Phenyl, s = singlet d = doublet, t = triplet, q = quartet, dd = doublet of doublets and m = multiplet.

2. Experimental Procedures

2.1 Synthesis of mPAN and mPAN-Cu Complex

About 1g of Polyacrylonitrile (20 mmol) (Molecular weight calculated using actual mass of single monomer) was mixed with 3.6 m1 of Monoethanolamine (MEA) (60 mmol) and the reaction was performed at 120°C for 3 h. After cooling the resultant mixture was diluted with ethanol and the modified polymer were precipitated out when the resultant mixture is poured into a beaker containing fourfold excess of acetone. The obtained modified polymer was dried at 50 °C for 24 h. After that about 2 mmol of dried modified polymer in 10 ml acetonitrile (CH_3CN)

was treated with 0.25 mmol (1% W/V) acetonitrile solution of $CuCl_2$ over a period of 30 minute under stirring. The reaction mixture was refluxed for 24 h at 78°C. The brown color complex thus formed was filtered, washed with ethanol and dried at room temperature under vacuum. (**Scheme S1**)



Scheme S1 Synthesis of the polymer supported copper catalyst

2.2 General Procedure for Click Reaction

To a 10 ml Round bottom flask, Benzylbromide (1 eq.), Phenylacetylene (1 eq.), sodium azide (1.2 eq.), mPAN-Cu (20 mol %) were added followed by the addition of methanol (3 ml). The reaction mixture was then stirred at room temperature and progress of the reaction was monitored by TLC. After completion of the reaction, the reaction mixture was extracted with ethyl acetate and water. The organic layer was separated and dried over anhydrous Na_2SO_4 and concentrated on rotary evaporator. The obtained crude product was separated by column chromatography using hexane: ethylacetate (90: 10) and the yields were noted. The structure of the products was characterized using spectroscopic analyses.

2.3 $CuCl_2$ Loading (mmol) in mPAN-Cu(II)

The catalyst is usually prepared by treating mPAN with 0.25 mmol of $CuCl_2$ loading. In order to examine the effect of metal loading we have prepared different batch of catalyst by varying copper loading to ensure that the catalyst surface has a sufficient number of active centers to carried out the reaction. For that we prepared three set of mPAN-Cu(II) catalyst with 0.15 mmol, 0.25 mmol and 0.50 mmol of $CuCl_2$ loading. Then we carried out the CuAAC in optimized conditions, the product obtained with 67, 91 and 93 % yield respectively. The results showed that the catalyst with the low metal loading has less number of active site while compare

with 0.25 mmol of $CuCl_2$ loading. But the catalyst with high copper loading (0.5 mmol) didn't show any drastic change in the yield of the product.

Table 1; $CuCl_2$ Loading (mmol) in mPAN-Cu(II)

Entry	$CuCl_2$ Loading (mmol) in mPAN-Cu(II)	Yield[b]
1	**0.15**	**67**
2	**0.25**	**91**
3	**0.50**	**93**

[a]Reaction conditions: **1a**(1 eq.), **2a**(1 eq.), **NaN_3**(1.2eq.), mPAN-Cu(II) (20mol %), NaAsc (30 mol%), H_2O (3ml), rt, 7h. [b]isolated yield.

3. Characterization of PAN, mPAN and mPAN-Cu(II)

3.1 XRD Analysis

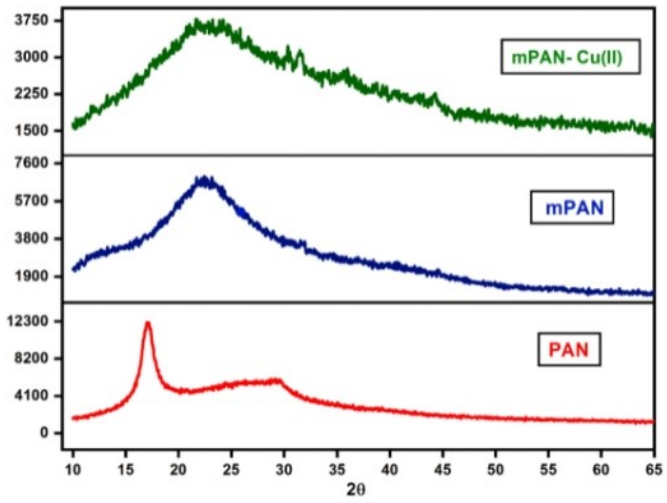


Figure S1: XRD pattern of PAN, mPAN, mPAN-Cu(II)

Figure S1 shows the XRD pattern of PAN, mPAN, mPAN-Cu(II) complex, the strong diffraction peaks at 2θ =17.27˚ and 29.38˚ indicating the semi crystalline nature of PAN, in addition to that these peaks disappeared after synthetic modification with monoethanolamine and

observed an amorphous pattern for mPAN . But in the case of mPAN-Cu(II) three diffraction peaks are observed at 2θ = 25.83˚, 30.63˚, 30.97˚ are attributed to the planes (1 0 1), (0 0 2) and (2 1 -1) which indicating the presence of copper (II) phase which is in close agreement with the jcpds card 00-034-0198.

3.2 Thermogravimetic Analysis (TGA)

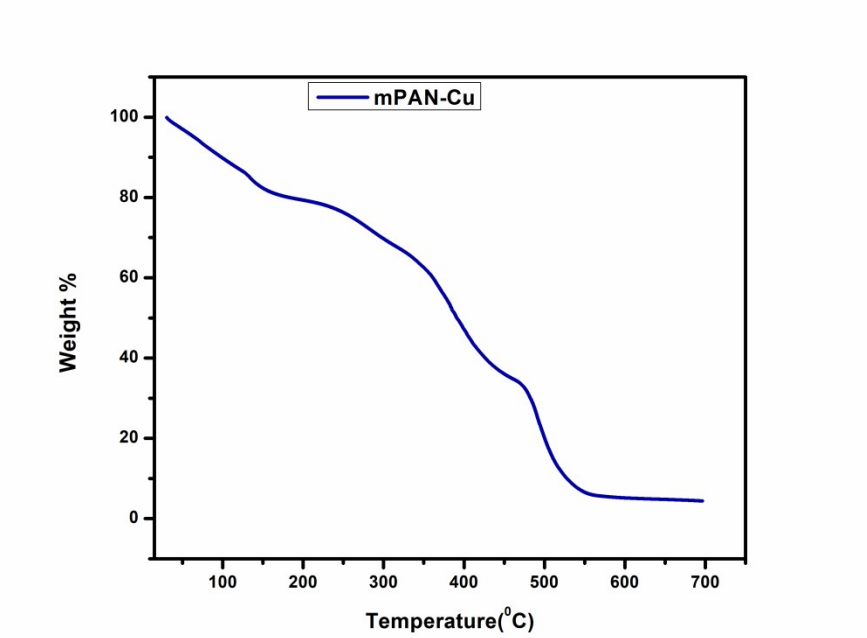


Figure S2:TGA Curve of mPAN-Cu (II)

TGA analysis of mPAN-Cu(II) (**Figure S2)** revealed the thermal stability of the complex and its weight loss consists of three stages. The first stage which occurs between 50 and 190°C with a weight loss of 18% was attributed to the loss of water molecules. The second stage is in between 190 and 472°C with weight loss of 45% corresponds to the decomposition of metal from the polymeric chain. The third stage involves the decomposition of remaining polyacrylonitrile chain with a weight loss of 28%.

3.3 FT-IR spectrum of Fresh and Reused Catalyst

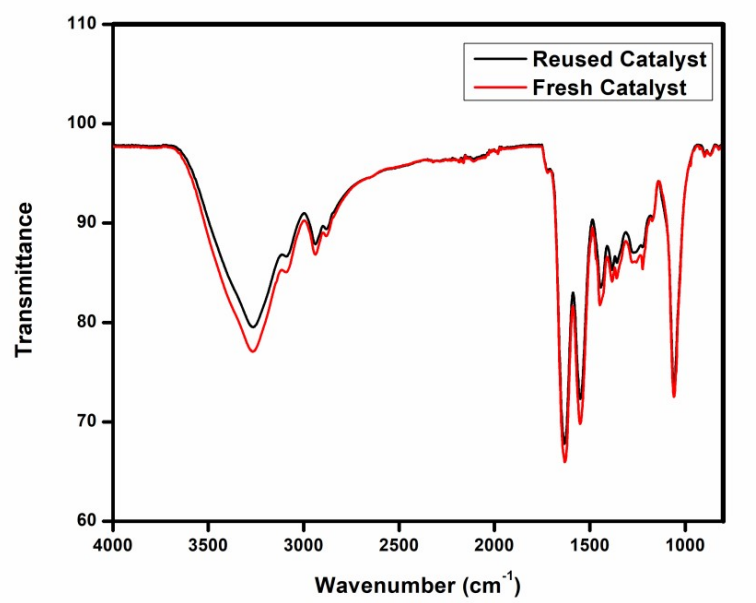


Figure S3: FT-IR Spectrum of fresh and reused catalyst

3.4 XRD pattern of Fresh and Reused catalyst

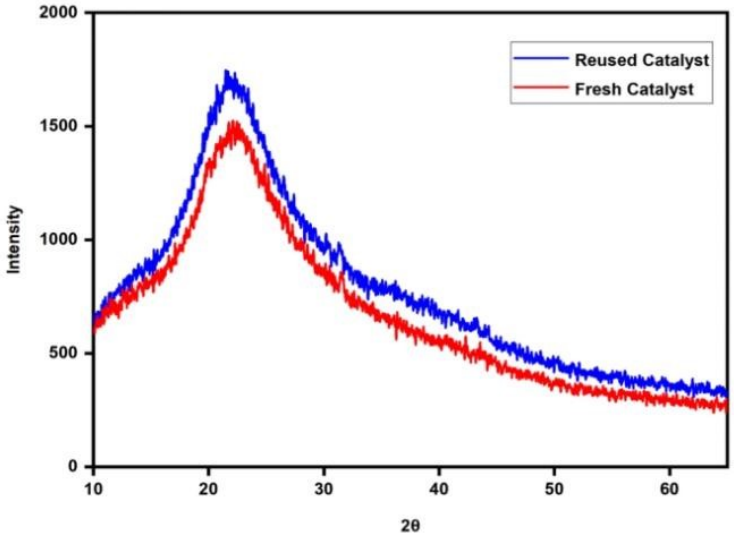
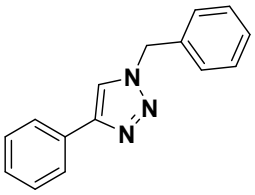


Figure S4: XRD pattern of fresh and reused catalyst

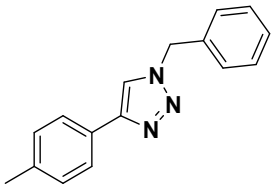
4. SPECTROSCOPIC DATA OF COMPOUNDS (3a-t)

1-benzyl-4-phenyl-1H-1, 2, 3-triazole (3a)



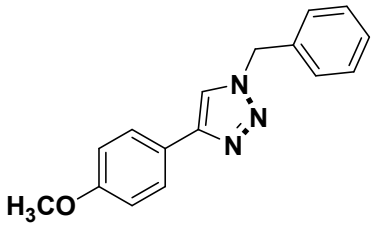
White solid; R_f = 0.35 (Hexane/EtOAc= 90:10); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 (d, *J* = 8.0 Hz, 2H), 7.69 (s, 1H), 7.39 – 7.25 (m, 8H), 5.50 (s, 2H);^{13}C NMR (100 MHz, $CDCl_3$): *δ* 148.2, 134.6, 130.5, 129.1, 128.8, 128.0, 125.7, 119.5, 54.2; FTIR (neat): 3141, 2922, 1605, 1449, 1222, 918, 856, 763 cm^{-1}; GC-MS (EI) [M]+:m/z calculated for $C_{15}H_{13}N_3$:235.11, found:235.00.

1-benzyl-4-(p-tolyl)-1H-1, 2, 3-triazole (3b)



White solid; R_f = 0.40 (Hexane/EtOAc = 90:10);^{1}H NMR (400 MHz, $CDCl_3$) δ= 7.67 (d, *J* = 8.1 Hz, 2H), 7.61 (s, 1H), 7.39 – 7.29 (m, 5H), 7.20 (d, *J* = 7.9 Hz, 2H), 5.56 (s, 2H), 2.35 (s, 3H); ^{13}C NMRδ=148.1, 134.7, 133.5, 130.9, 130.4, 129.1, 128.8, 128.0, 125.7, 119.8, 54.1, 29.4; FTIR (neat): 3143, 2917, 2850, 1729, 1494, 1221, 1046, 825, 788 cm^{-1}; GC-MS (EI) [M]+:m/z calculated for $C_{16}H_{15}N_3$:249.13, found: 249.00.

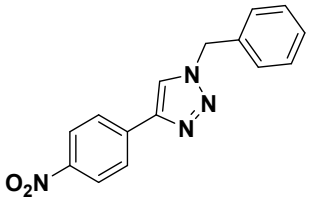
1-benzyl-4-(4-methoxyphenyl)-1H-1, 2, 3-triazole (3c)



White solid; R_f = 0.15 (Hexane/EtOAc = 90:10); ^{1}H NMR (400 MHz, $CDCl_3$): *δ* 7.70 (d, *J* = 8.8 Hz, 2H), 7.58 (s, 1H), 7.36 – 7.28 (m, 5H), 6.91 (d, *J* = 8.8 Hz, 2H), 5.51 (s, 2H), 3.79 (s, 3H);

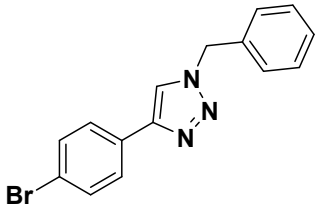
^{13}C NMR (100 MHz, $CDCl_3$): δ 159.6, 148.0, 134.7, 129.1, 128.7, 128.0, 127.0, 123.2, 118.8, 114.2, 55.3, 54.1; FTIR (neat): 3135, 2958, 2923, 1725, 1450, 1214, 1033, 973, 760 cm^{-1}; GC-MS(EI) [M]+:m/z calculated for $C_{16}H_{15}N_3O$:265.12, found:256.00

1-benzyl-4-(4-nitrophenyl)-1H-1, 2, 3-triazole (3d)



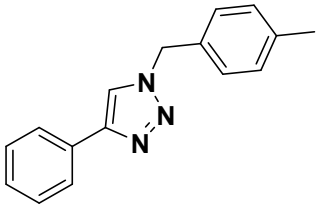
Light Yellow solid; R_f = 0.25 (Hexane/EtOAc = 90:10); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.24 (d, J = 8.9 Hz, 2H), 7.96 – 7.94 (m, 2H), 7.80 (s, 1H), 7.40 (dq, J = 4.8, 1.0 Hz, 3H), 7.39 – 7.32 (m, 2H), 5.60 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.3, 146.0, 136.7, 134.1, 1129.3, 129.1, 128.2, 126.1, 124.3, 121.0, 54.2; FTIR (neat): 3124, 2928, 2850, 1732, 1075, 1026, 978, 839, 756 cm^{-1}.GC-MS (EI) [M]+:m/z calculated for $C_{15}H_{12}N_4O_2$:280.10, found: 281.00.

1-benzyl-4-(4-bromophenyl)-1H-1, 2, 3-triazole (3e)



White solid; R_f = 0.35 (Hexane/EtOAc = 90:10); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.66 (d, J = 3.8 Hz, 2H), 7.63 (s, 1H), 7.49 (d, J = 8.6 Hz, 2H), 7.39 – 7.26 (m, 5H), 5.54 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$):δ 147.1, 134.5, 131.9, 130.9, 129.4, 128.9, 128.1, 127.2, 122.0, 119.7, 54.3; FTIR (neat): 3121, 2923, 2855, 1725, 1453, 1223, 1068, 969, 810, 724 cm^{-1}.GC-MS(EI) [M]+:m/z calculated for $C_{15}H_{12}BrN_3$: 313.02, found:313.02

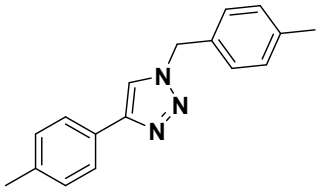
1-(4-methylbenzyl)-4-phenyl-1H-1, 2, 3-triazole (3f)



White solid; R_f = 0.50 (Hexane/EtOAc = 90:10); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.79 (d, J = 7.4 Hz, 2H), 7.68 (s, 1H), 7.37 – 7.25 (m, 3H), 7.18 – 7.12 (m, 4H), 5.44 (s, 2H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.0, 138.6, 131.8, 130.6, 129.8, 128.8, 128.1, 125.7, 119.7, 53.95,

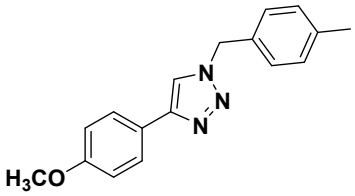
21.2; FTIR(neat):3117, 2962, 2923, 1608, 1514, 1222, 1079, 973, 831, 763 cm^{-1}; GC-MS(EI) [M]+:m/z calculated for $C_{16}H_{15}N_3$: 249.13, found: 249.13

1-(4-methylbenzyl)-4-(p-tolyl)-1H-1, 2, 3-triazole (3g)



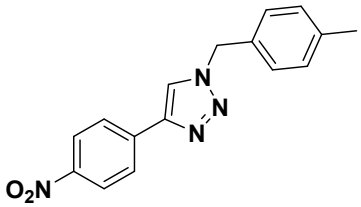
White solid; R_f = 0.45 (Hexane/EtOAc = 90:10); **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.67 (d, J = 7.8 Hz, 2H), 7.59 (s, 1H), 7.21 – 7.16 (m, 6H), 5.49 (s, 2H), 2.34 (s, 6H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 148.1, 138.0, 131.6, 130.9, 129.4, 128.1, 127.7, 125.6, 119.1, 54.0, 21.0; FTIR (neat): 3124, 2919, 2850, 1733, 1454, 1244, 1072, 1024, 975, 827, 814, 741cm^{-1}; GC-MS (EI) [M]+:m/z calculated for $C_{17}H_{17}N_3$:263.14, found: 264.10

4-(4-methoxyphenyl)-1-(4-methylbenzyl)-1H-1, 2, 3-triazole (3h)



White solid; R_f = 0.18 (Hexane/EtOAc = 90:10); ^{1}H NMR (400 MHz, $CDCl_3$):δ 7.69 (d, J = 8.0 Hz, 2H), 7.56 (s, 1H), 7.16 (t, J = 2.5 Hz, 4H), 6.89 (d, J = 8.0 Hz, 2H), 5.46 (s, 2H), 3.78 (s, 3H), 1.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.5, 147.9, 138.6, 132.4, 131.7, 130.9, 12.8, 128.1, 127.0, 123.3, 118.7, 114.2, 55.2, 53.9, 21.1; FTIR (neat): 3129, 2914, 2850, 1614, 1514, 1431, 1223, 1069, 1048, 974, 810 cm^{-1}; GC-MS (EI) [M]+:m/z calculated for $C_{17}H_{17}N_3O$:279.14, found:279.14.

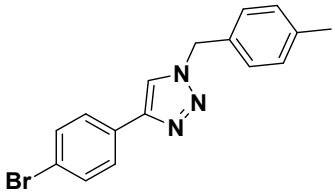
1-(4-methylbenzyl)-4-(4-nitrophenyl)-1H-1, 2, 3-triazole (3i)



Yellow solid; R_f = 0.25 (Hexane/EtOAc = 90:10); ^{1}H NMR (400 MHz, $CDCl_3$):δ 8.24 (d, J = 7.7 Hz, 1H), 7.94 (d, J = 7.6 Hz, 1H), 7.78 (s, 1H), 7.21 (q, J = 6.8, 4.8 Hz, 4H), 5.55 (s, 2H), 2.36

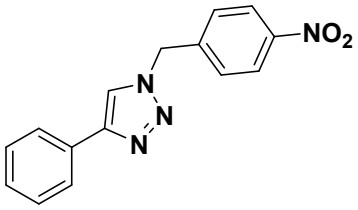
(s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$):δ 147.3, 145.9, 139.1, 136.8, 131.1, 129.9, 128.3, 126.1, 124.2, 120.9, 54.3, 21.2; FTIR (neat): 3123, 2923, 2859, 1726, 1605, 1330, 1222, 1074, 972, 853, 831, 758 cm^{-1}; GC-MS(EI) [M]+:m/z calculated for $C_{16}H_{14}N_4O_2$: 294.11, found: 294.10

4-(4-bromophenyl)-1-(4-methylbenzyl)-1H-1, 2, 3-triazole (3j)



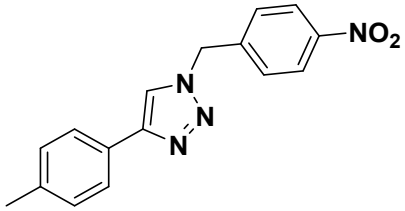
White solid; R_f = 0.4 (Hexane/EtOAc = 90:10); ^{1}H NMR (400 MHz, $CDCl_3$):δ 7.64 (d, J = 8.4 Hz, 2H), 7.62 (s, 1H), 7.50 (d, J = 8.1 Hz, 2H), 7.19 (d, J = 1.4 Hz, 4H), 5.51 (s, 2H), 1.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$):δ 147.1, 138.9, 131.9, 131.4, 129.8, 128.2, 127.2, 122.0, 119.5, 54.2, 21.2; FTIR (neat): 3121, 2923, 2855, 1738, 1604, 1384, 1182, 1064, 972, 810, 757 cm^{-1}; GC-MS (EI) [M]+:m/z calculated for $C_{16}H_{14}BrN_3$: 327.04, found: 327.00

1-(4-nitrobenzyl)-4-phenyl-1H-1, 2, 3-triazole (3k)



Pale Yellow Solid; R_f = 0.40 (Hexane/EtOAc = 85:15); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.22 (d, J = 5.1 Hz, 2H), 8.18 (d, J = 4.9 Hz, 2H), 7.56 – 7.47 (m, 5H), 7.47 (s, 1H), 4.49 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.7, 147.6, 144.8, 142.7, 129.9, 128.6, 124.2, 124.0, 123.8, 53.7; FTIR (neat):3120, 2916, 2864, 1603, 1452, 1057, 986, 912, 850, 749 cm^{-1}; GC-MS (EI) [M]+:m/z calculated for $C_{15}H_{12}N_4O_2$: 280.10, found:281.10.

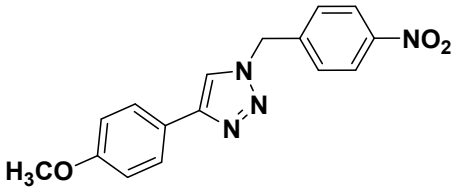
1-(4-nitrobenzyl)-4-(p-tolyl)-1H-1, 2, 3-triazole (3l)



Pale Yellow solid; R_f = 0.43 (Hexane/EtOAc = 90:10); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.22 (d, J = 7.8 Hz, 2H), 7.72 (s, 1H), 7.70 – 7.68 (m, 2H), 7.44 (d, J = 8.0 Hz, 2H), 7.21 (d, J = 7.3 Hz, 2H), 5.68 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.6, 148.1, 141.6, 138.5, 129.6, 128.6,

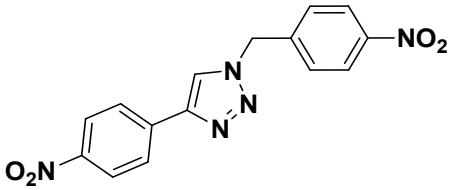
126.9, 125.7, 124.3, 119.5, 53.2, 21.3; FTIR (neat): 3126, 2928, 1736,1616, 1337, 1079, 956, 889, 725 cm^{-1}; GC-MS(EI) [M]+:m/z calculated for $C_{16}H_{14}O_2N_4$: 294.11, found: 294.0

4-(4-methoxyphenyl)-1-(4-nitrobenzyl)-1H-1, 2, 3-triazole (3m)



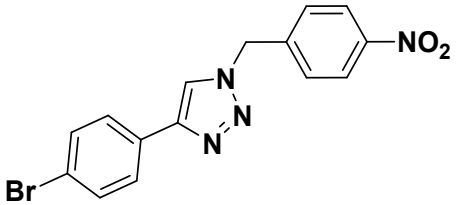
Light Brown solid; R_f = 0.16 (Hexane/EtOAc = 90:10); ^{1}H NMR (400 MHz, $CDCl_3$):δ 8.19 (d, *J* = 8.4 Hz, 2H), 7.71 (d, *J* = 8.6 Hz, 2H), 7.67 (s, 1H), 7.40 (s, 2H), 6.92 (d, *J* = 8.6 Hz, 2H), 5.65 (s, 2H), 3.81 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$):δ 159.8, 148.5, 148.0, 141.8, 128.5, 127.0, 124.3, 122.7, 119.0, 114.3, 55.3, 53.1; FTIR (neat): 3104, 2923, 2859, 1608, 1595, 1223, 1199, 1104, 857, 798 cm^{-1}; GC-MS(EI) [M]+:m/z calculated for $C_{16}H_{14}N_4O_3$: 310.11, found: 311.10

1-(4-nitrobenzyl)-4-(4-nitrophenyl)-1H-1, 2, 3-triazole (3n)



Pale yellow solid; R_f = 0.16 (Hexane/EtOAc = 90:10);^{1}H NMR (400 MHz, $CDCl_3$): δ 8.28 (t, *J* = 8.9 Hz, 4H), 7.99 (d, *J* = 8.5 Hz, 2H), 7.88 (s, 1H), 7.48 (d, *J* = 8.3 Hz, 2H), 5.73 (s, 2H); FTIR(neat): 3210, 2920, 2850, 1744, 1603, 1515, 1231, 1107, 1048, 973, 853, 805, 779 cm^{-1}; GC-MS(EI) [M]+:m/z calculated for $C_{15}H_{11}N_5O_4$:325.08, found:325.00

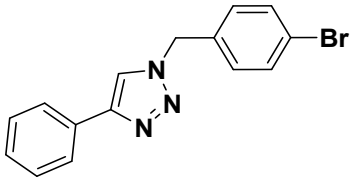
4-(4-bromophenyl)-1-(4-nitrobenzyl)-1H-1, 2, 3-triazole (3o)



White solid; R_f = 0.22 (Hexane/EtOAc = 90:10); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.23 (d, *J* = 8.7 Hz, 2H), 7.74 (s, 1H), 7.67 (d, *J* = 8.6 Hz, 2H), 7.53 (d, *J* = 8.6 Hz, 2H), 7.44 (d, *J* = 8.7 Hz, 2H), 5.68 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.1, 141.5, 132.5, 130.9, 129.0, 128.6, 127.2,

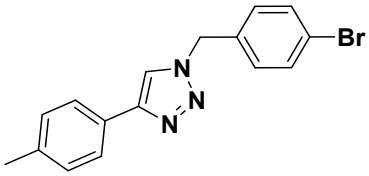
124.4, 122.4, 119.8, 53.2; FTIR (neat): 3110, 2923, 2855, 1728, 1510, 1227, 1068, 978, 861, 823, 732 cm^{-1}; GC-MS(EI) [M]+:m/z calculated for $C_{15}H_{11}N_4O_2Br$: 358.01, found:358.00

1-(4-bromobenzyl)-4-phenyl-1H-1, 2, 3-triazole (3p)



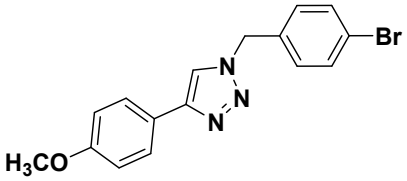
White solid; R_f = 0.15 (Hexane/EtOAc = 90:10); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 (dd, *J* = 8.3, 1.3 Hz, 2H), 7.66 (s, 1H), 7.53 – 7.46 (m, 2H), 7.42 – 7.28 (m, 3H), 7.19 – 7.13 (m, 2H), 5.50 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): *δ* 148.4, 133.7, 132.2, 130.3, 129.6, 128.8, 128.3, 125.7, 122.9, 119.2, 53.5; FTIR (neat): 3120, 3081, 2921, 2851, 1737, 1442, 1206, 1190, 1025, 976 cm^{-1}; GC-MS(EI) [M]+:m/z calculated for $C_{15}H_{12}BrN_3$:313.02, found:314.00

1-(4-bromobenzyl)-4-(p-tolyl)-1H-1, 2, 3-triazole (3q)



White solid; R_f = 0.25 (Hexane/EtOAc = 90:10); ^{1}H NMR (400 MHz, $CDCl_3$): *δ* 7.67 (d, *J* = 8.1 Hz, 2H), 7.63 (s, 1H), 7.48 (d, *J* = 8.4 Hz, 2H), 7.22 – 7.12 (m, 4H), 5.48 (s, 2H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): *δ* 148.4, 138.2, 133.7, 132.3, 129.5, 128.8, 127.4, 125.0, 122.9, 119.2, 53.5, 21.3; FTIR (neat): 3133, 2973, 1738, 1454, 1362, 1216, 1072, 977, 814, 758 cm^{-1}; GC-MS(EI) [M]+:m/z calculated for $C_{16}H_{14}BrN_3$: 327.04, found: 329.00

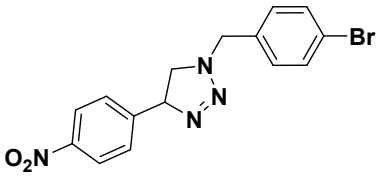
1-(4-bromobenzyl)-4-(4-methoxyphenyl)-1H-1, 2, 3-triazole (3r)



White solid; R_f = 0.15 (Hexane/EtOAc = 90:10); ^{1}HNMR (400 MHz, $CDCl_3$); δ= 7.71 (d, *J* = 8.9 Hz, 2H), 7.58 (s, 1H), 7.49 (d, *J* = 8.4 Hz, 2H), 7.16 (d, *J* = 8.4 Hz, 2H), 6.92 (d, *J* = 8.9 Hz, 2H), 5.50 (s, 2H), 3.81 (s, 3H); ^{13}C NMR (100 MHz,$CDCl_3$) δ= 159.7, 148.2, 133.7, 132.3, 129.6,

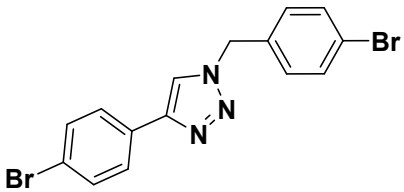
127.0, 122.9, 118.7, 114.2, 53.3, 53.5; FTIR(neat): 3122, 2919, 2855, 1982, 1733, 1617, 1217, 1175, 1073, 975, 831, 761 cm^{-1}.GC-MS(EI) [M]+:m/z calculated for $C_{16}H_{14}BrN_3O$: 343.00 , found: 345.00

1-(4-bromobenzyl)-4-(4-nitrophenyl)-1H-1, 2, 3-triazole (3s)



Pale Yellow solid; R_f = 0.22 (Hexane/EtOAc = 90:10); ^1H NMR (400 MHz, $CDCl_3$): δ 8.27 – 8.22 (m, 2H), 7.98 – 7.92 (m, 2H), 7.82 (s, 1H), 7.54 – 7.49 (m, 2H), 7.20 (d, J = 8.4 Hz, 2H), 5.55 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.3, 146.1, 136.6, 133.1, 132.5, 129.8, 126.1, 124.3, 123.3, 120.9, 53.8.; FTIR (neat): 3119, 2912, 1737, 1604, 1341, 1110, 1071, 975, 845, 789 cm^{-1}.GC-MS (EI) [M]+:m/z calculated for $C_{15}H_{13}N_4O_2Br$:360.02, found:360.00

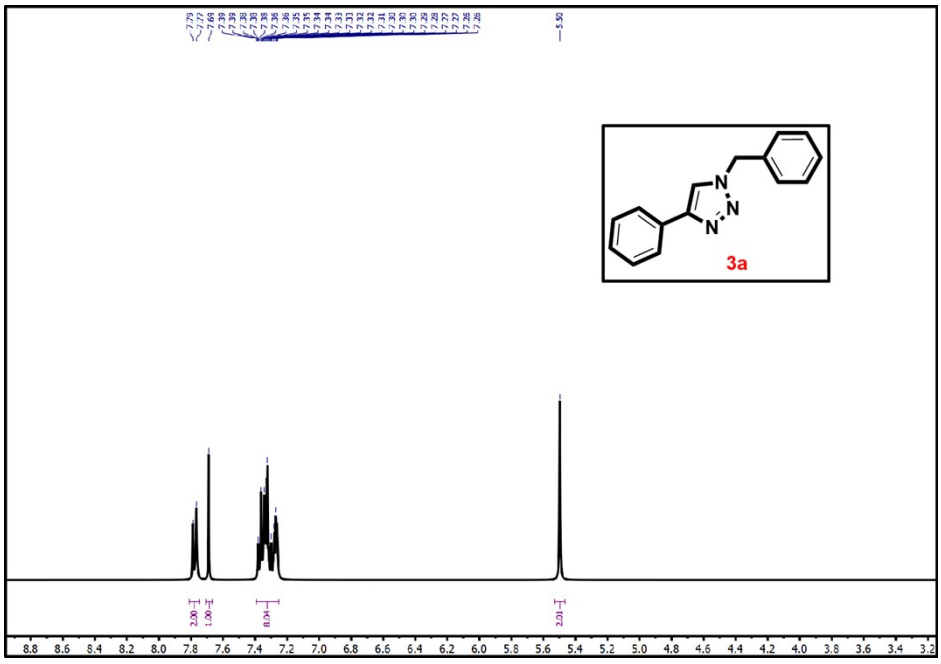
1-(4-bromobenzyl)-4-(4-bromophenyl)-1H-1, 2, 3-triazole (3t)

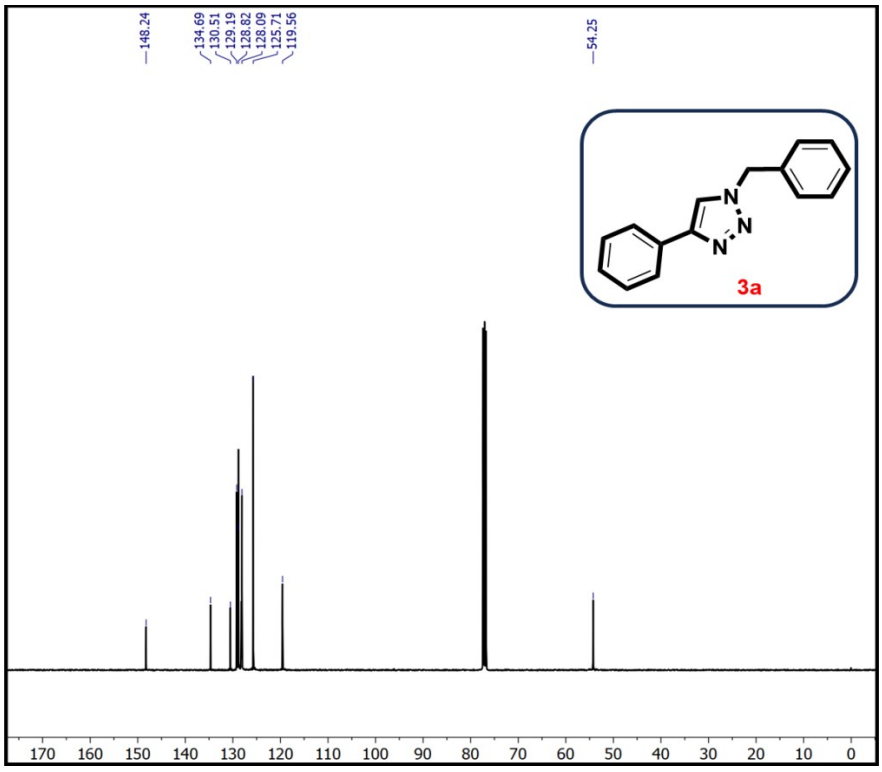


White solid; R_f = 0.37 (Hexane/EtOAc = 90:10); ^1H NMR (400 MHz, $CDCl_3$): δ7.66 (s, 1H), 7.65 – 7.61 (m, 2H), 7.51 – 7.47 (m, 4H), 7.16 (d, J = 8.5 Hz, 2H), 5.49 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.3, 133.4, 132.3, 132.0, 129.7, 129.2, 127.2, 123.0, 122.2, 119.6, 53.6; FTIR (neat): 3114, 2923, 1729, 1547, 1193, 1045, 973, 886, 754 cm^{-1};GC-MS(EI) [M]+:m/z calculated for $C_{15}H_{11}Br_2N_3$: 390.03, found:392.00.

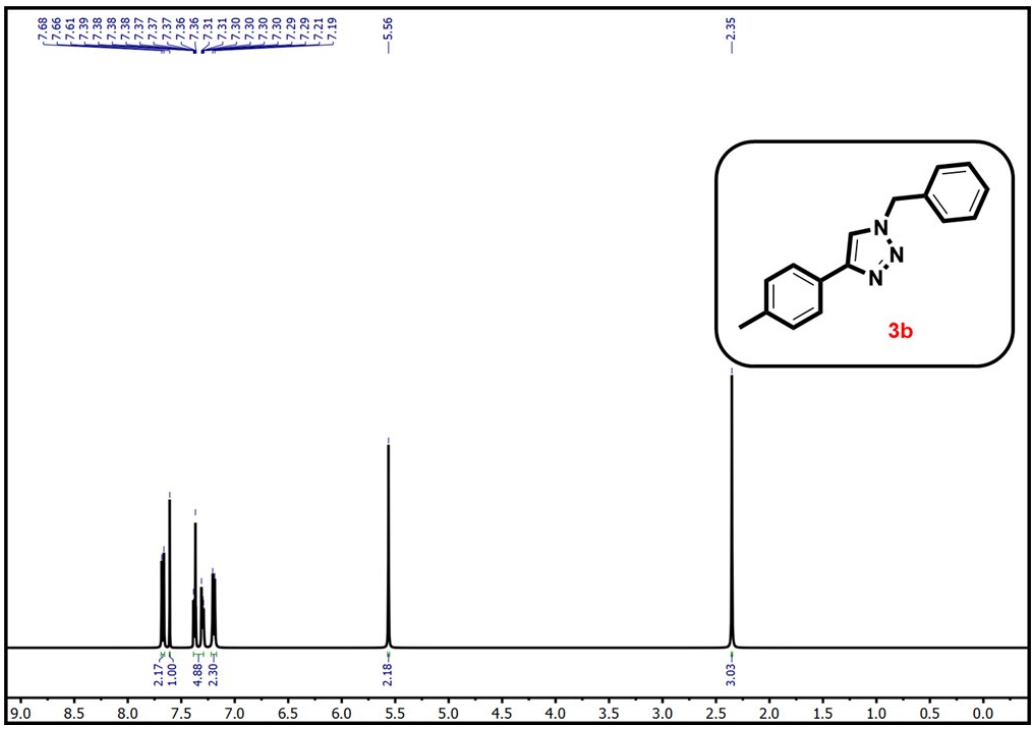
^{1}H and ^{13}C NMR spectra of products (3a-t)

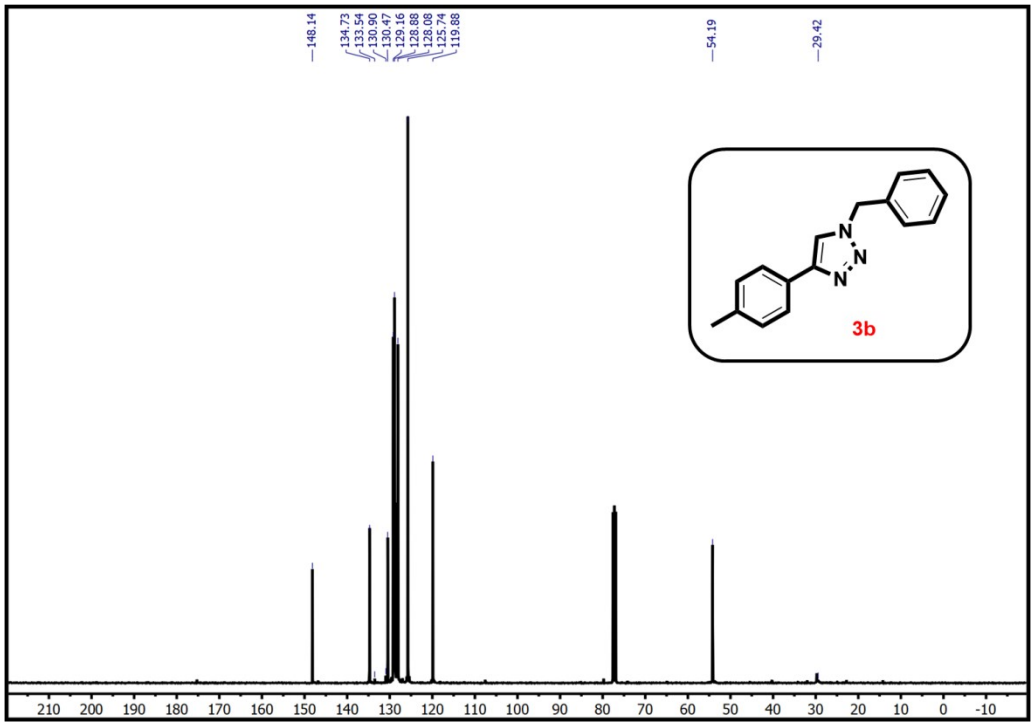
1. 1-benzyl-4-phenyl-1H-1,2,3-triazole (3a)



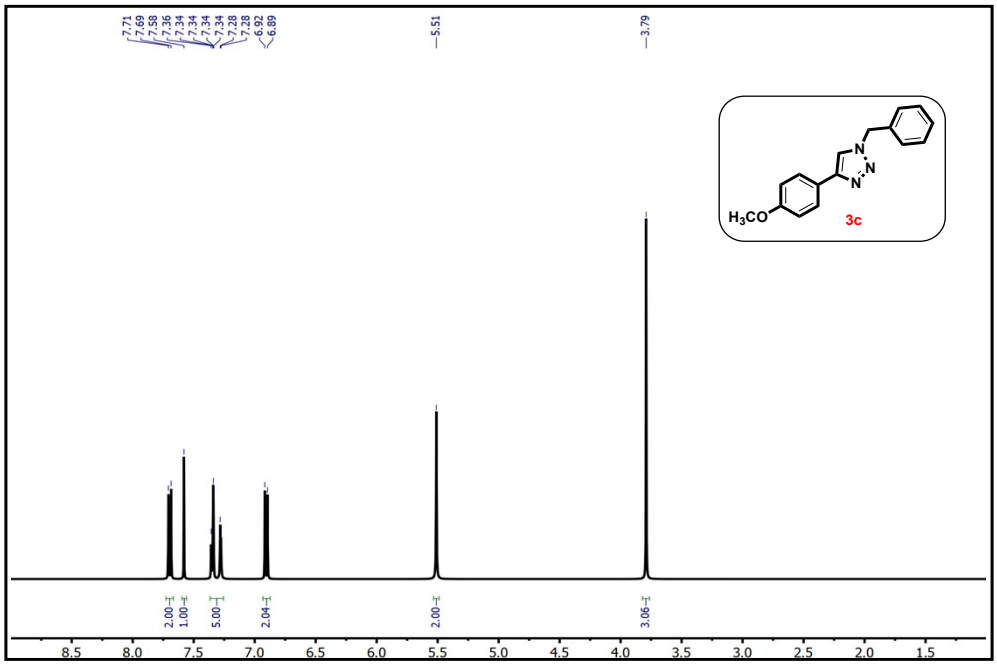


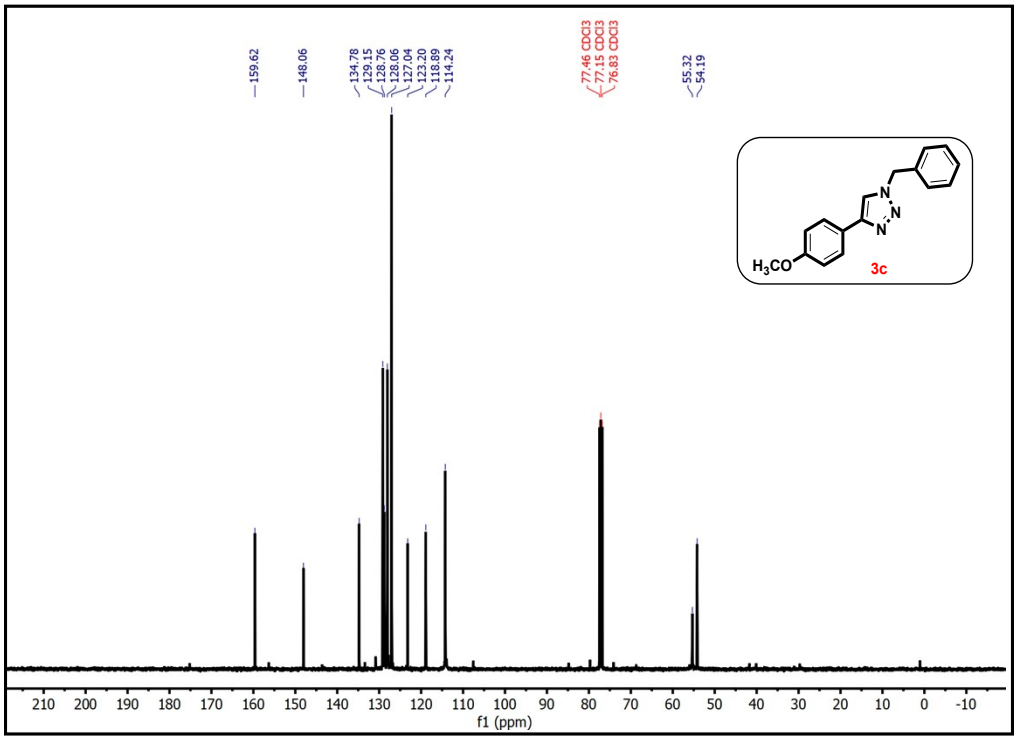
2. 1-benzyl-4-(p-tolyl)-1H-1,2,3-triazole (3b)



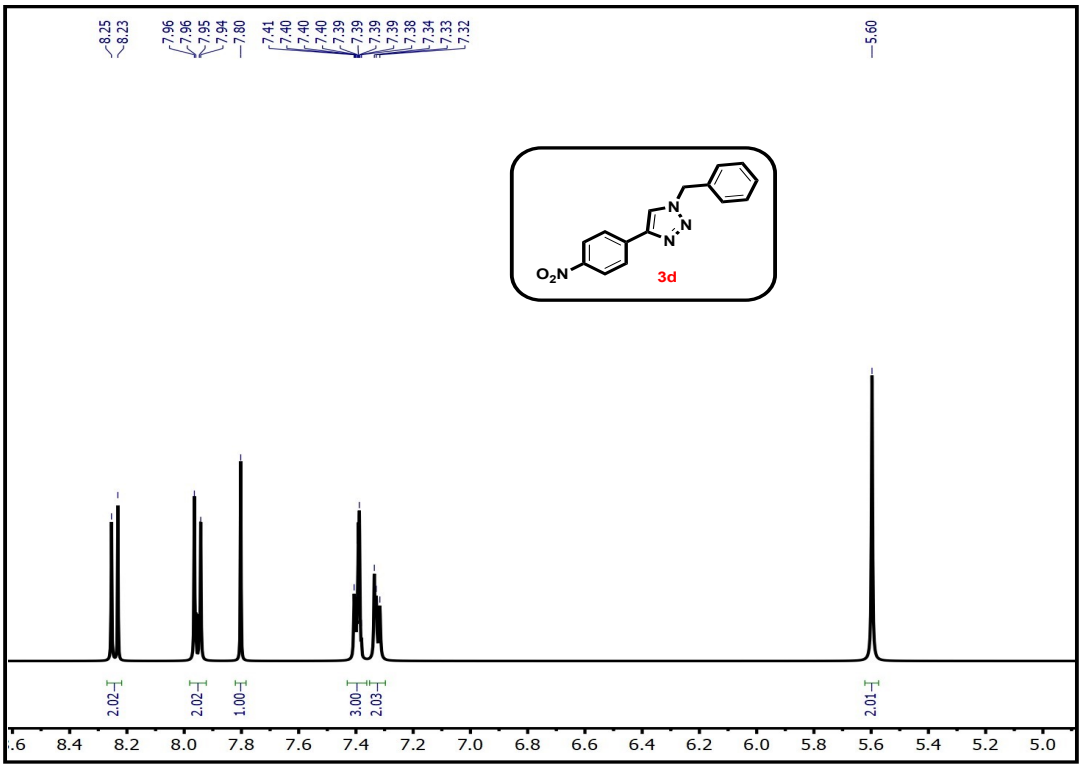


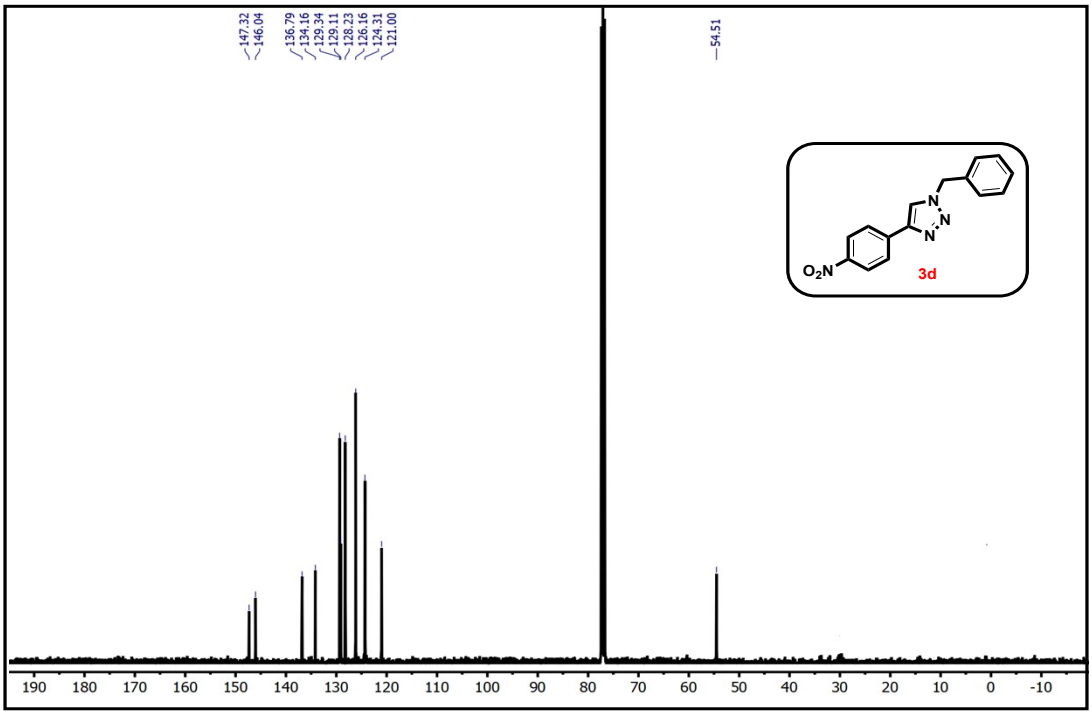
3. 1-benzyl-4-(4-methoxyphenyl)-1H-1,2,3-triazole (3c)



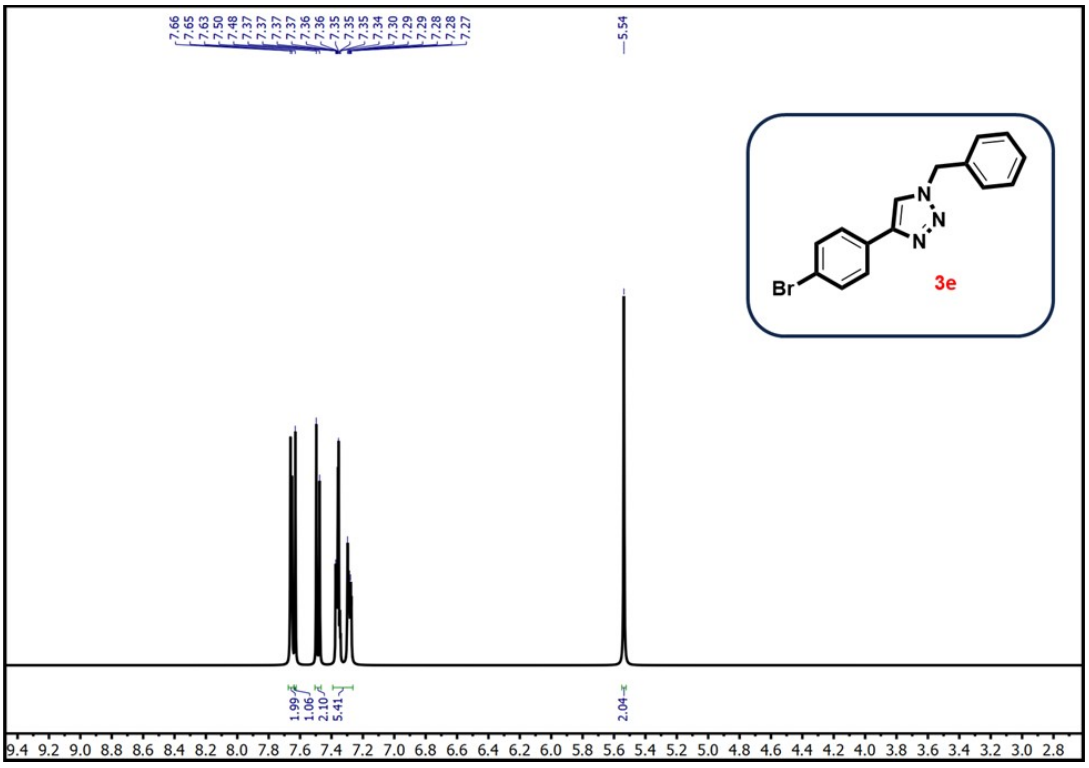


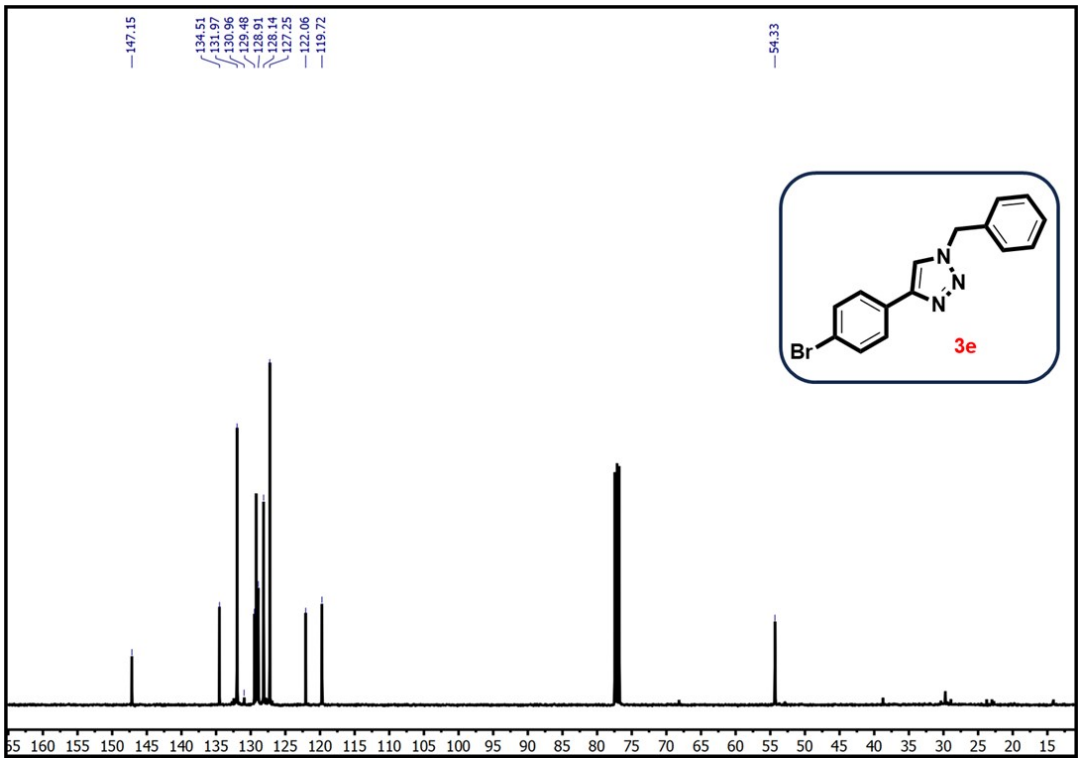
4. 1-benzyl-4-(4-nitrophenyl)-1H-1,2,3-triazole (3d)



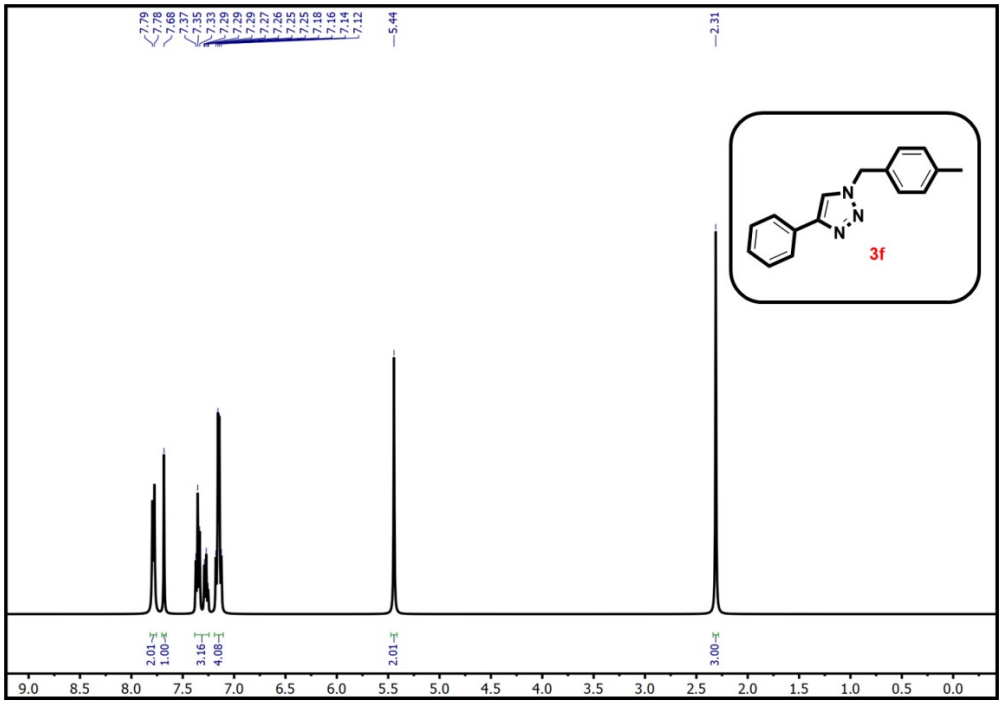


5. 1-benzyl-4-(4-bromophenyl)-1H-1,2,3-triazole (3e)

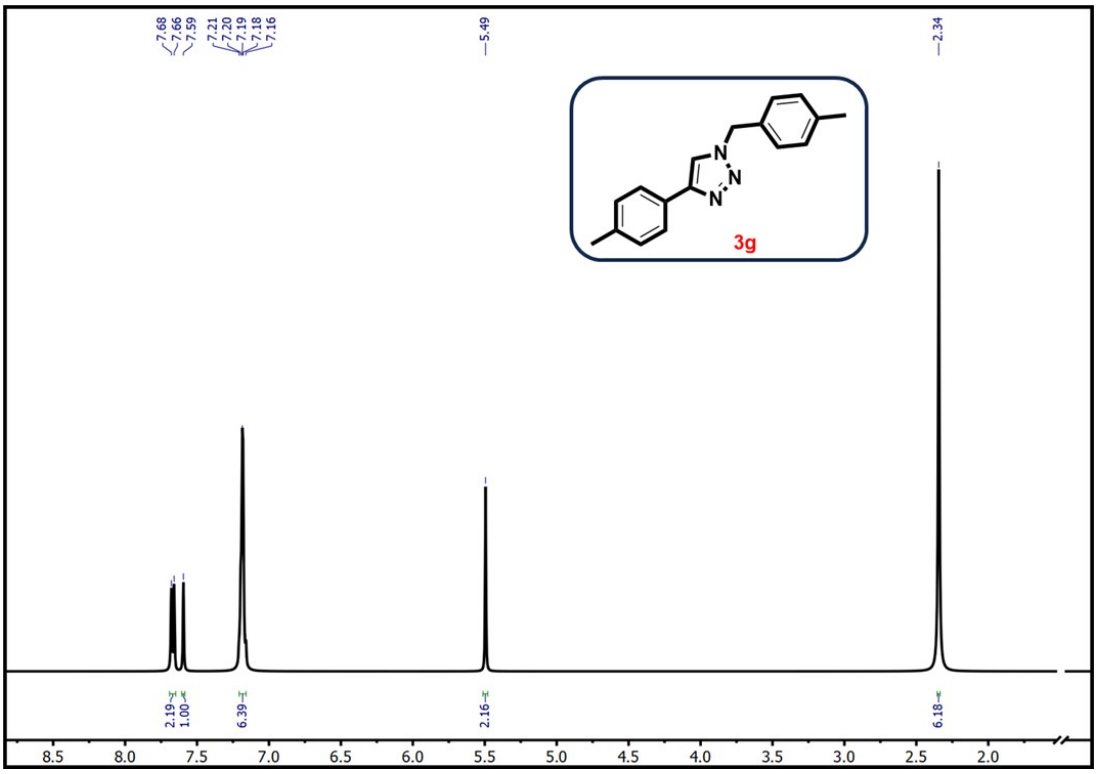


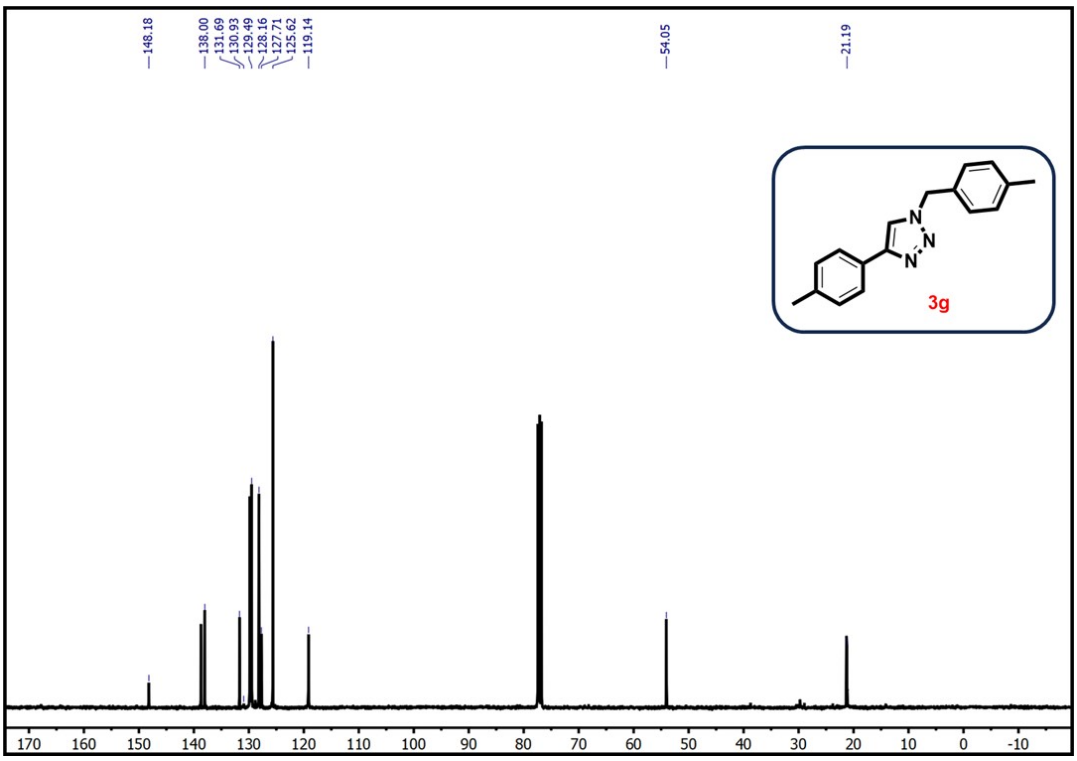


6. 1-(4-methylbenzyl)-4-phenyl-1H-1,2,3-triazole (3f)

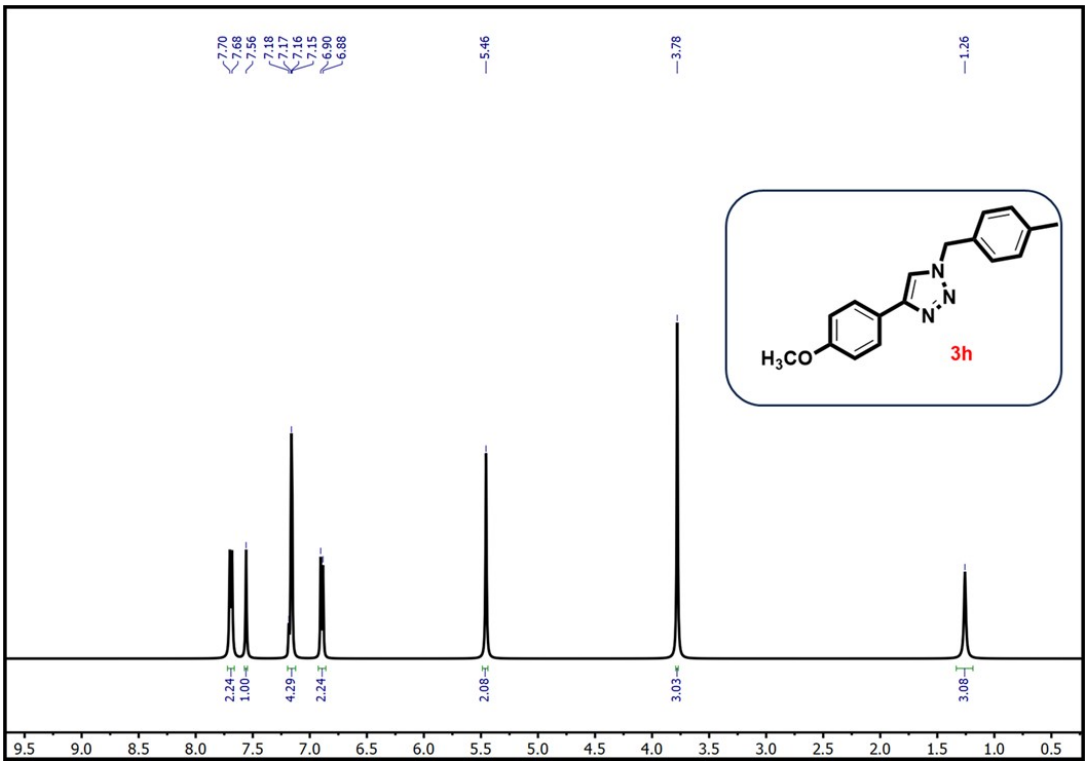


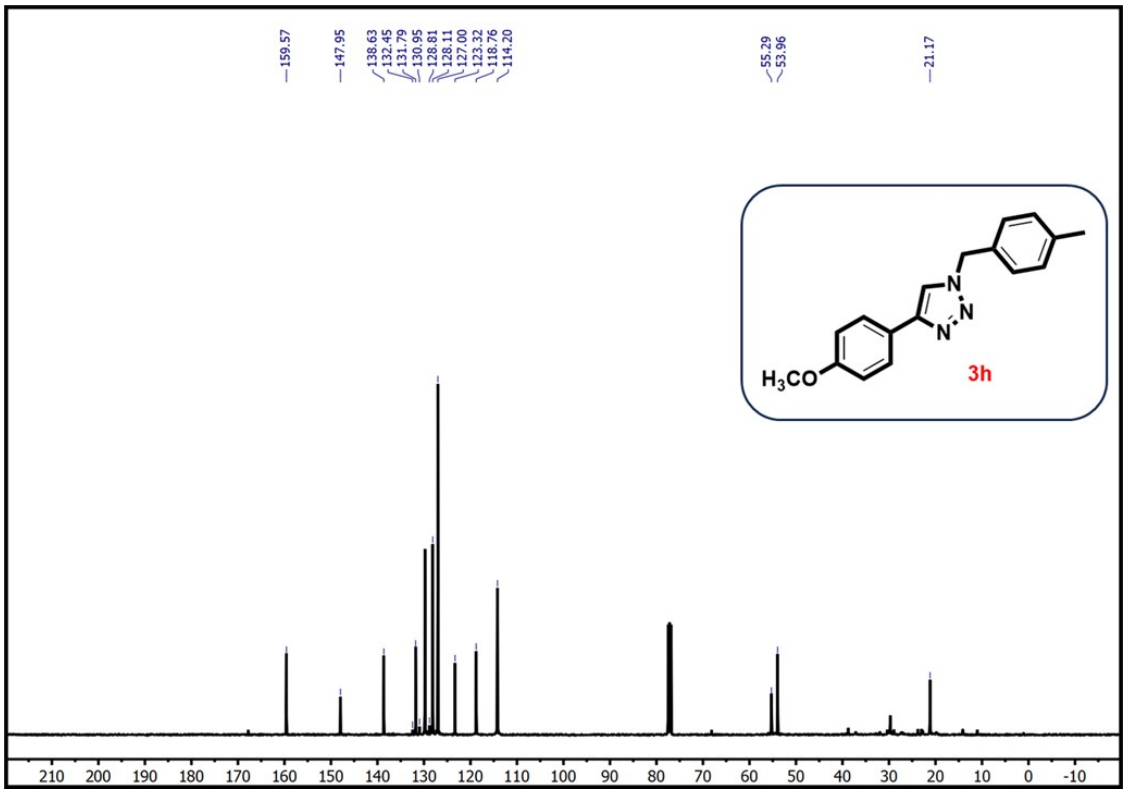
7. 1-(4-methylbenzyl)-4-(p-tolyl)-1H-1,2,3-triazole (3g)



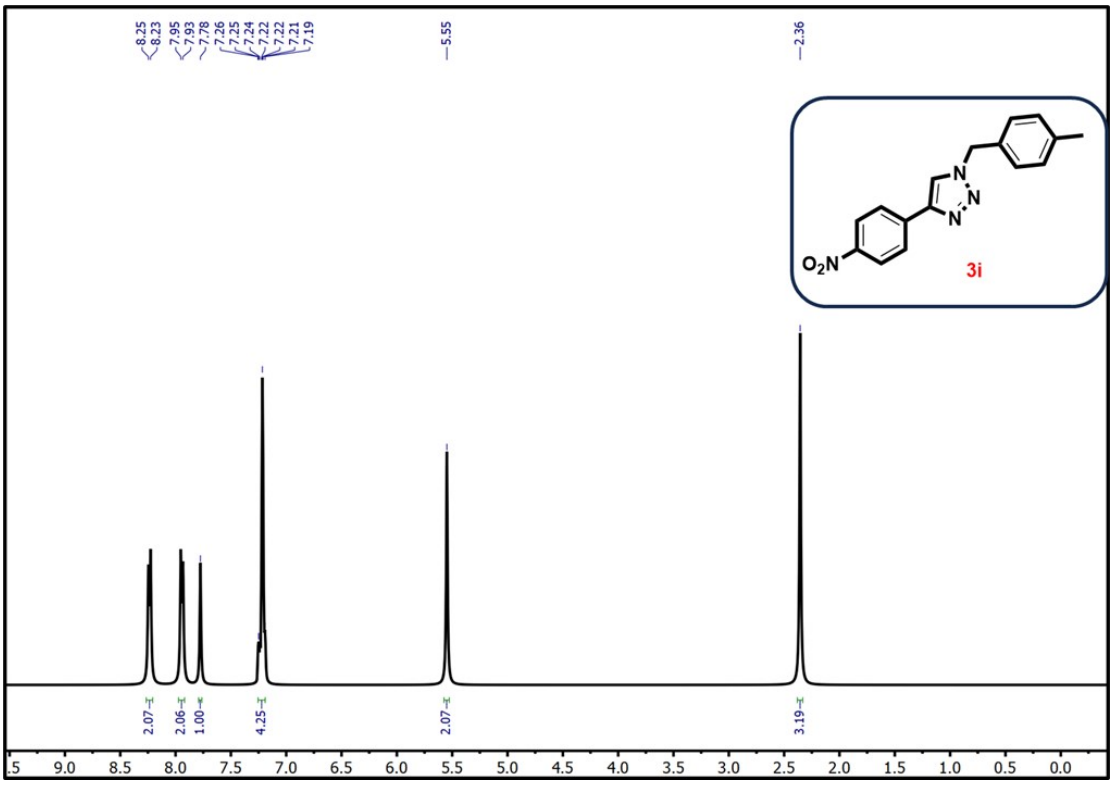


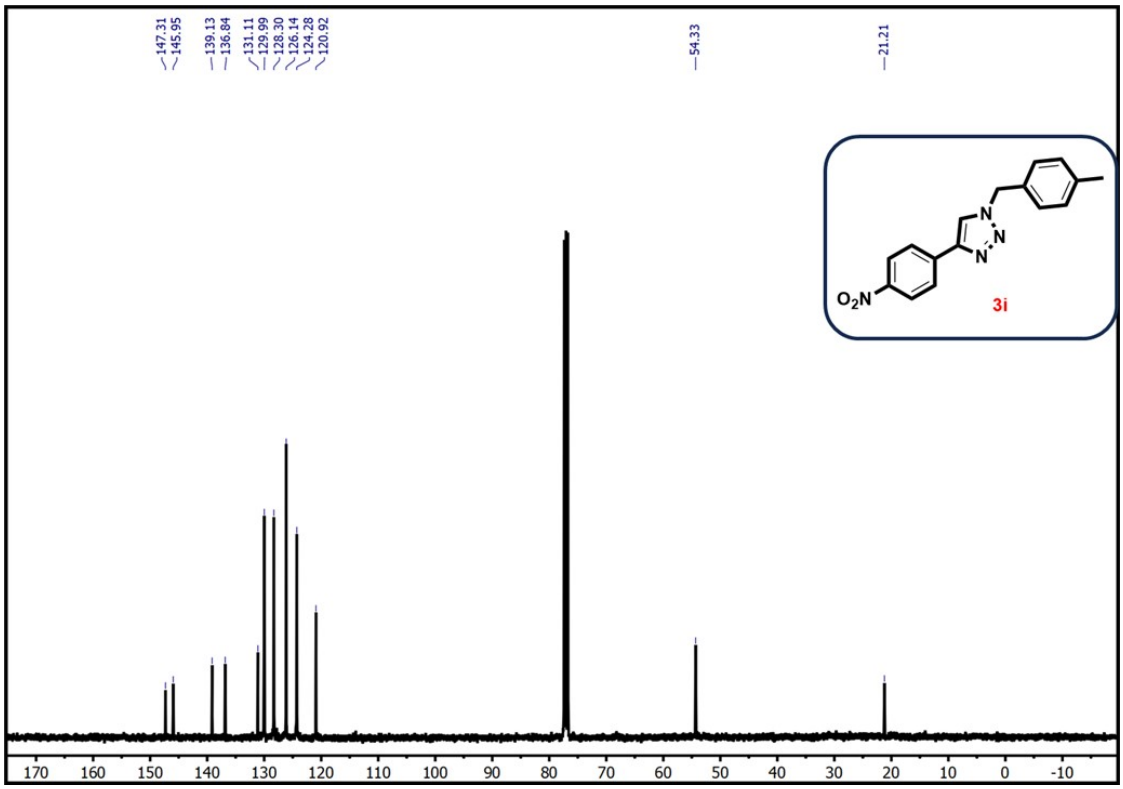
8. 4-(4-methoxyphenyl)-1-(4-methylbenzyl)-1H-1,2,3-triazole (3h)



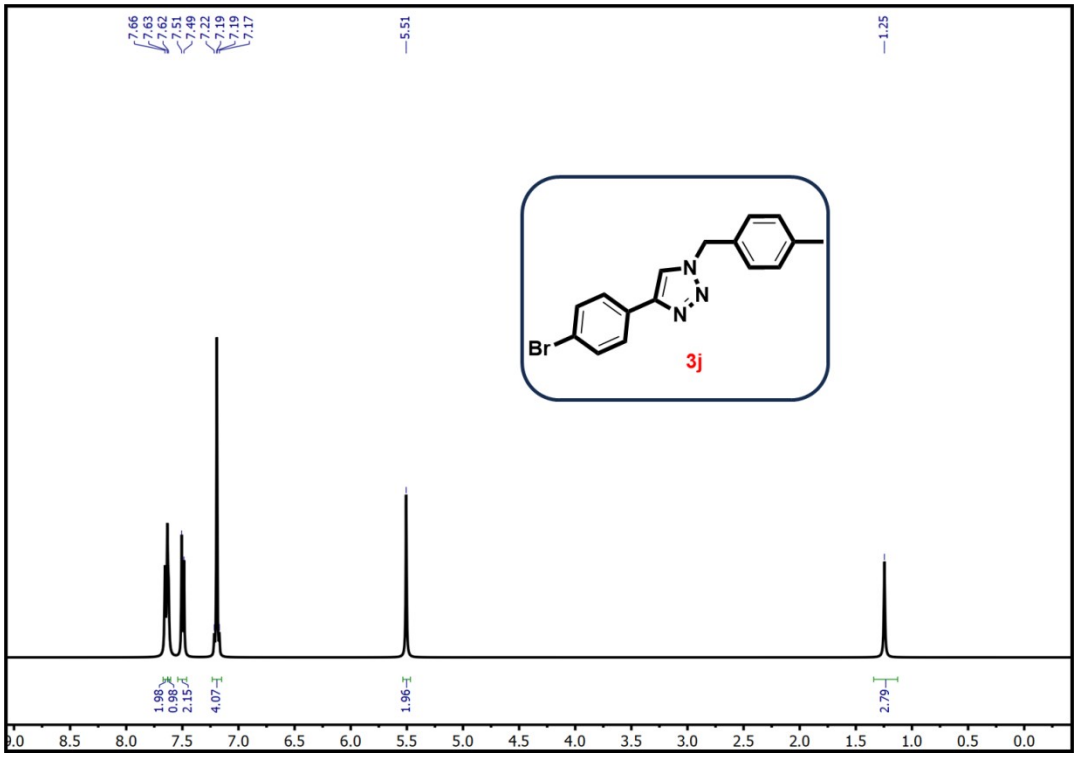


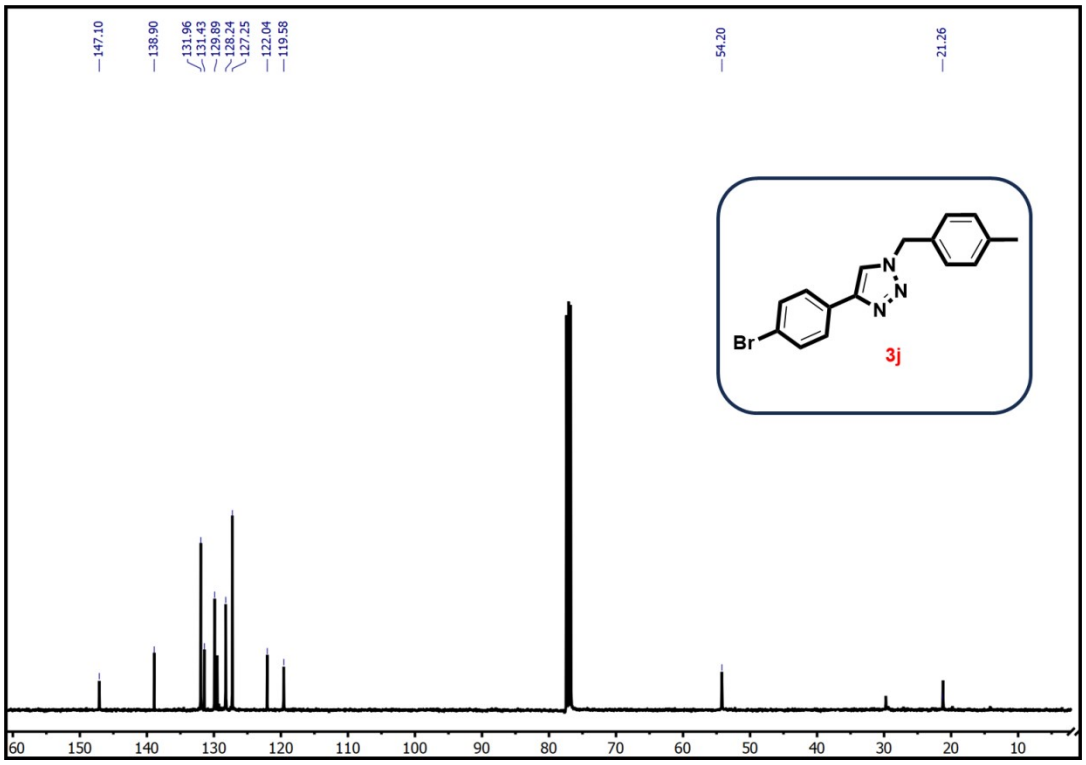
9. 1-(4-methylbenzyl)-4-(4-nitrophenyl)-1H-1,2,3-triazole (3i)



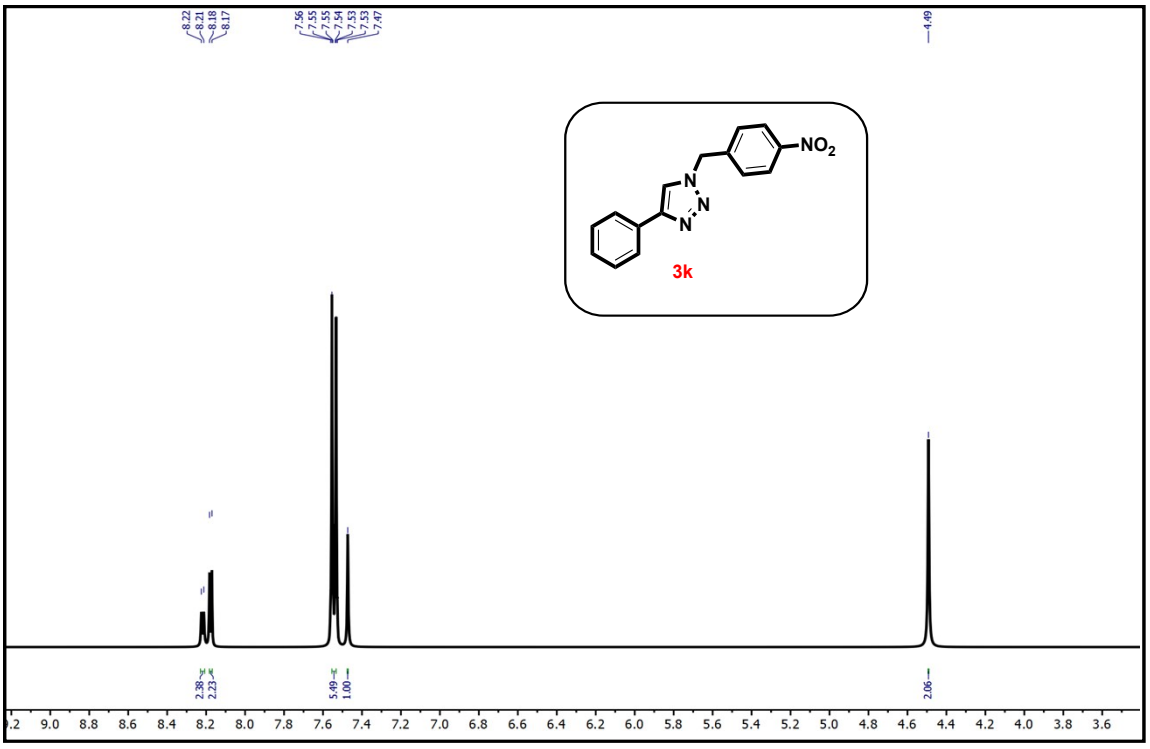


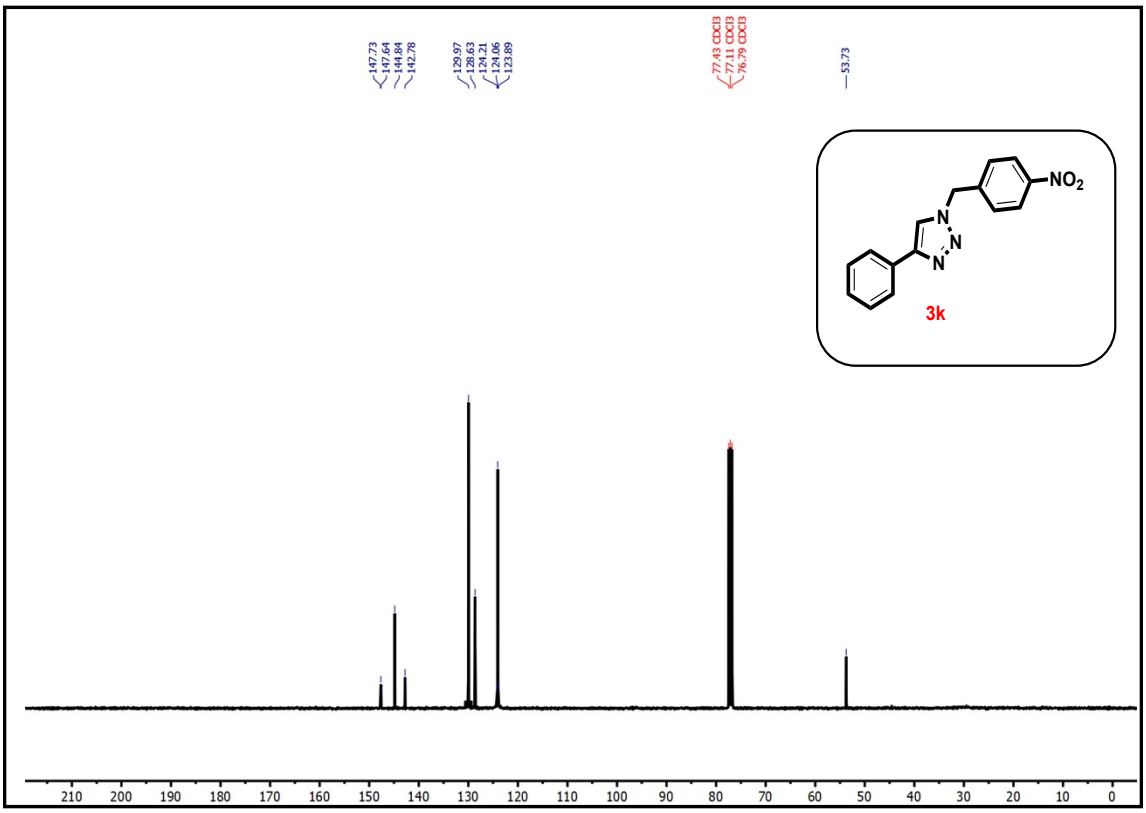
10. 4-(4-bromophenyl)-1-(4-methylbenzyl)-1H-1,2,3-triazole (3j)



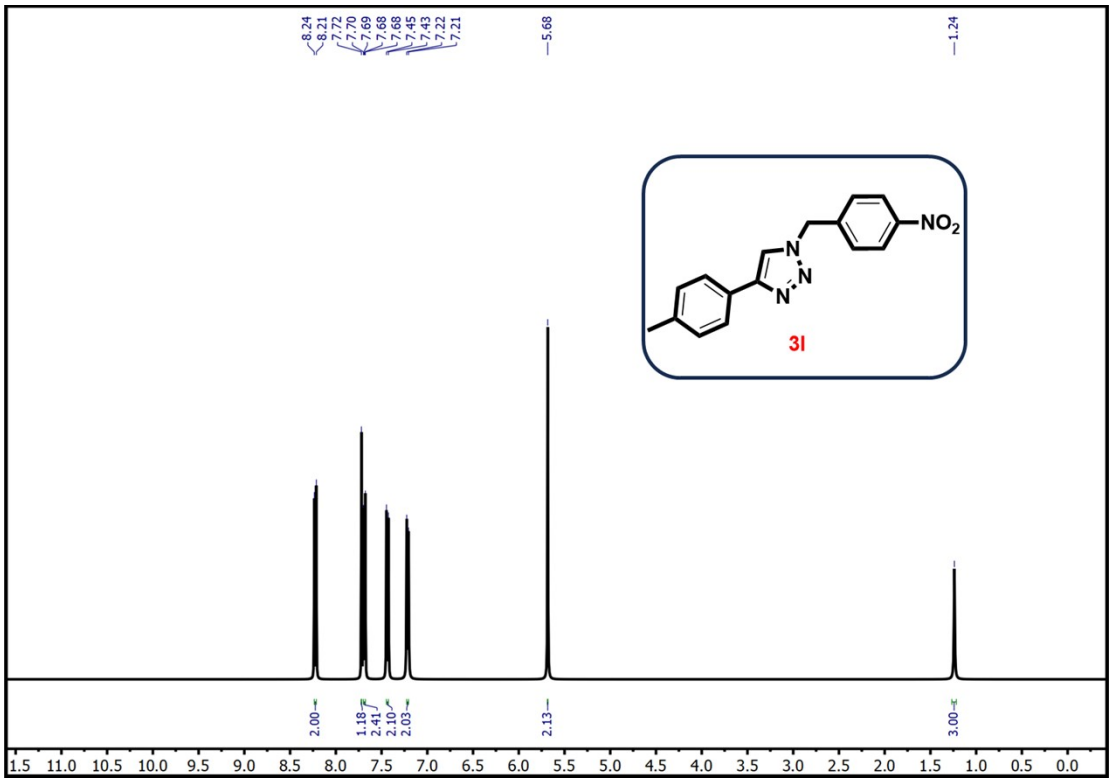


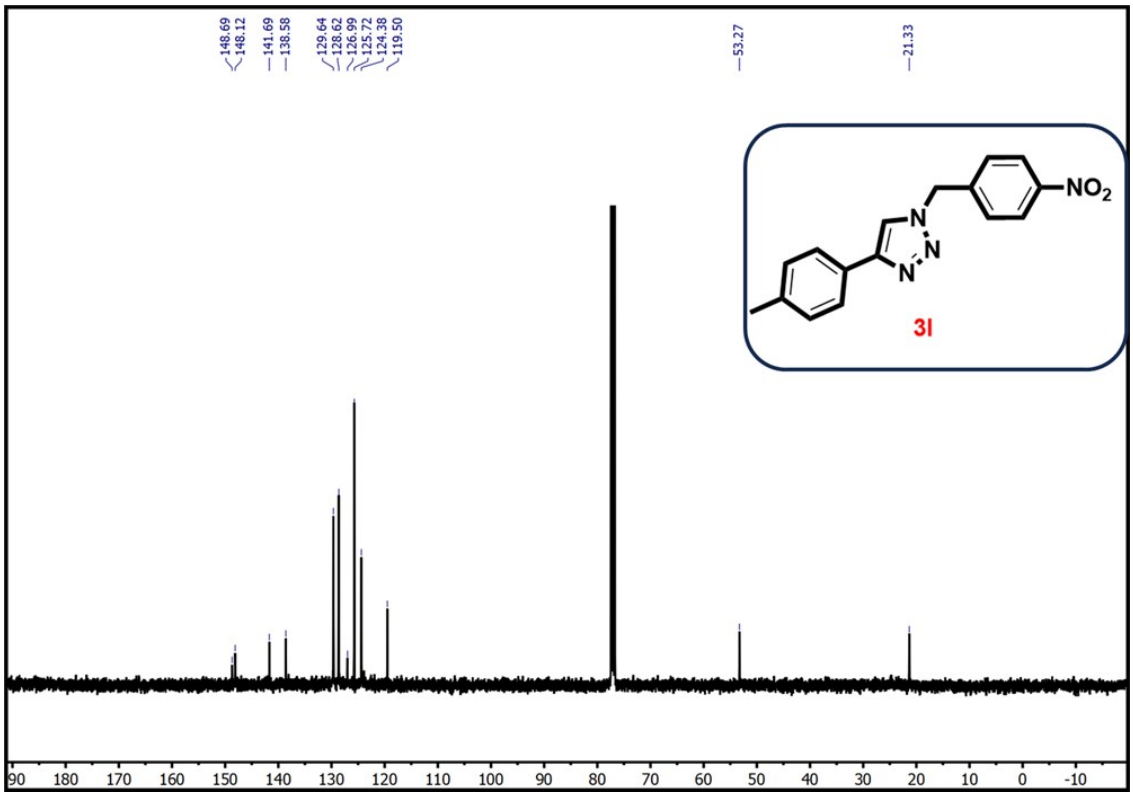
11. 1-(4-nitrobenzyl)-4-phenyl-1H-1,2,3-triazole (3k)



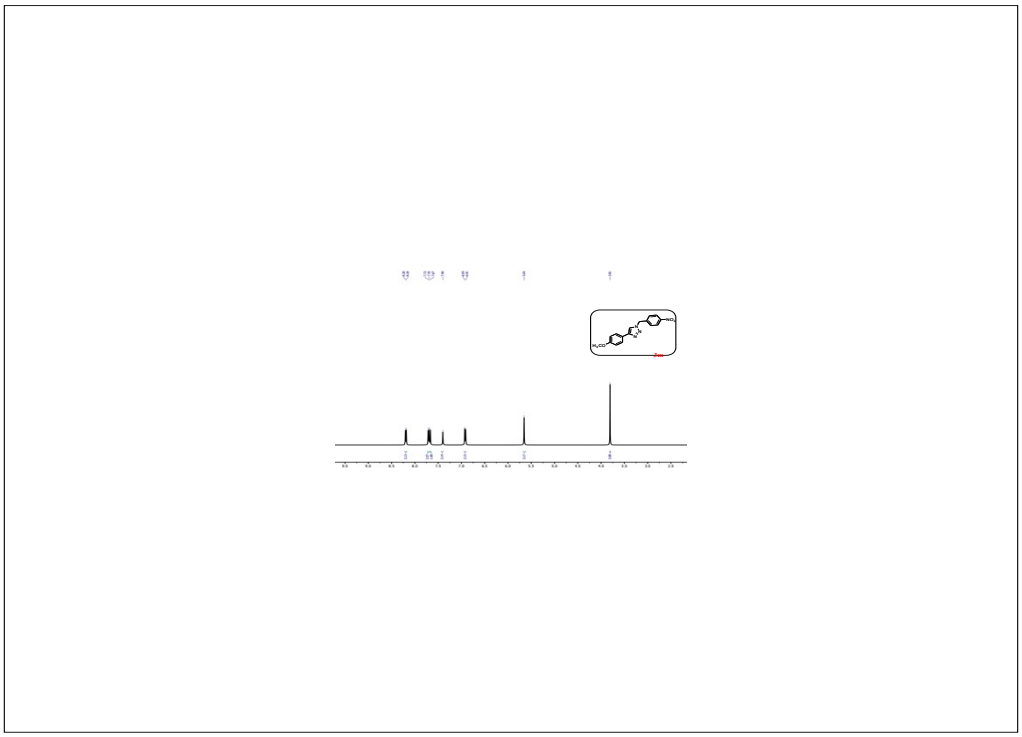


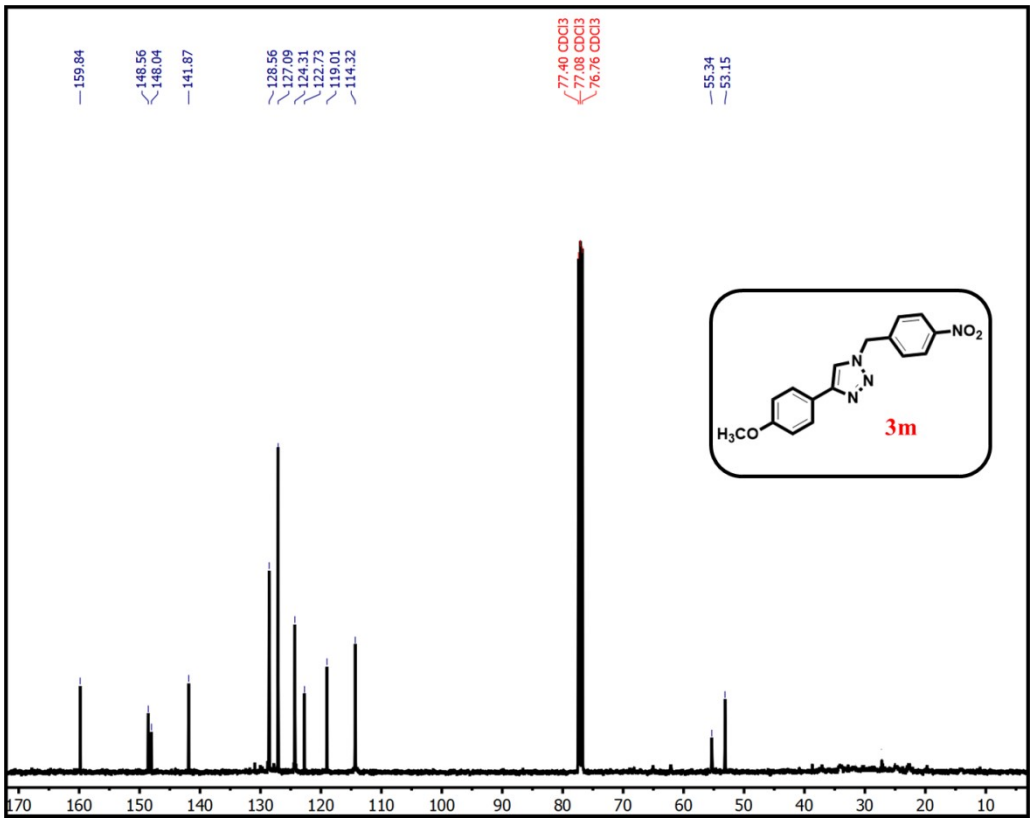
12. 1-(4-nitrobenzyl)-4-(p-tolyl)-1H-1,2,3-triazole (3l)


8.24
8.21
7.72
7.70
7.69
7.68
7.68
7.45
7.43
7.22
7.21
5.68
1.24
NO2
N
N
N
3l
2.00
1.18
2.41
2.10
2.03
2.13
3.00
1.5 11.0 10.5 10.0 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

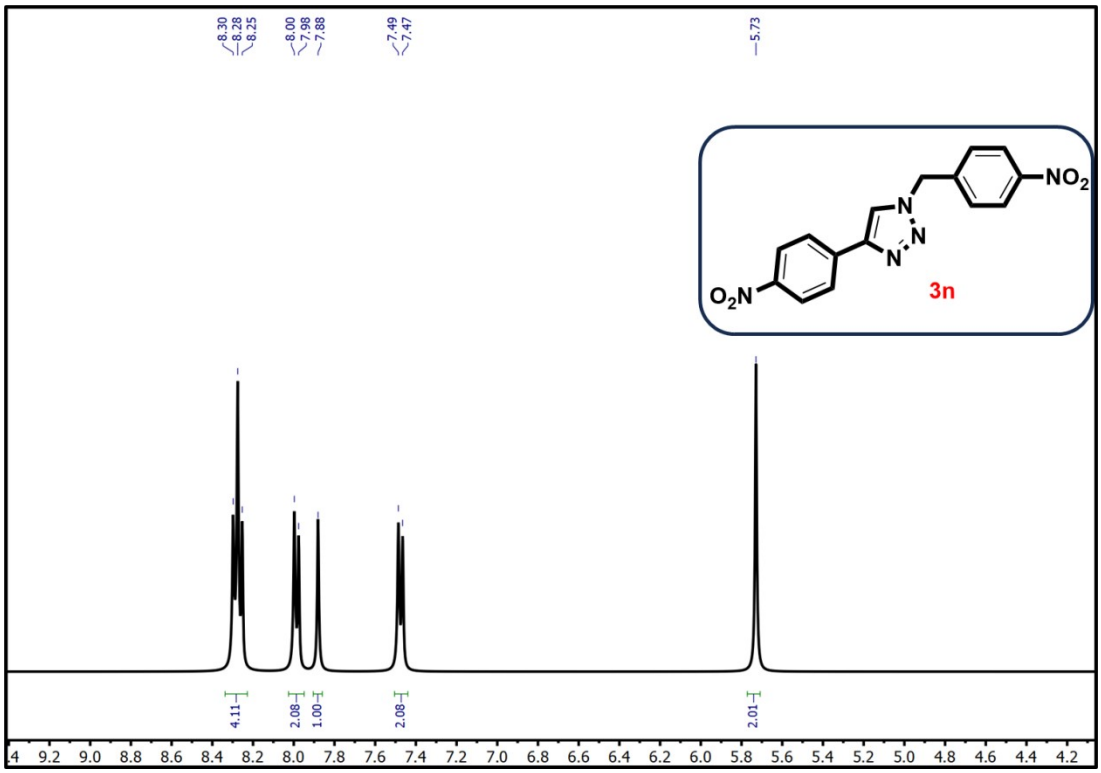

148.69
148.12
141.69
138.58
129.64
128.62
126.99
125.72
124.38
119.50
53.27
21.33
NO2
N
N
N
3l
90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

13. 4-(4-methoxyphenyl)-1-(4-nitrobenzyl)-1H-1,2,3-triazole (3m)

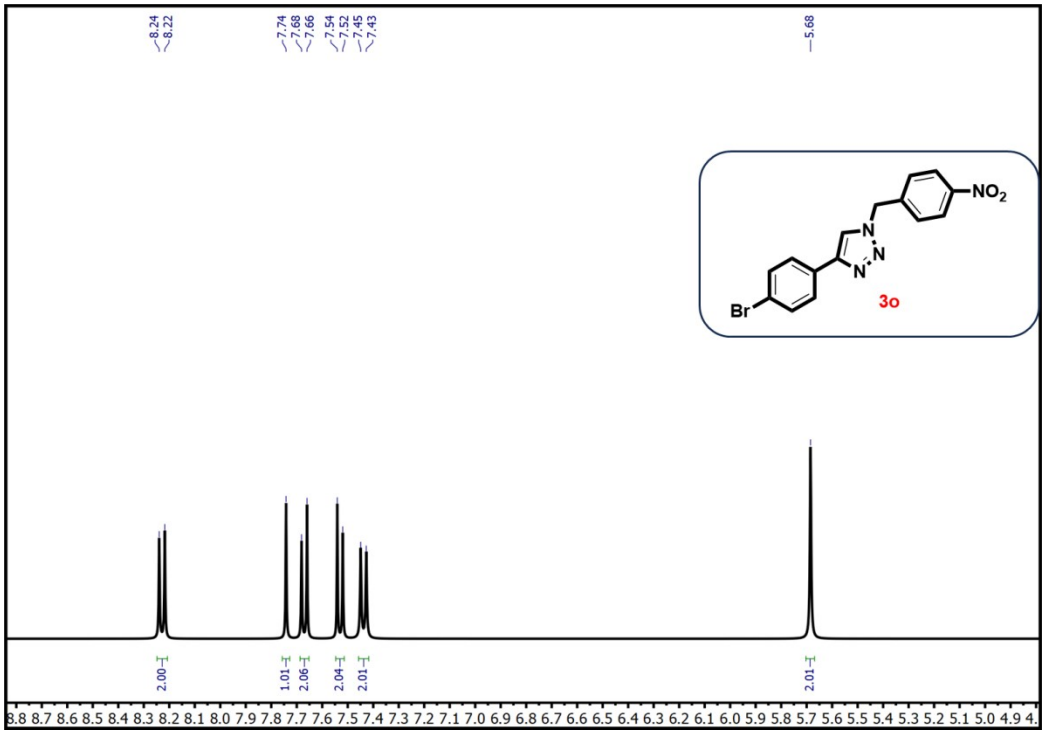


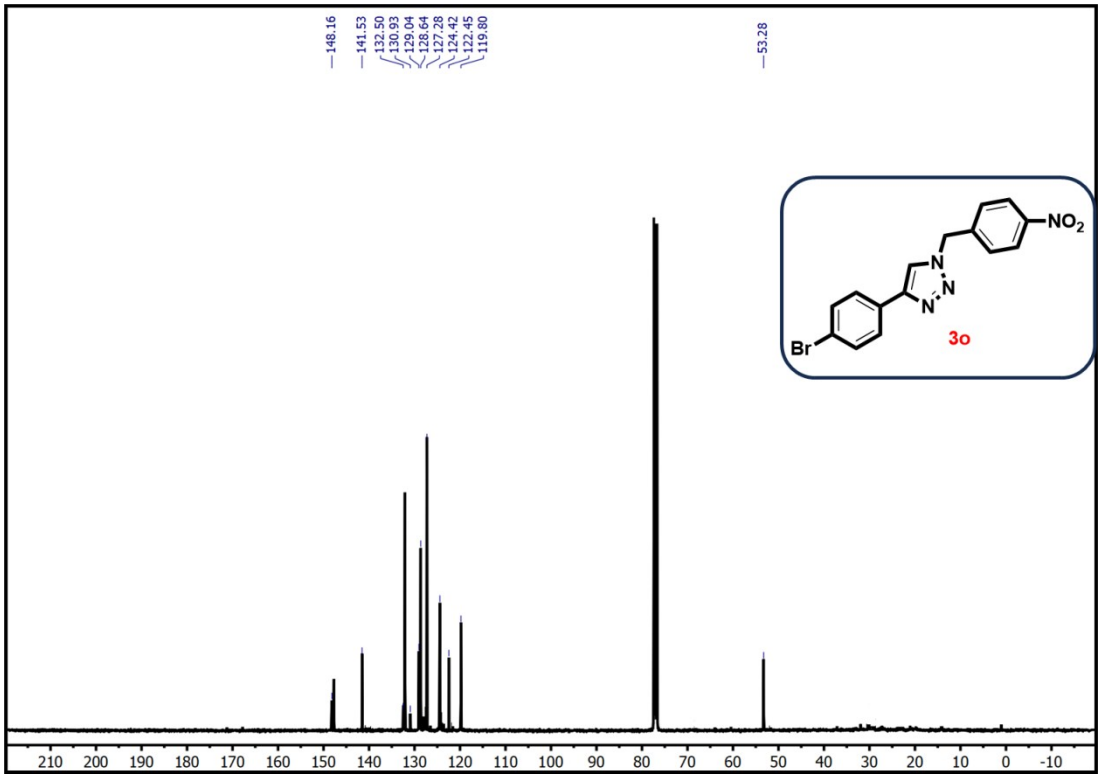


14. 1-(4-nitrobenzyl)-4-(4-nitrophenyl)-1H-1,2,3-triazole (3n)

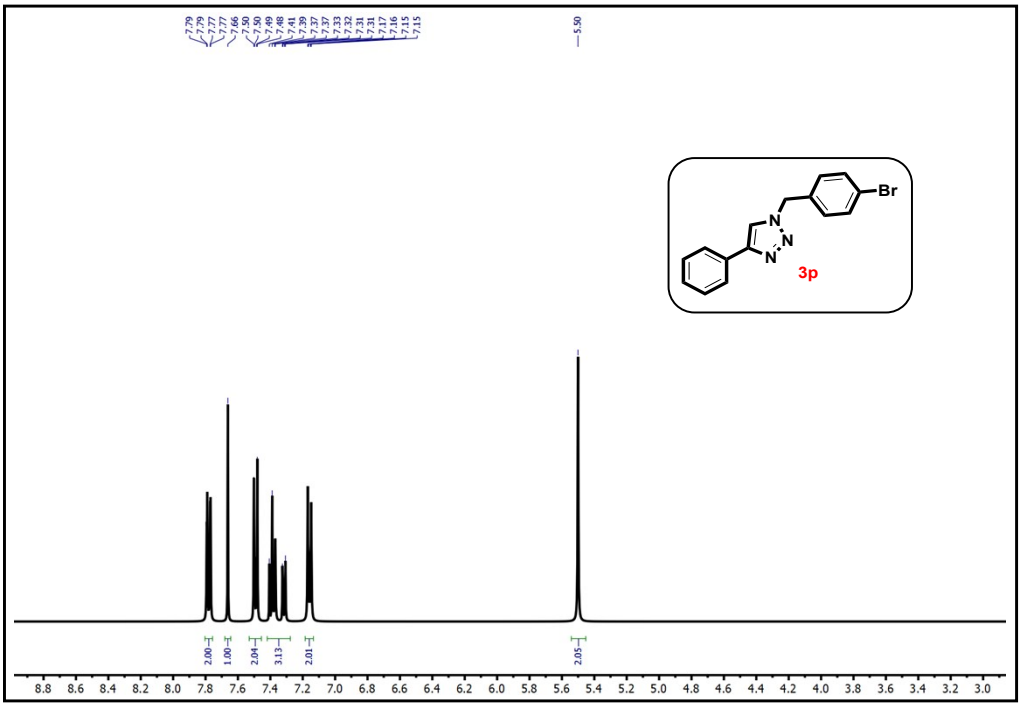


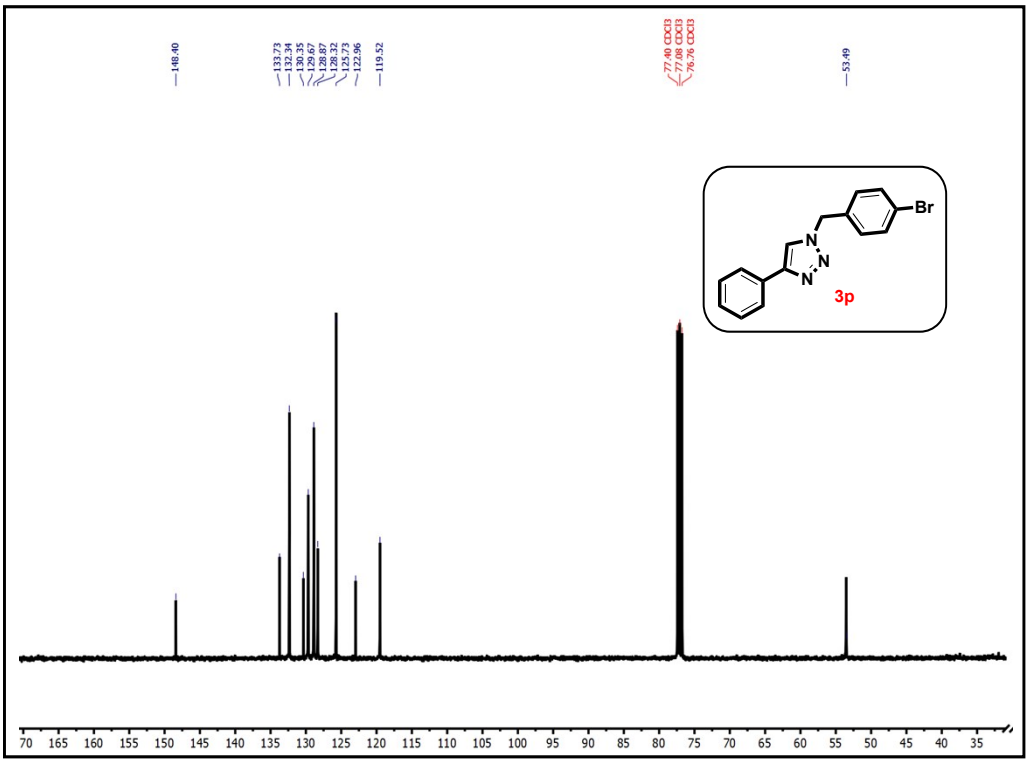
15. 4-(4-bromophenyl)-1-(4-nitrobenzyl)-1H-1,2,3-triazole (3o)



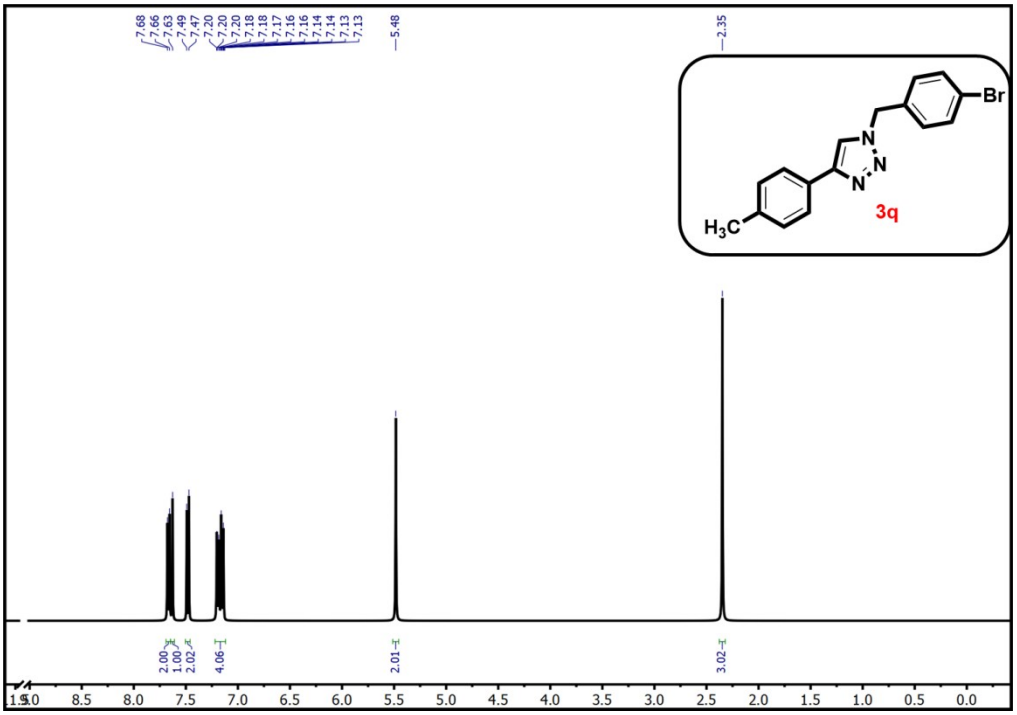


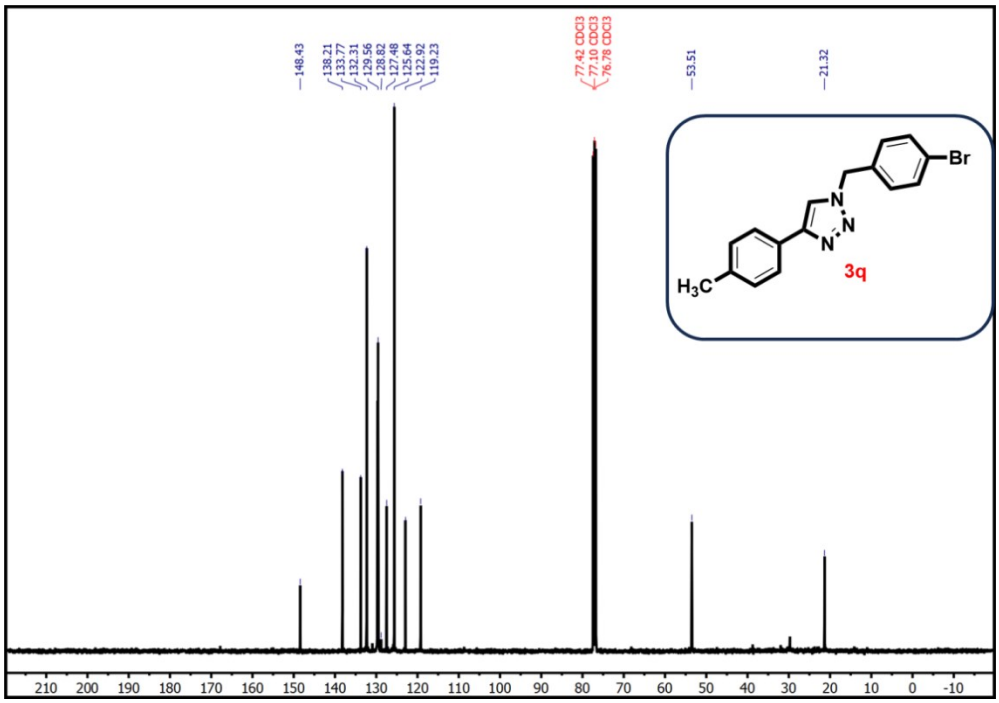
16. 1-(4-bromobenzyl)-4-phenyl-1H-1,2,3-triazole (3p)


7.79
7.79
7.77
7.77
7.66
7.50
7.50
7.49
7.48
7.41
7.39
7.37
7.33
7.32
7.31
7.31
7.17
7.16
7.15
7.15
5.50
Br
N
N
N
3p
2.00
1.00
2.04
3.13
2.01
2.05
8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0

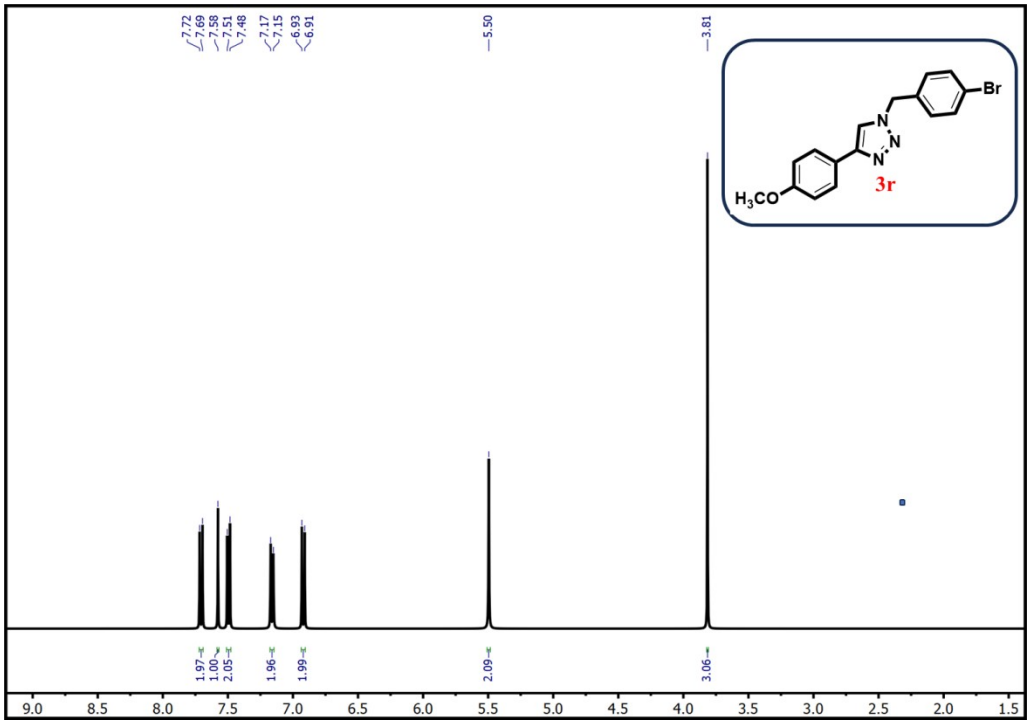

148.40
133.73
132.24
130.35
129.67
128.87
128.32
125.73
122.96
119.52
77.40 CDCl3
77.08 CDCl3
76.76 CDCl3
53.49
Br
N
N
N
3p
70 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35

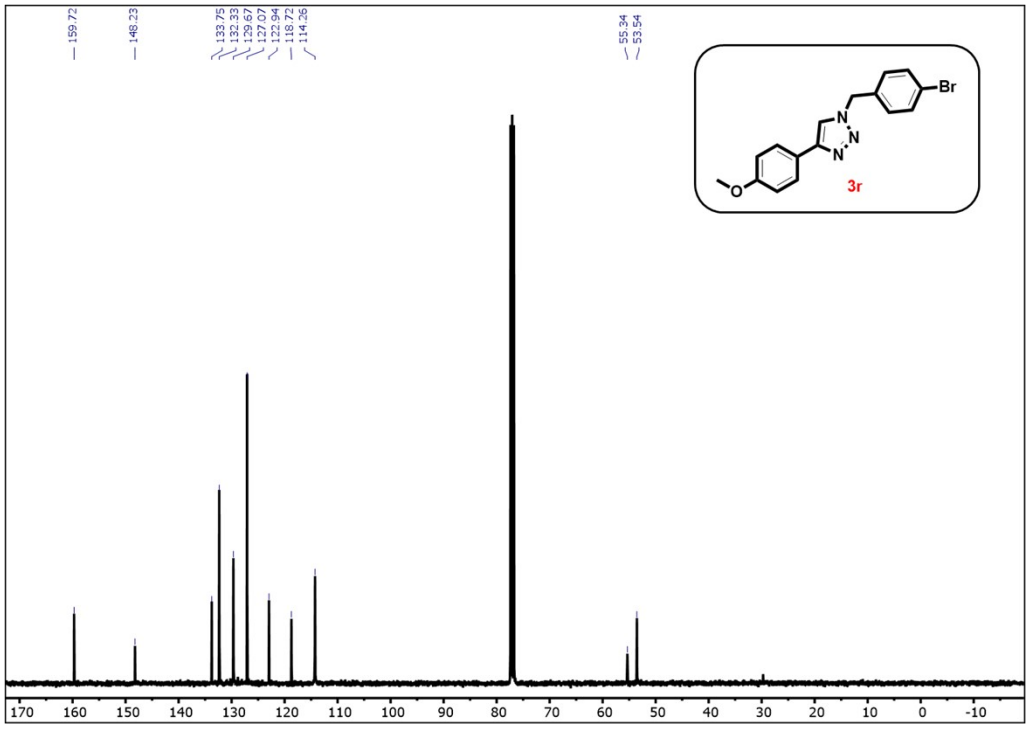
17. 1-(4-bromobenzyl)-4-(p-tolyl)-1H-1,2,3-triazole (3q)



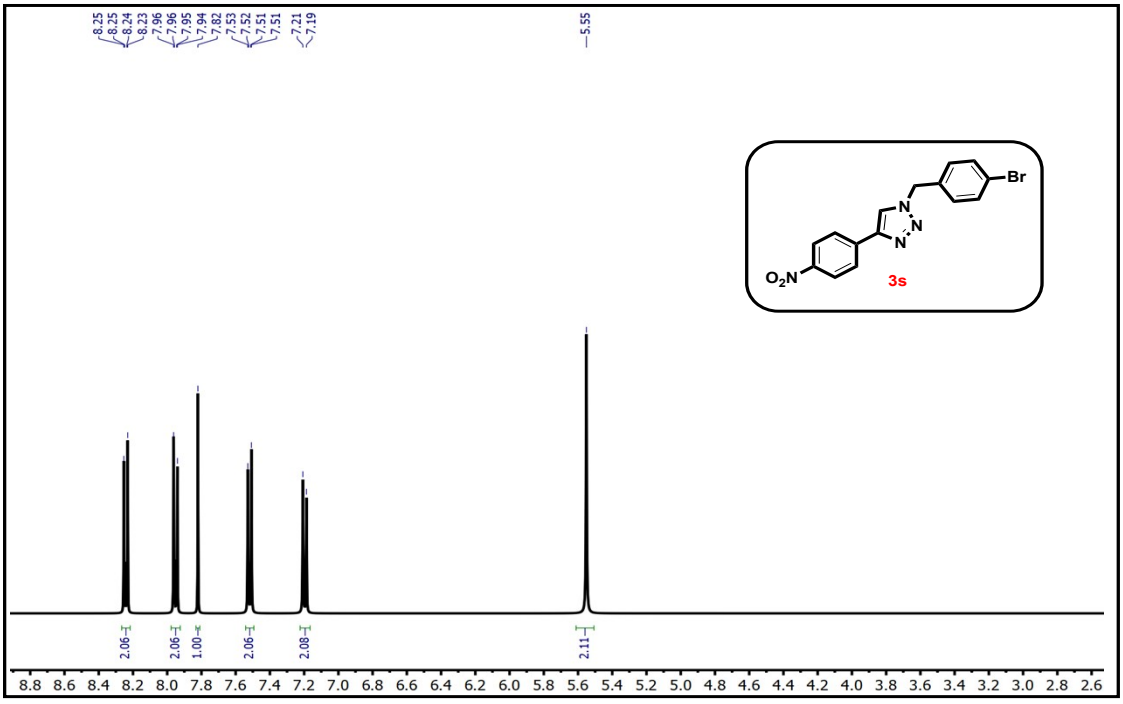


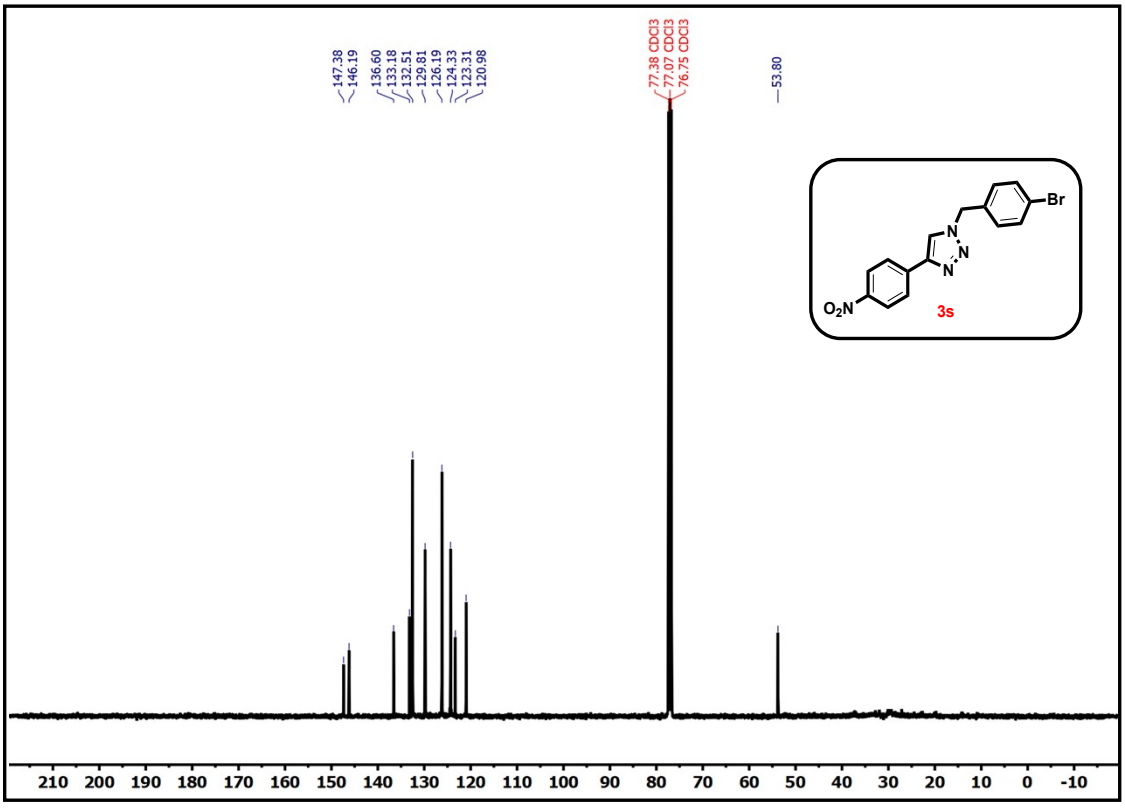
18. 1-(4-bromobenzyl)-4-(4-methoxyphenyl)-1H-1,2,3-triazole (3r)





19. 1-(4-bromobenzyl)-4-(4-nitrophenyl)-1H-1,2,3-triazole (3s)





20. 1-(4-bromobenzyl)-4-(4-bromophenyl)-1H-1,2,3-triazole (3t)