Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Cu^{II} immobilized on guanidinated epibromohydrin functionalized γ-Fe_2O_3@TiO_2 (γ-Fe_2O_3@TiO_2-EG-Cu^{II}): a novel magnetically recyclable heterogeneous nanocatalyst for the green one-pot synthesis of 1,4-disubstituted 1,2,3-triazoles through alkyne-azide cycloaddition in water

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Experimental

General

The purity determinations of the products and the progress of the reactions were accomplished by TLC on silica gel polygram STL G/UV 254 plates. The melting points of the products were determined with an Electrothermal Type 9100 melting point apparatus. The FTIR spectra were recorded on pressed KBr pellets using an AVATAR 370 FT-IR spectrometer (Therma Nicolet spectrometer, USA) at room temperature in the range between 4000 and 400 cm^{-1} with a resolution of 4 cm^{-1}, and each spectrum was the average of 32 scans. NMR spectra were recorded on a NMR Bruker Avance spectrometer at 400 and 300 MHz in $CDCl_3$ as solvent in the presence of tetramethylsilane as the internal standard and the coupling constants (*J* values) are given in Hz. Elemental analyses were performed using a Thermo Finnigan Flash EA 1112 Series instrument (furnace: 900 ˚C, oven: 65 ˚C, flow carrier: 140 mL min^{-1}, flow reference: 100 mL min^{-1}). Mass spectra were recorded with a CH7A Varianmat Bremem instrument at 70 eV electron impact ionization, in m/z (rel %). Thermogravimetric analyses (TGA and DTG) were carried out using a Shimadzu Thermogravimetric Analyzer (TG-50) in the temperature range of 25–900 ˚C at a heating rate of 10 ˚C min^{-1}, under air atmosphere. HRTEM analysis was performed using HRTEM microscope (Philips CM30). Inductively coupled plasma (ICP) was carried out on a Varian, VISTA-PRO, CCD, Australia. Elemental compositions were determined with an SC7620 Energy-dispersive X-ray analysis (EDX) presenting a 133 eV resolution at 20 kV. Room temperature magnetization isotherms were obtained using a vibrating sample magnetometer (VSM, LakeShore 7400). X-ray powder diffraction (XRD) was performed on a X'Pert Pro MPD diffractometer with Cu K_α (λ = 0.154 nm) radiation. Most of the obtained triazoles (**4a-j**, **4m-p** and **4r-v**) were known and their physical (color, melting points) and spectral (mass spectrometry) data found to be identical with

those of authentic compounds. The selected compounds were further identified by FT-IR, ^{1}H NMR and ^{13}C NMR spectroscopy which compared with literature data. The novel synthesized compounds (**4k**, **4l** and **4q**) were also characterized by using elemental analysis technique. All yields refer to isolated products after purification by recrystallization.

1-Benzyl-4-phenyl-1*H*-1,2,3-triazole (4a) (0.22 g, 94%); white solid (crystals); mp 127-128 ºC (from EtOH) (Lit.[1] 128–129 ºC); FT-IR (KBr): ν_{max}/cm^{-1} 3133, 3051, 2949, 1611, 1461 (CH_2), 1443, 1427, 1352, 1222 (N–N=N–), 1188 (C–N), 1072, 1049, 972, 914, 816 (=C–H oop, triazole ring), 767, 720, 696, 581; ^{1}H NMR: δH (300 MHz; $CDCl_3$; Me_4Si) 7.83 (2 H, d, *J* = 7.65 Hz, Ar-H), 7.70 (1 H, s, C=C<u>H</u>), 7.44-7.38 (5 H, m, Ar-H), 7.36-7.29 (3 H, m, Ar-H), 5.58 (2 H, s, C<u>H</u>$_2$); ^{13}C NMR: δC (75 MHz; $CDCl_3$; Me_4Si) 148, 134, 130, 129, 128.83, 128.79, 128.18, 128.07, 125, 119, 54; MS, *m/z* 235 (M^+, 13%), 234 (75, M – H), 206 (55, M – N_2), 129 (63, M – C_7H_7N), 116 (95, M – $C_8H_7N_2$), 104 (75, M – $C_8H_6N_2$), 91 (100, M – $C_8H_6N_3$), 77 (74, M – $C_9H_8N_3$), 29 (50, M – $C_{15}H_{13}N$).

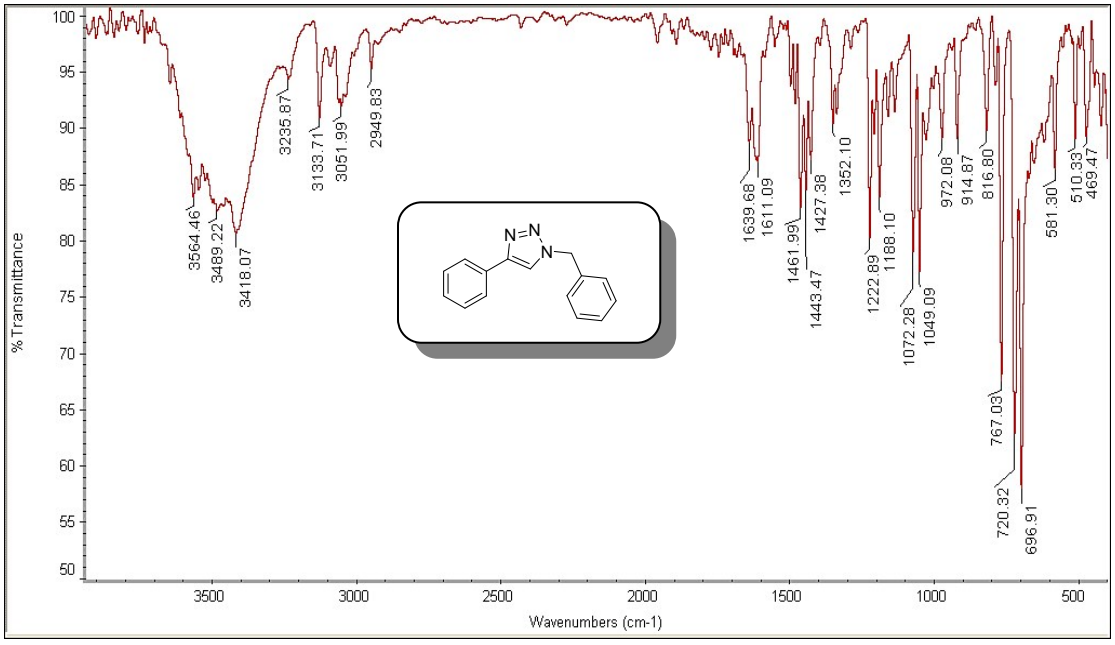

Figure 1: FT-IR (KBr) of 1-Benzyl-4-phenyl-1*H*-1,2,3-triazole (**4a**).

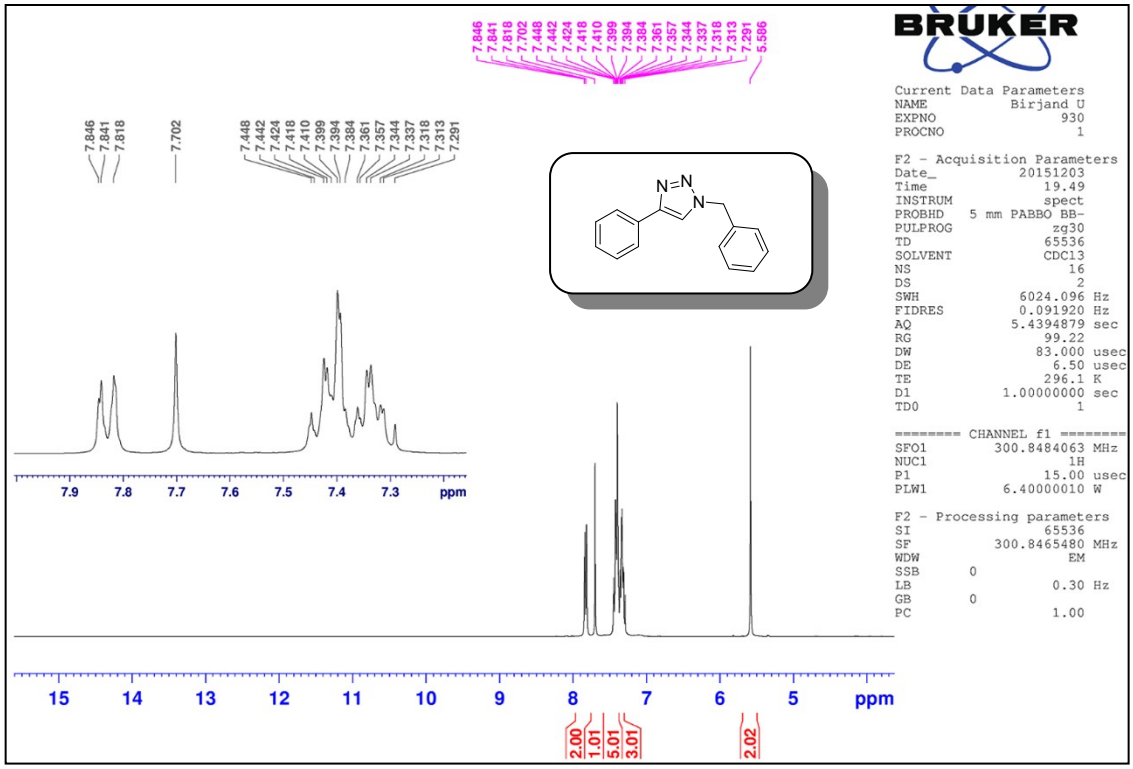

Figure 2: ^{1}H NMR (300 MHz, $CDCl_3$) of 1-Benzyl-4-phenyl-1*H*-1,2,3-triazole (**4a**).

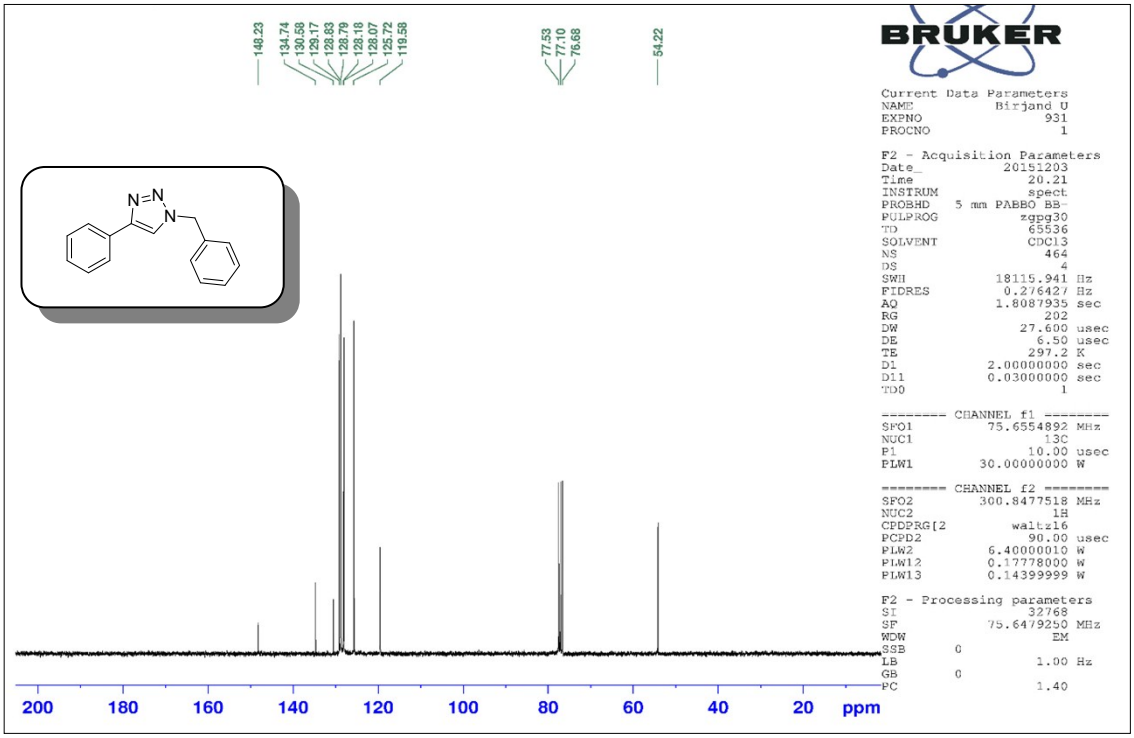

Figure 3: ^{13}C NMR (75MHz, $CDCl_3$) of 1-Benzyl-4-phenyl-1*H*-1,2,3-triazole (**4a**).

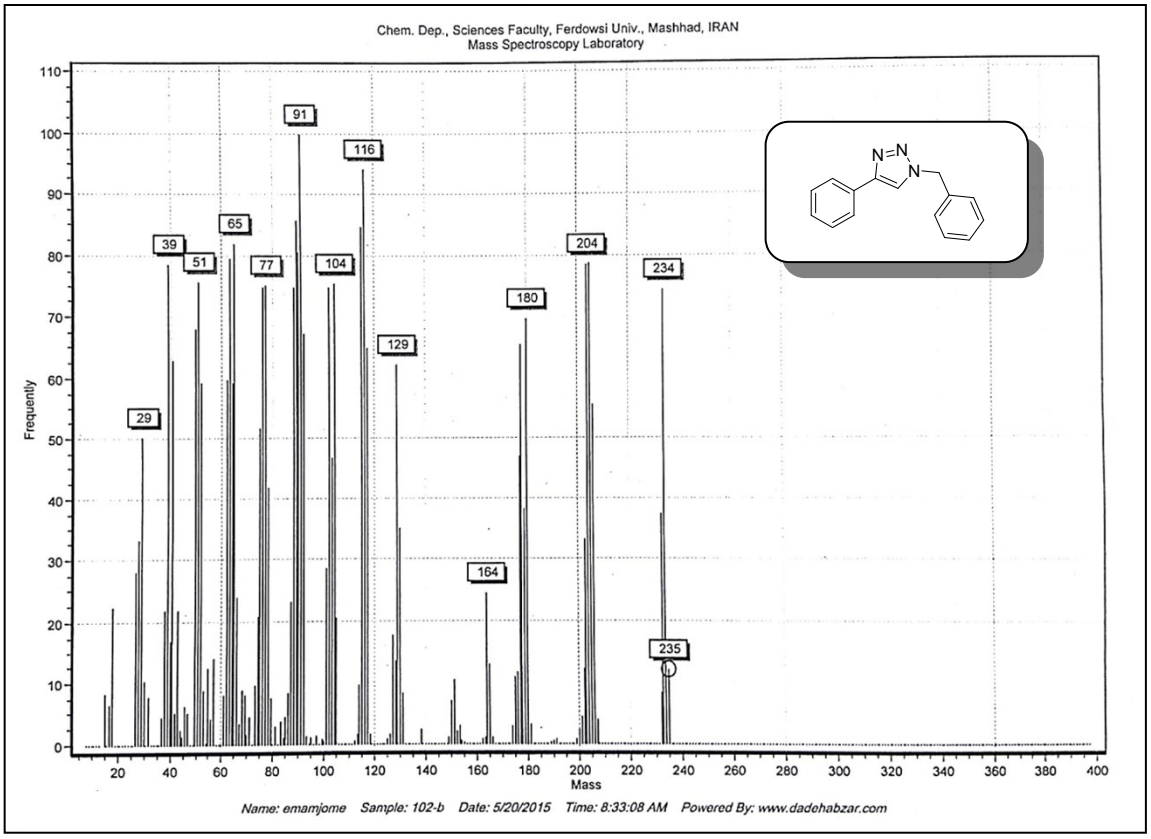

Figure 4: Mass spectrum of 1-Benzyl-4-phenyl-1*H*-1,2,3-triazole (**4a**).

1-Benzyl-4-(*p*-tolyl)-1*H*-1,2,3-triazole (4b) (0.23 g, 92%); white solid (crystals); mp 142-144 ºC (from EtOH) (Lit.[2] 142–146 ºC); FT-IR (KBr): ν_{max}/cm^{-1} 3145, 3015, 2913, 1495, 1456 (CH_2), 1431, 1347, 1222 (N–N=N–), 1180 (C–N), 1065, 1046, 976, 827 (=C–H oop, triazole ring), 793, 721, 583, 512; ^{1}H NMR: δH (300 MHz; $CDCl_3$; Me_4Si) 7.71 (2 H, d, *J* = 8.1 Hz, Ar-H), 7.65 (1 H, s, C=C<u>H</u>), 7.43-7.29 (5 H, m, Ar-H), 7.23 (2 H, d, *J* = 7.8 Hz, Ar-H), 5.59 (2 H, s, C<u>H</u>$_2$), 2.39 (3 H, s, C<u>H</u>$_3$); MS, *m/z* 249 (M^+, 3%), 248 (32, M – H), 247 (86, M – 2 H), 220 (70, M – N_2), 130 (99, M – C_8H_8N), 115 (55, M – $C_7H_7N_3$), 103 (86, M – $C_9H_{10}N_2$), 91 (100, M – $C_9H_8N_3$), 77 (86, M – $C_{10}H_{10}N_3$), 28 (85, M – $C_{16}H_{15}N$).

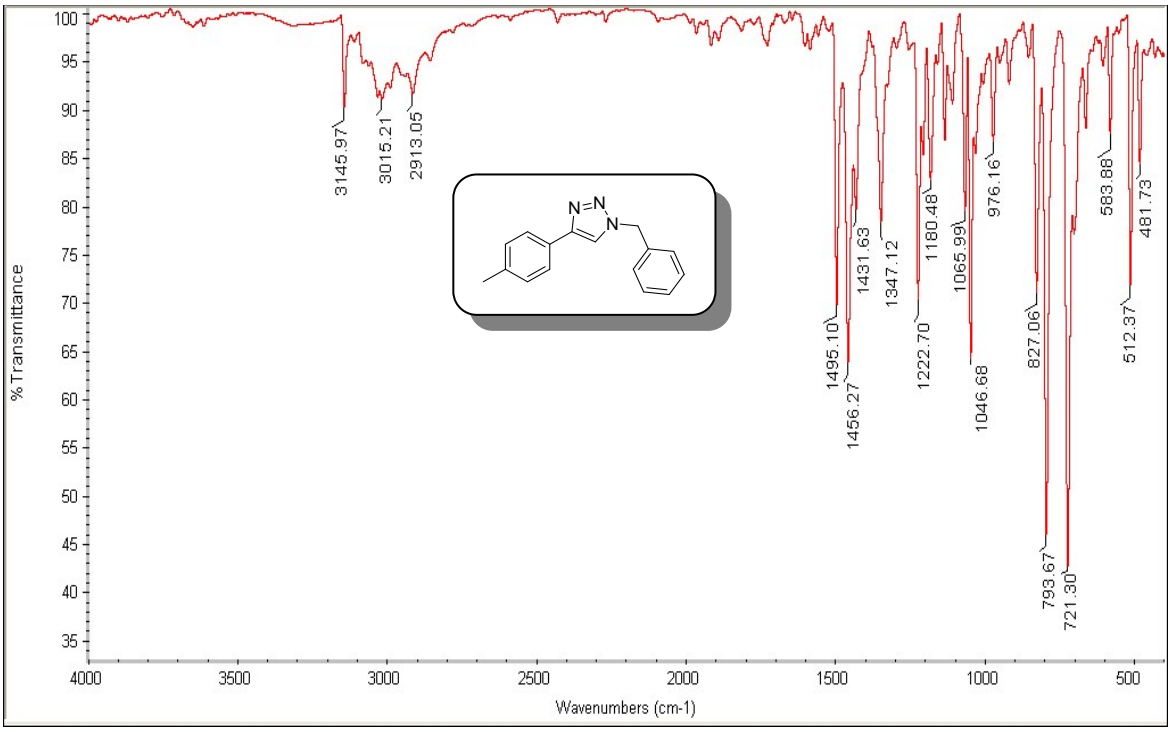

Figure 5: FT-IR (KBr) of 1-Benzyl-4-(*p*-tolyl)-1*H*-1,2,3-triazole (**4b**).

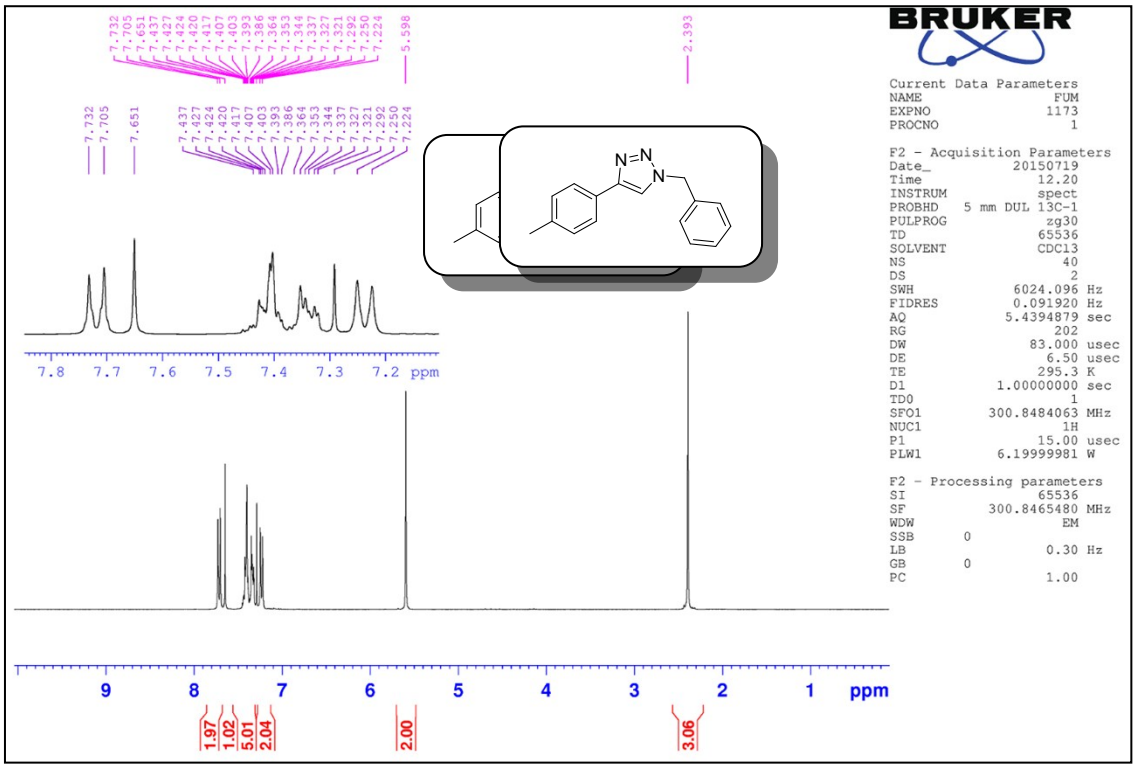

Figure 6: ^{1}H NMR (300 MHz, $CDCl_3$) of 1-Benzyl-4-(*p*-tolyl)-1*H*-1,2,3-triazole (**4b**).

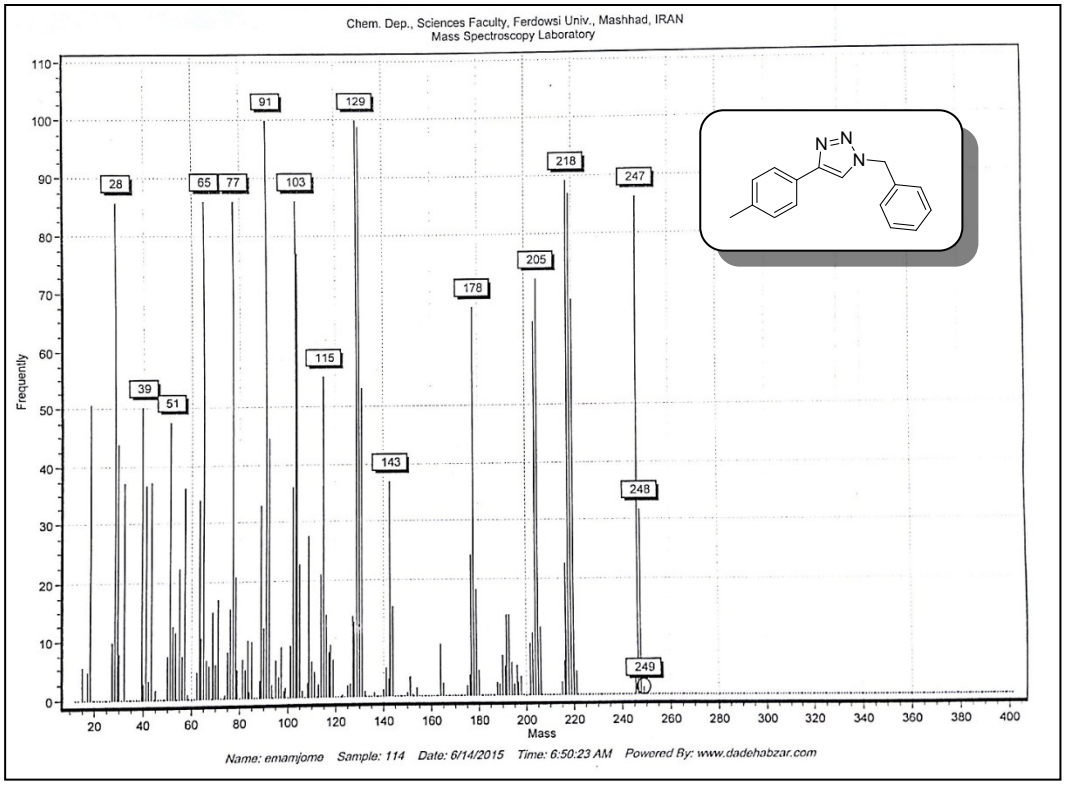

Figure 7: Mass spectrum of 1-Benzyl-4-(*p*-tolyl)-1*H*-1,2,3-triazole (**4b**).

1-Benzyl-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (4c) (0.24 g, 91%); white solid (crystals); mp 139–141 ºC (from EtOH) (Lit.[3] 140–142 ºC); FT-IR (KBr): ν_{max}/cm^{-1} 3137, 3035, 2966, 2952, 2855, 2835, 1617, 1580, 1556, 1500, 1455 (CH_2), 1352, 1266 (N–N=N–), 1250, 1221, 1172 (C–N), 1074, 1027, 980, 834 (=C–H oop, triazole ring), 796, 720, 579; ^{1}H NMR: δH (300 MHz; $CDCl_3$; Me_4Si) 7.78-7.29 (8 H, m, Ar-H, C=C<u>H</u>), 6.96 (2 H, d, *J* = 7.2 Hz, Ar-H), 5.58 (2 H, s, C<u>H</u>$_2$), 3.85 (3 H, s, OC<u>H</u>$_3$); ^{13}C NMR: δC (75 MHz; $CDCl_3$; Me_4Si) 159, 148, 134, 129, 128.76, 128.08, 126, 123, 114, 55, 54; MS, *m/z* 265 (M^+, 6%), 263 (78, M – 2 H), 262 (98, M – 3 H), 234 (58, M – CH_3O), 145 (99, M – $C_7H_7N_2$), 91 (100, M – $C_9H_8N_3O$), 28 (98, M – $C_{16}H_{15}NO$).

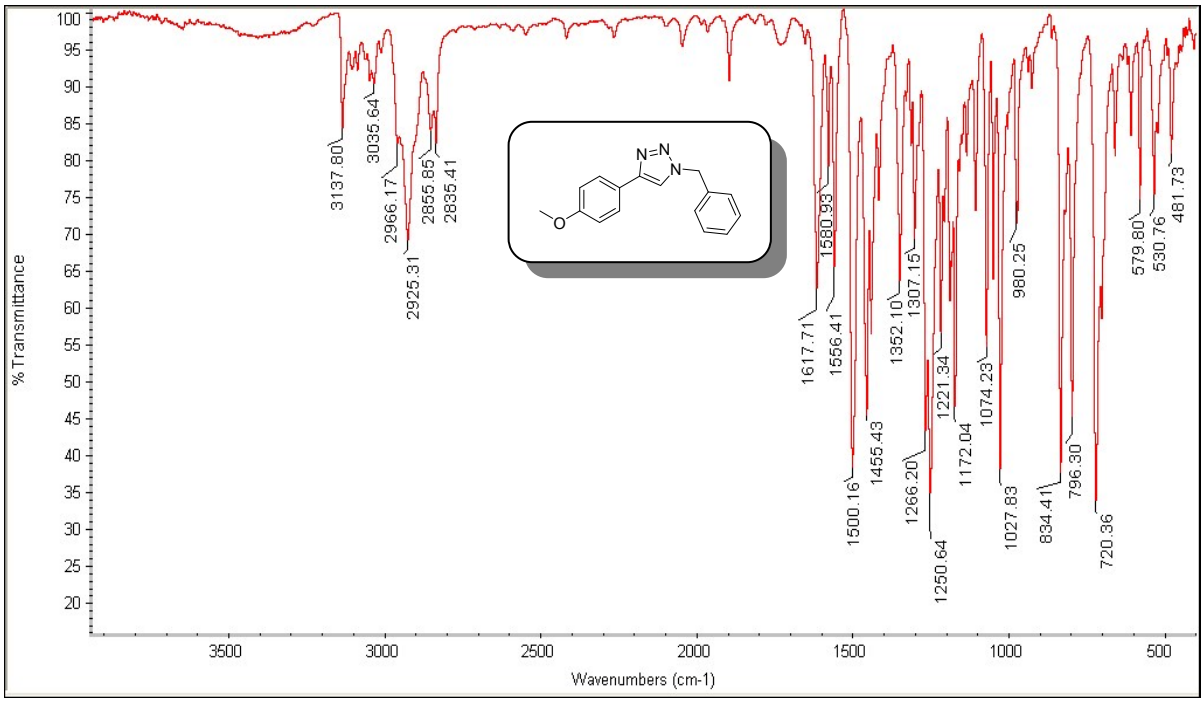

Figure 8: FT-IR (KBr) of 1-Benzyl-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (**4c**).

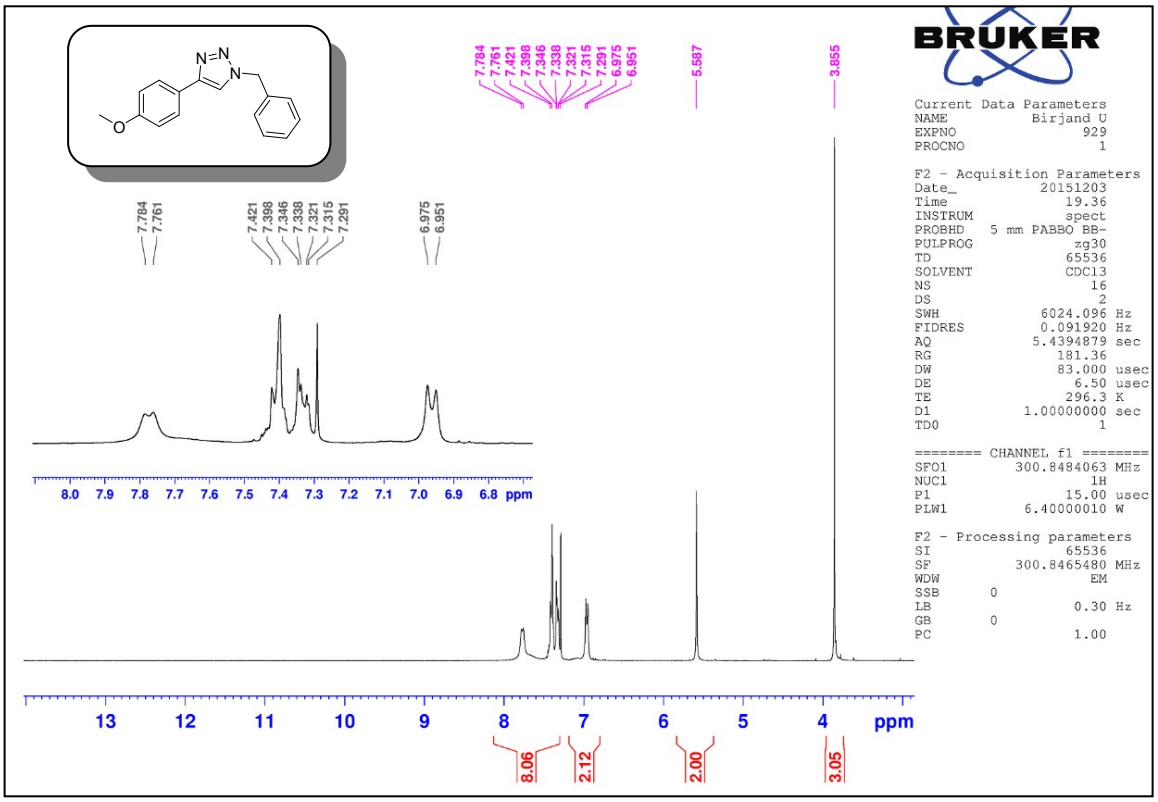

Figure 9: ^{1}H NMR (300 MHz, $CDCl_3$) of 1-Benzyl-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (**4c**).

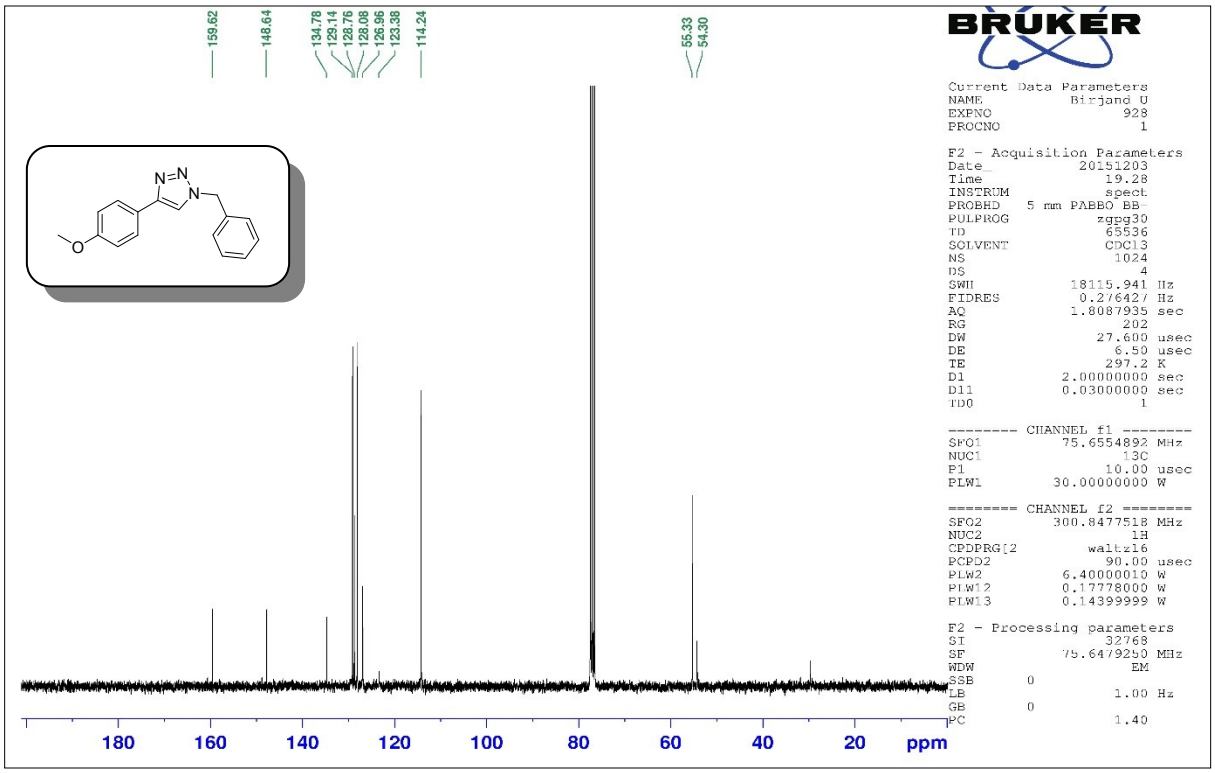

Figure 10: ^{13}C NMR (75MHz, $CDCl_3$) of 1-Benzyl-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (**4c**).

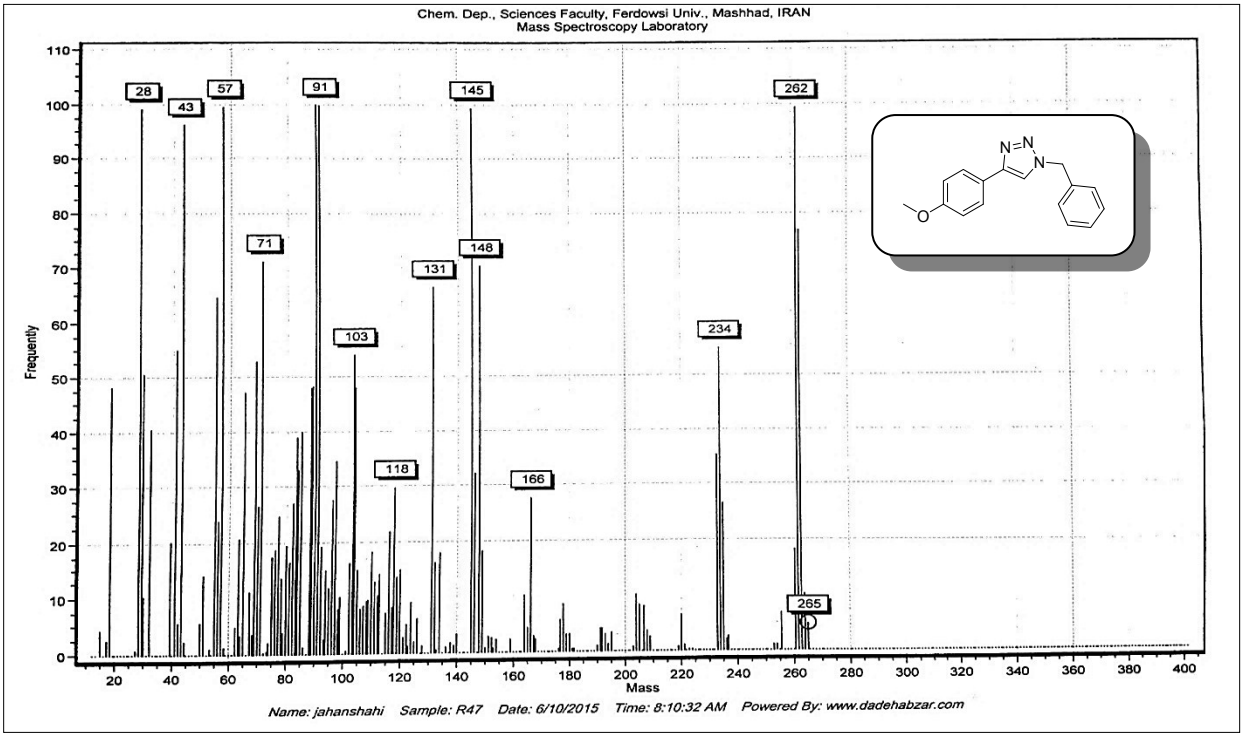

Figure 11: Mass spectrum of 1-Benzyl-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (**4c**).

1-benzyl-4-(4-(*tert*-butyl)phenyl)-1*H*-1,2,3-triazole (4d) (0.25 g, 88%); white solid (crystals); mp 112–113 ºC (from EtOH) (Lit.[4] 112–114 ºC); FT-IR (KBr): ν_{max}/cm^{-1} 3084, 3035, 2959, 2865, 1495, 1457 (CH_2), 1363, 1221 (N–N=N–), 1189 (C–N), 1071, 1048, 976, 832 (=C–H oop, triazole ring), 739, 719, 693, 559; ^{1}H NMR: δH (400 MHz; $CDCl_3$; Me_4Si) 7.73 (2 H, d, *J* = 8 Hz, Ar-H), 7.63 (1 H, s, C=C<u>H</u>), 7.43-7.21 (7 H, m, Ar-H,), 5.58 (2 H, s, C<u>H</u>$_2$), 1.37 (9 H, s, 3 C<u>H</u>$_3$); MS, *m/z* 291 (M^+, 4%), 290 (27, M – H), 289 (88, M – 2 H), 171 (99, M – $C_7H_7N_2$), 157 (43, M – $C_7H_7N_3$), 91 (100, M – $C_{12}H_{14}N_3$), 57 (45, M – $C_{15}H_{12}N_3$), 29 (96, M – $C_{19}H_{21}N$).

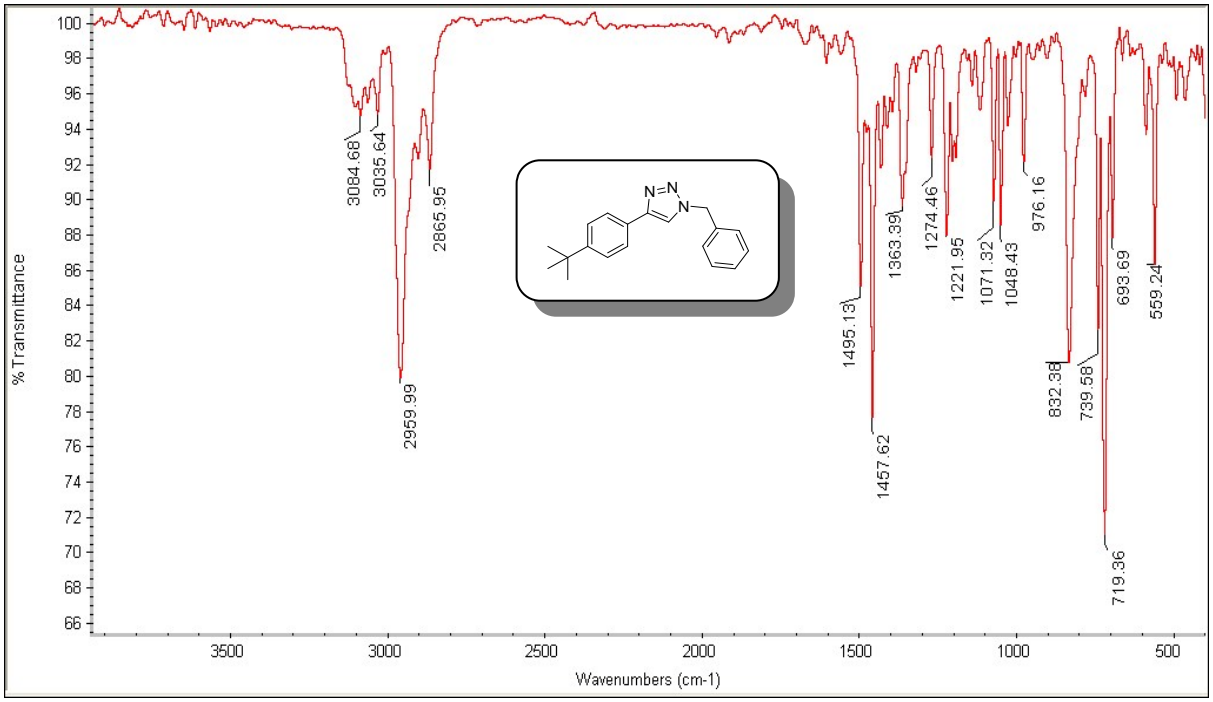

Figure 12: FT-IR (KBr) of 1-benzyl-4-(4-(*tert*-butyl)phenyl)-1*H*-1,2,3-triazole (**4d**).

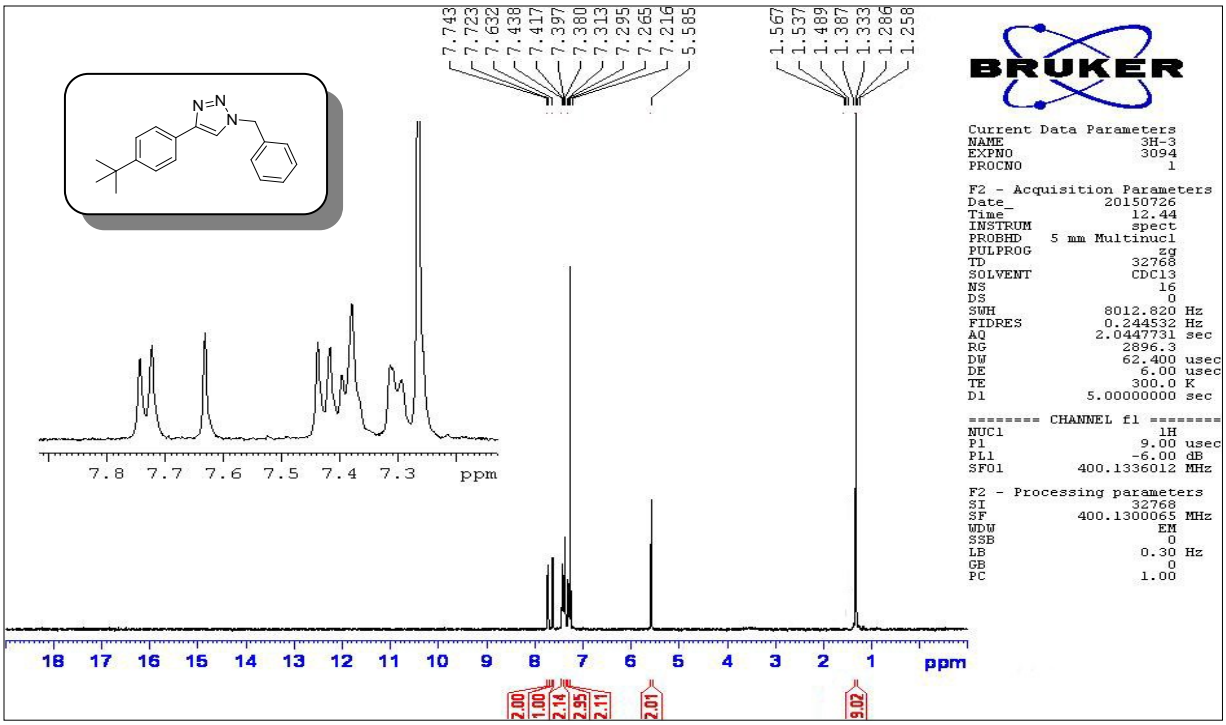

Figure 13: ^{1}H NMR (400 MHz, $CDCl_3$) of 1-benzyl-4-(4-(*tert*-butyl)phenyl)-1*H*-1,2,3-triazole (**4d**).

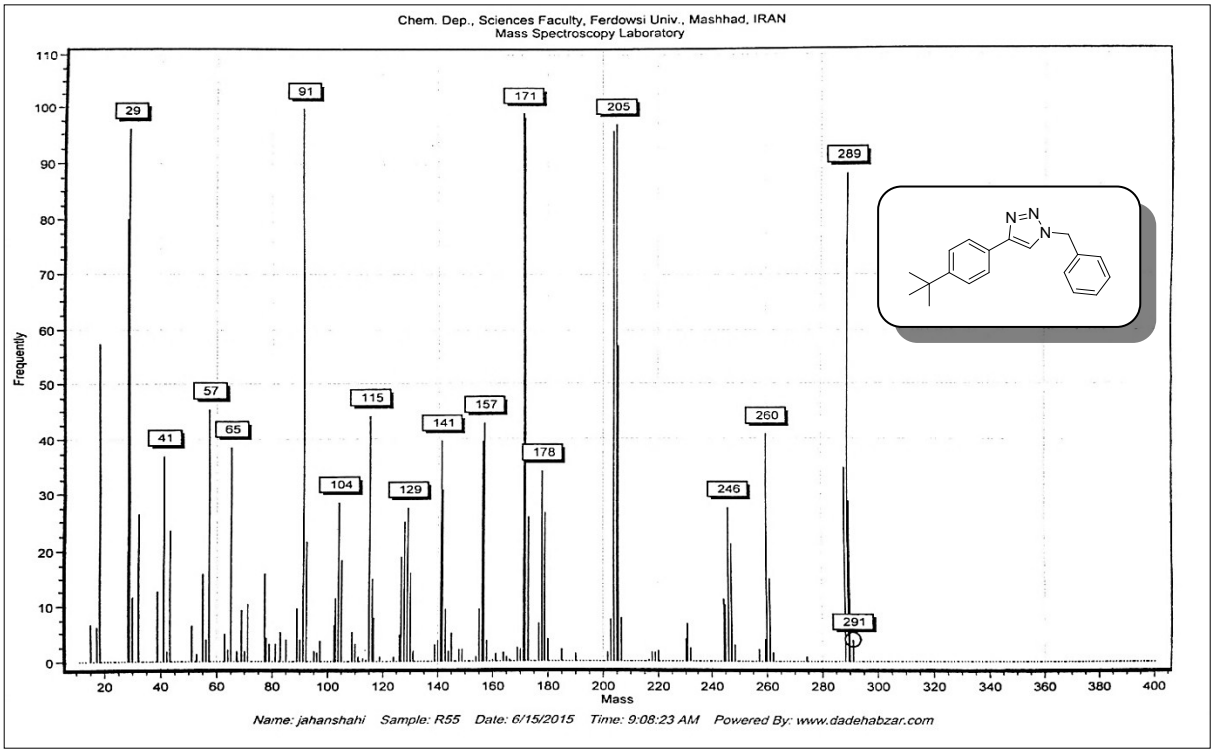

Figure 14: Mass spectrum of 1-benzyl-4-(4-(*tert*-butyl)phenyl)-1*H*-1,2,3-triazole (**4d**).

1-benzyl-4-(4-chlorophenyl)-1*H*-1,2,3-triazole (4e) (0.25 g, 95%); white solid (crystals); mp 125–126 ºC (from EtOH) (Lit.[5] 125–127 ºC); ^{1}H NMR: δH (300 MHz; $CDCl_3$; Me_4Si) 7.74 (2 H, d, *J* = 8.4 Hz, Ar-H), 7.69 (1 H, s, C=C<u>H</u>), 7.40-7.29 (7 H, m, Ar-H), 5.57 (2 H, s, C<u>H</u>$_2$); ^{13}C NMR: δC (75 MHz; $CDCl_3$; Me_4Si) 147, 134, 133, 129.21, 129.11, 129.01, 128.87, 128.11, 126, 119, 54; MS, *m/z* 269 (M^+, 8%), 271 (2, M + 2), 268 (60, M – H), 267 (65, M – 2 H), 241 (32, M – N_2), 178 (65, M – C_7H_7), 149 (94, M – $C_7H_7N_2$), 123 (69, M – $C_8H_8N_3$), 104 (65, M – $C_8H_5ClN_2$), 91 (100, M – $C_8H_5ClN_3$), 28 (62, M – $C_{15}H_{12}ClN$).

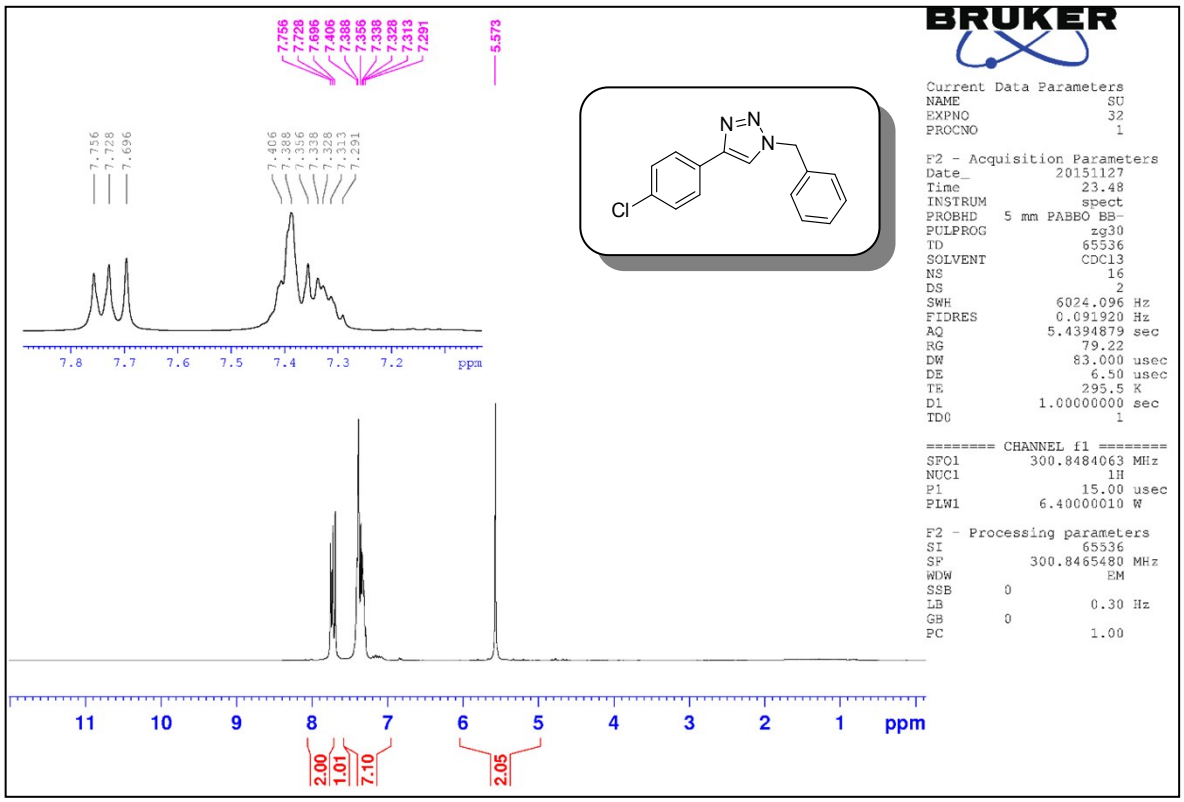

Figure 15: ^{1}H NMR (300 MHz, $CDCl_3$) of 1-benzyl-4-(4-chlorophenyl)-1*H*-1,2,3-triazole (**4e**).

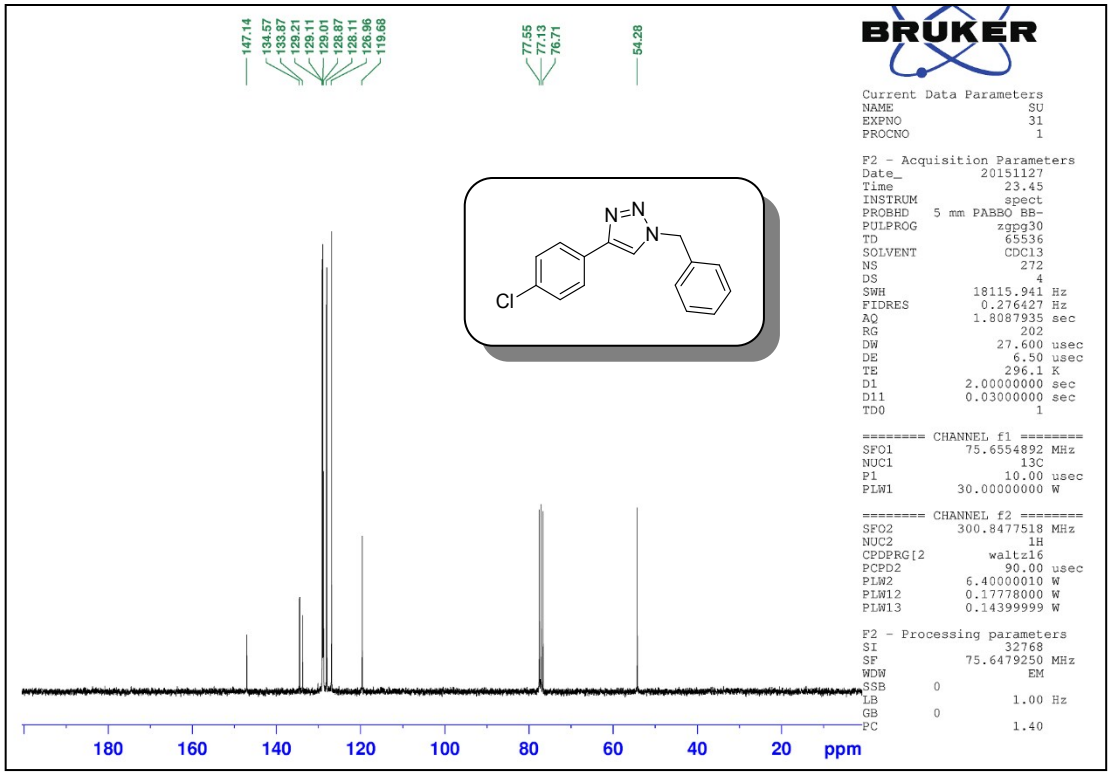

Figure 16: ^{13}C NMR (75MHz, $CDCl_3$) of 1-benzyl-4-(4-chlorophenyl)-1*H*-1,2,3-triazole (**4e**).

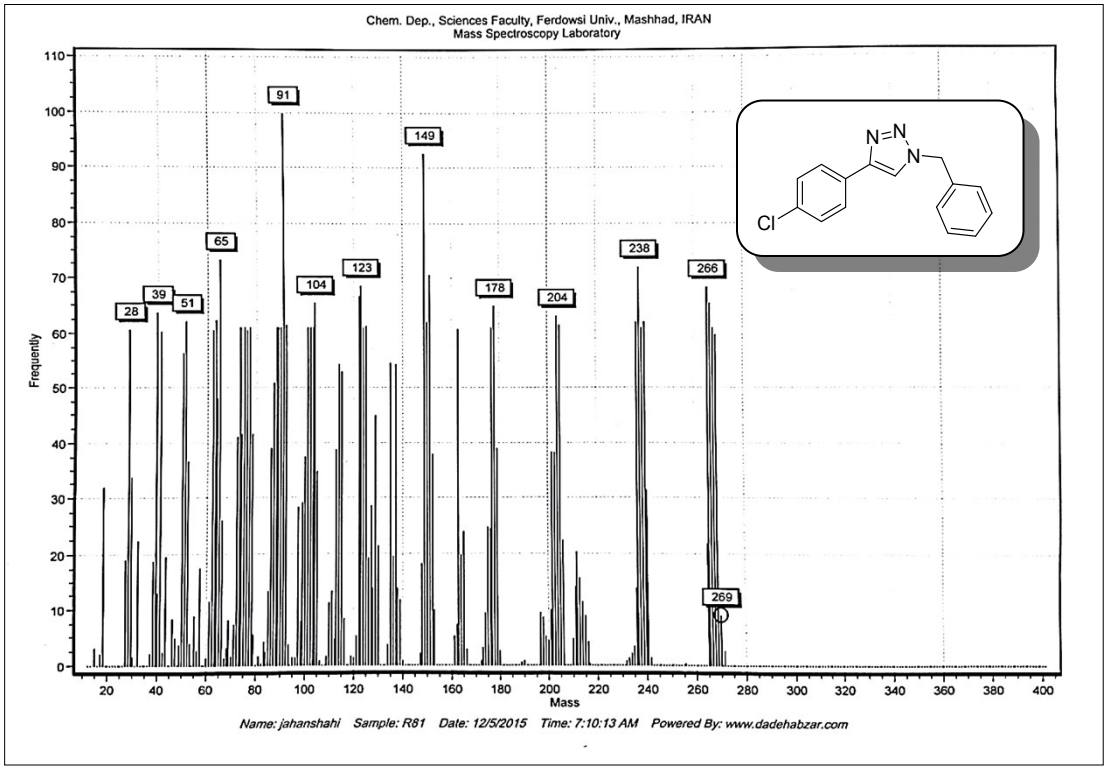

Figure 17: Mass spectrum of 1-benzyl-4-(4-chlorophenyl)-1*H*-1,2,3-triazole (**4e**).

1-benzyl-4-(4-bromophenyl)-1*H*-1,2,3-triazole (4f) white solid (crystals); mp 144 ºC (from EtOH) (Lit.[5] 143–145 ºC); ^{1}H NMR: δH (300 MHz; $CDCl_3$; Me_4Si) 7.69 (2 H, d, *J* = 1.8 Hz, Ar-H), 7.67 (1 H, s, C=C<u>H</u>), 7.53 (2 H, d, *J* = 6.9 Hz, Ar-H), 7.29-7.43 (5 H, m, Ar-H), 5.58 (2 H, s, C<u>H</u>$_2$); ^{13}C NMR: δC (75 MHz; $CDCl_3$; Me_4Si) 147, 134, 131, 129.54, 129.22, 128.89, 128.12, 127, 122, 119, 54; MS, *m/z* 314 (M^+, 7%), 316 (6, M + 2), 313 (56, M – H), 312 (72, M – 2 H), 285 (13, M – N_2), 194 (88, M – C_8H_8N), 104 (82, M – $C_8H_5BrN_2$), 91 (100, M – $C_8H_5BrN_3$), 28 (24, M – $C_{15}H_{12}BrN$).

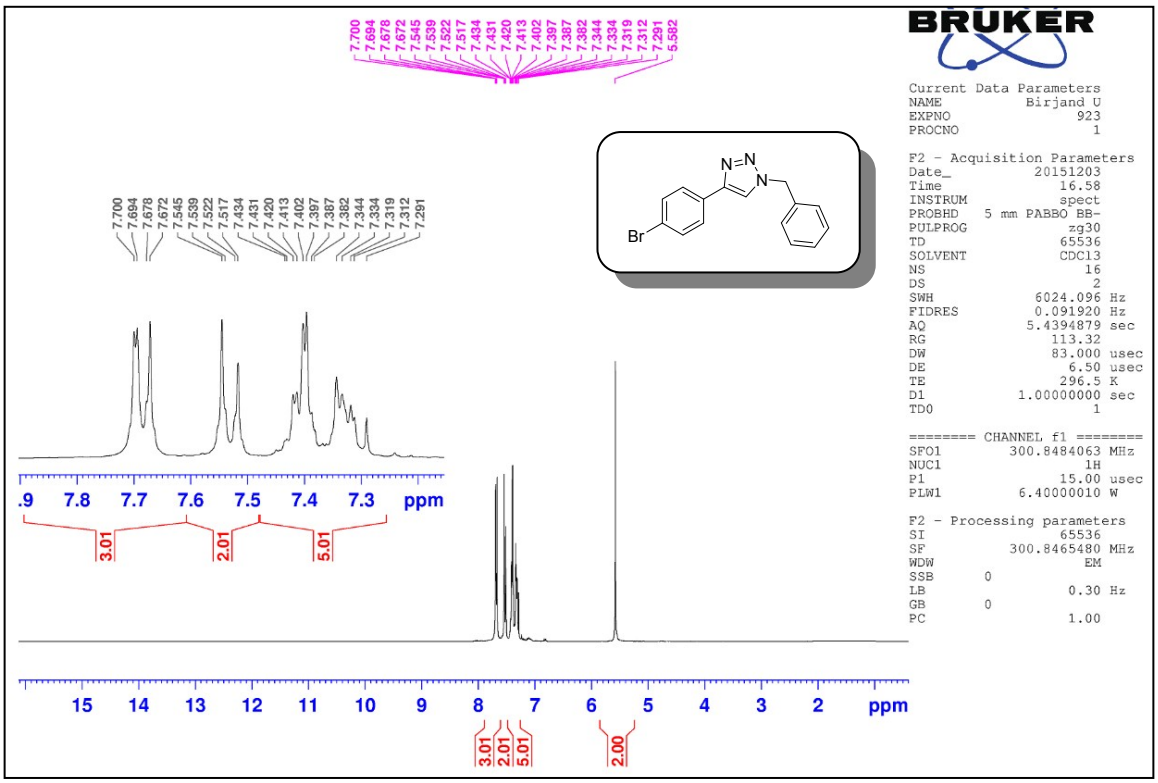

Figure 18: ^{1}H NMR (300 MHz, $CDCl_3$) of 1-benzyl-4-(4-bromophenyl)-1*H*-1,2,3-triazole (**4f**).

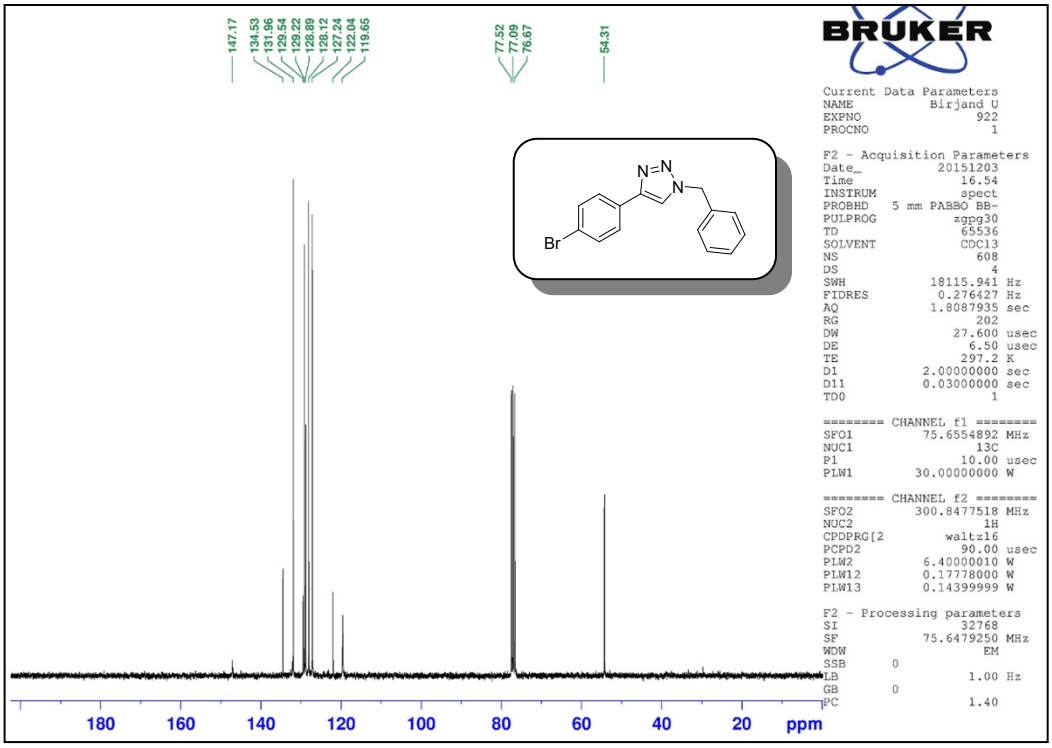

Figure 19: ^{13}C NMR (75MHz, $CDCl_3$) of 1-benzyl-4-(4-bromophenyl)-1*H*-1,2,3-triazole (**4f**).

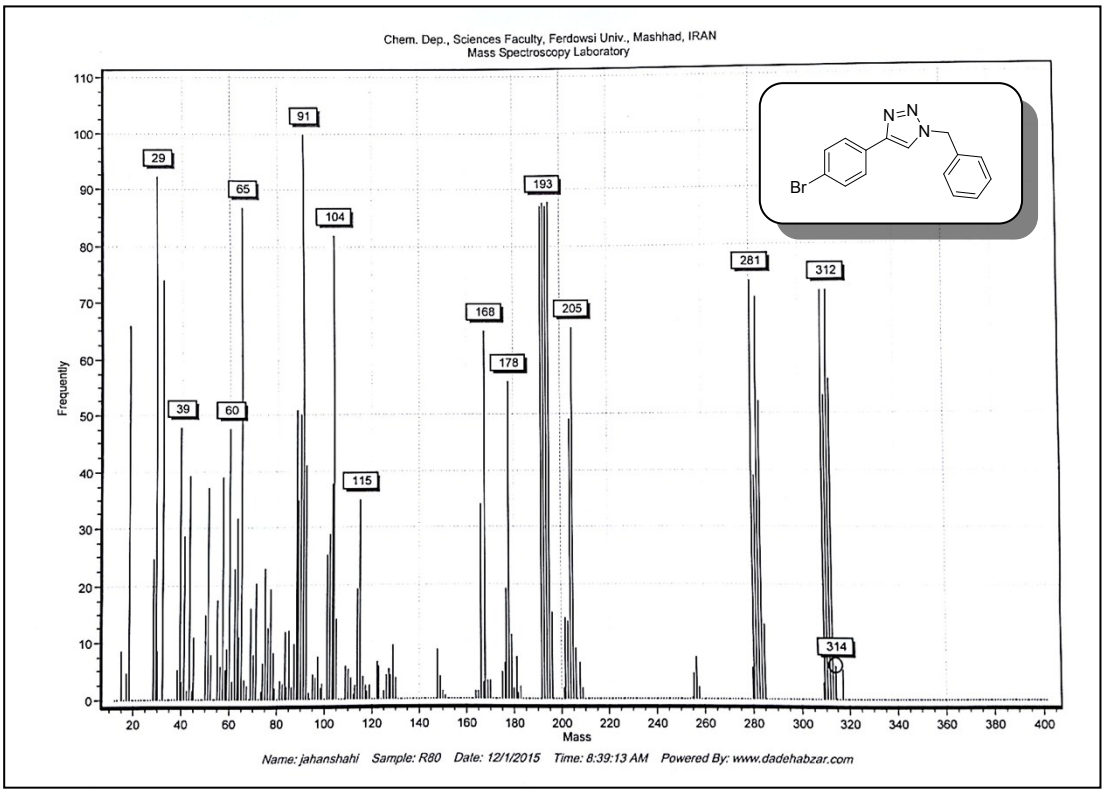

Figure 20: Mass spectrum of 1-benzyl-4-(4-bromophenyl)-1*H*-1,2,3-triazole (**4f**).

1-benzyl-4-(4-nitrophenyl)-1*H*-1,2,3-triazole (4g) (0.27 g, 96%); yellow solid (crystals); mp 167–168 ºC (from EtOH) (Lit.[6] 168–170 ºC); ^{1}H NMR: δH (300 MHz; $CDCl_3$; Me_4Si) 8.27 (2 H, d, *J* = 8.7 Hz, Ar-H), 7.99 (2 H, d, *J* = 8.7 Hz, Ar-H), 7.85 (1 H, s, C=C<u>H</u>), 7.29-7.44 (5 H, m, Ar-H), 5.63 (2 H, s, C<u>H</u>$_2$); ^{13}C NMR: δC (75 MHz; $CDCl_3$; Me_4Si) 147, 146, 136, 134, 129.33, 129.09, 128, 126, 124, 121, 54; MS, *m/z* 280 (M^+, 5%), 279 (57, M – H), 278 (68, M – 2 H), 252 (8, M – N_2), 233 (24, M – NO_2), 148 (37, M – $C_8H_8N_2$), 105 (39, M – $C_8H_5N_3O_2$), 91 (100, M – $C_8H_5N_4O_2$), 28 (58, M – $C_{15}H_{12}N_2O_2$).

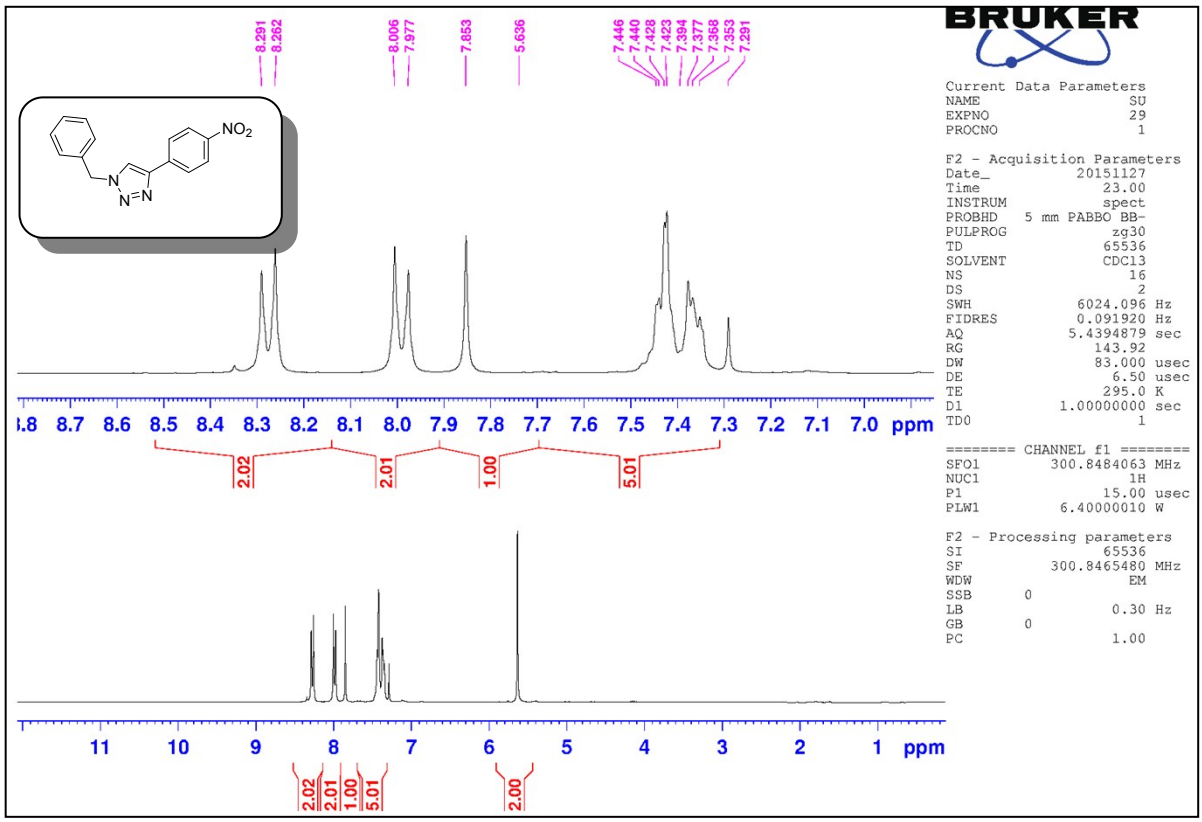

Figure 21: ^{1}H NMR (300 MHz, $CDCl_3$) of 1-benzyl-4-(4-nitrophenyl)-1*H*-1,2,3-triazole (**4g**).

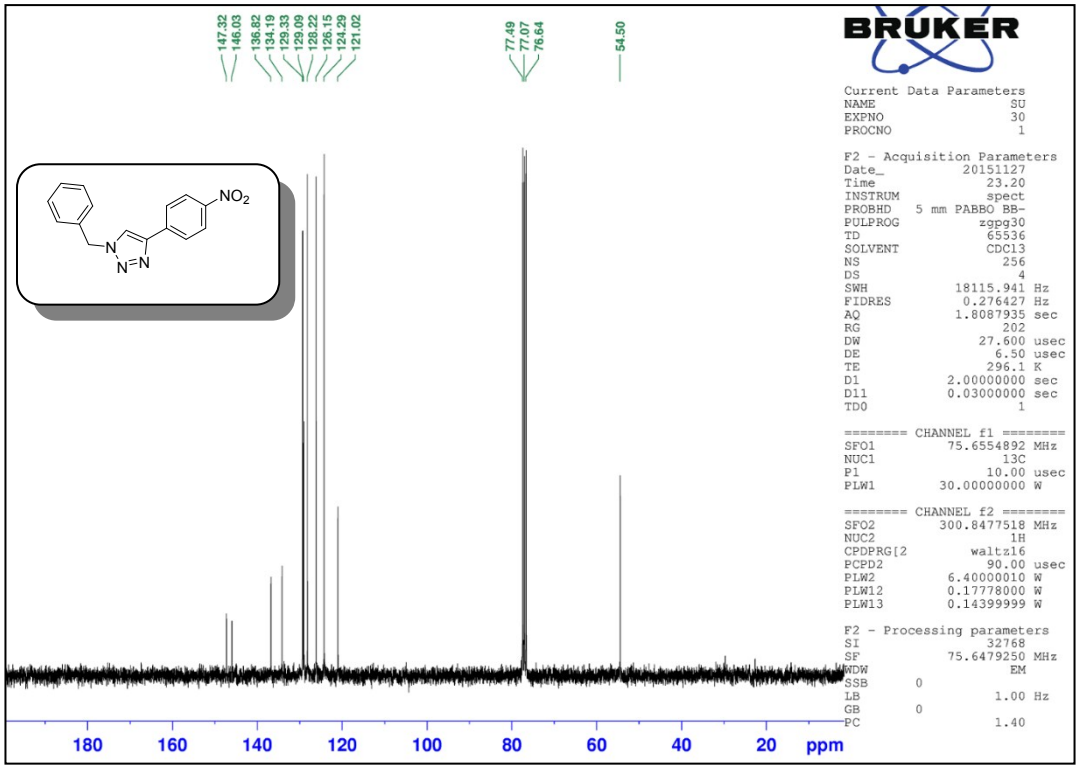

Figure 22: ^{13}C NMR (75MHz, $CDCl_3$) of 1-benzyl-4-(4-nitrophenyl)-1*H*-1,2,3-triazole (**4g**).

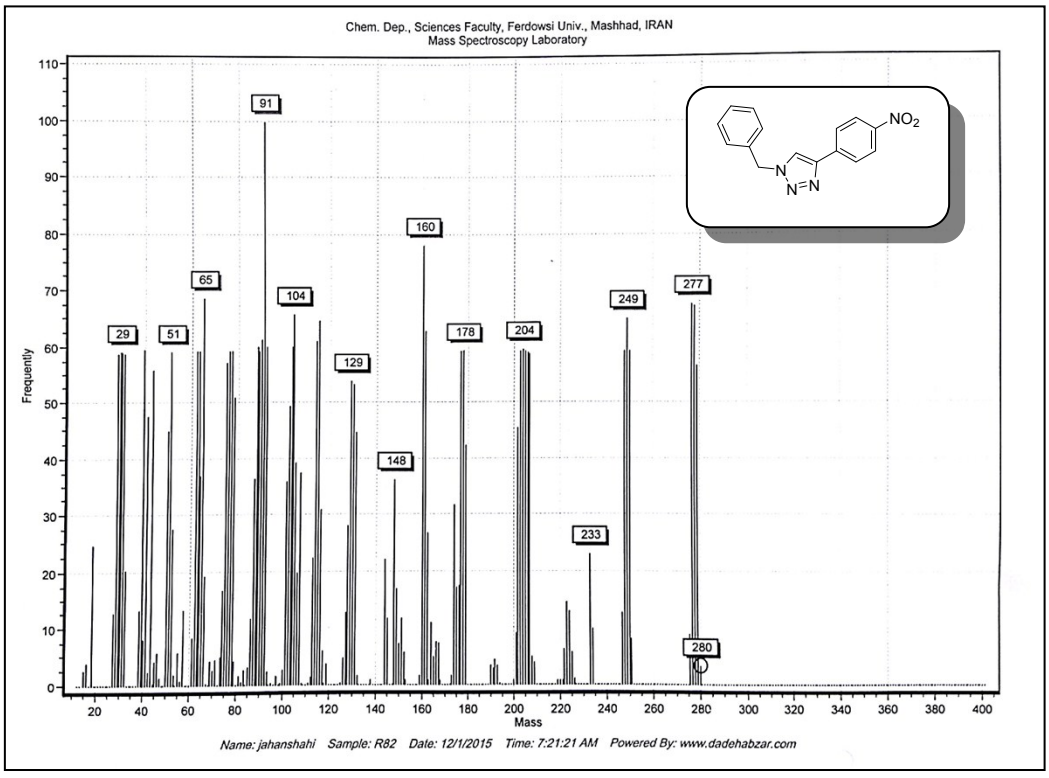

Figure 23: Mass spectrum of 1-benzyl-4-(4-nitrophenyl)-1*H*-1,2,3-triazole (**4g**).

2-(1-benzyl-1*H*-1,2,3-triazol-4-yl)pyridine (4h) (0.21 g, 90%); white solid (crystals); mp 112–113 ºC (from EtOH) (Lit.[7] 113–114 ºC); FT-IR (KBr): ν_{max}/cm^{-1} 3137, 3105, 3084, 3002, 2949, 1599, 1568, 1455 (CH_2), 1419, 1352, 1223 (N–N=N–), 1196 (C–N), 1082, 1044, 996, 857 (=C–H oop, triazole ring), 786, 727, 711, 579; ^{1}H NMR: δH (300 MHz; $CDCl_3$; Me_4Si) 8.55 (1 H, d, J = 4.2 Hz, Py-H), 8.19 (1 H, d, J = 8.1 Hz, Py-H), 8.06 (1 H, s, C=C<u>H</u>), 7.78 (1 H, td, J_1 = 7.8 Hz, J_2 = 1.8 Hz, Py-H), 7.41-7.33 (5 H, m, Ar-H, Py-H), 7.24-7.20 (1 H, m, Ar-H), 5.60 (2 H, s, C<u>H</u>$_2$); ^{13}C NMR: δC (75 MHz; $CDCl_3$; Me_4Si) 150, 149, 148, 136, 134, 129, 128.86, 128.33, 122, 121, 120, 54.MS, *m/z* 236 (M^+, 5%), 235 (41, M – H), 234 (82, M – 2 H), 207 (95, M – N_2), 78 (35, M – $C_9H_8N_3$), 91 (92, M – $C_7H_5N_4$).

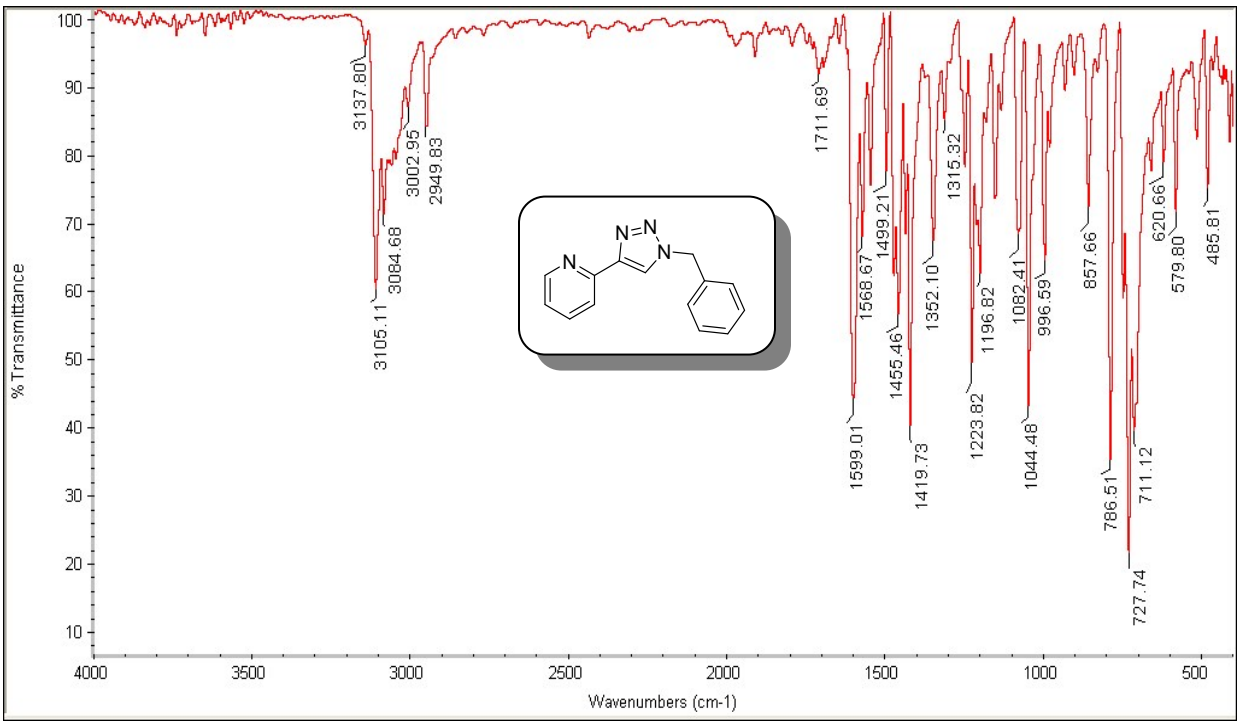

Figure 24: FT-IR (KBr) of 2-(1-benzyl-1*H*-1,2,3-triazol-4-yl)pyridine (**4h**).

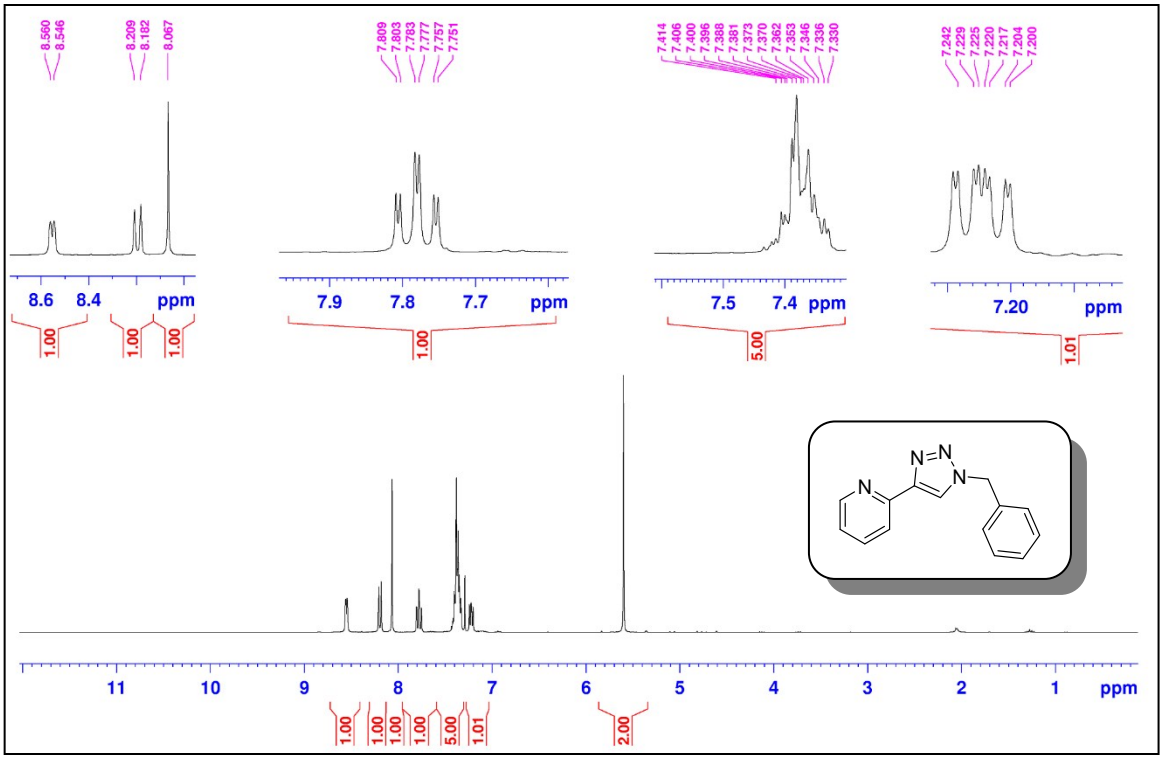

Figure 25: ^{1}H NMR (300 MHz, $CDCl_3$) of 2-(1-benzyl-1*H*-1,2,3-triazol-4-yl)pyridine (**4h**).

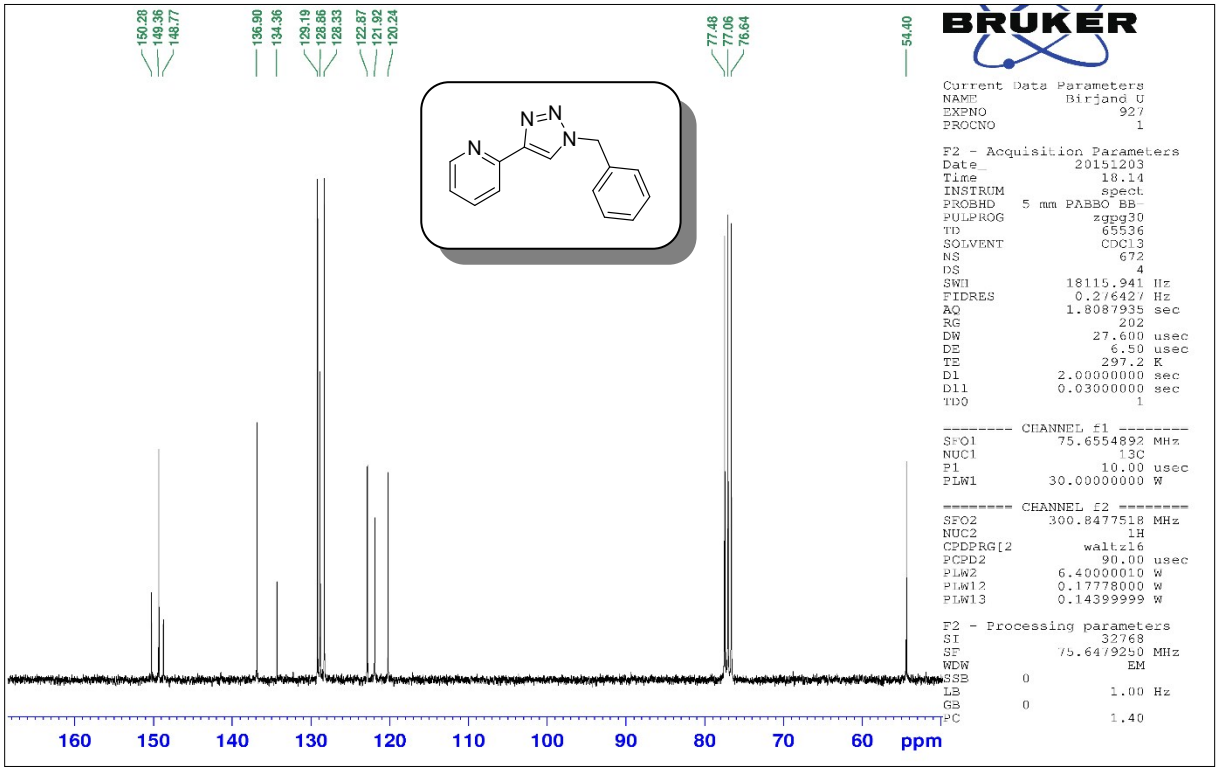

Figure 26: ^{13}C NMR (75MHz, $CDCl_3$) of 2-(1-benzyl-1*H*-1,2,3-triazol-4-yl)pyridine (**4h**).

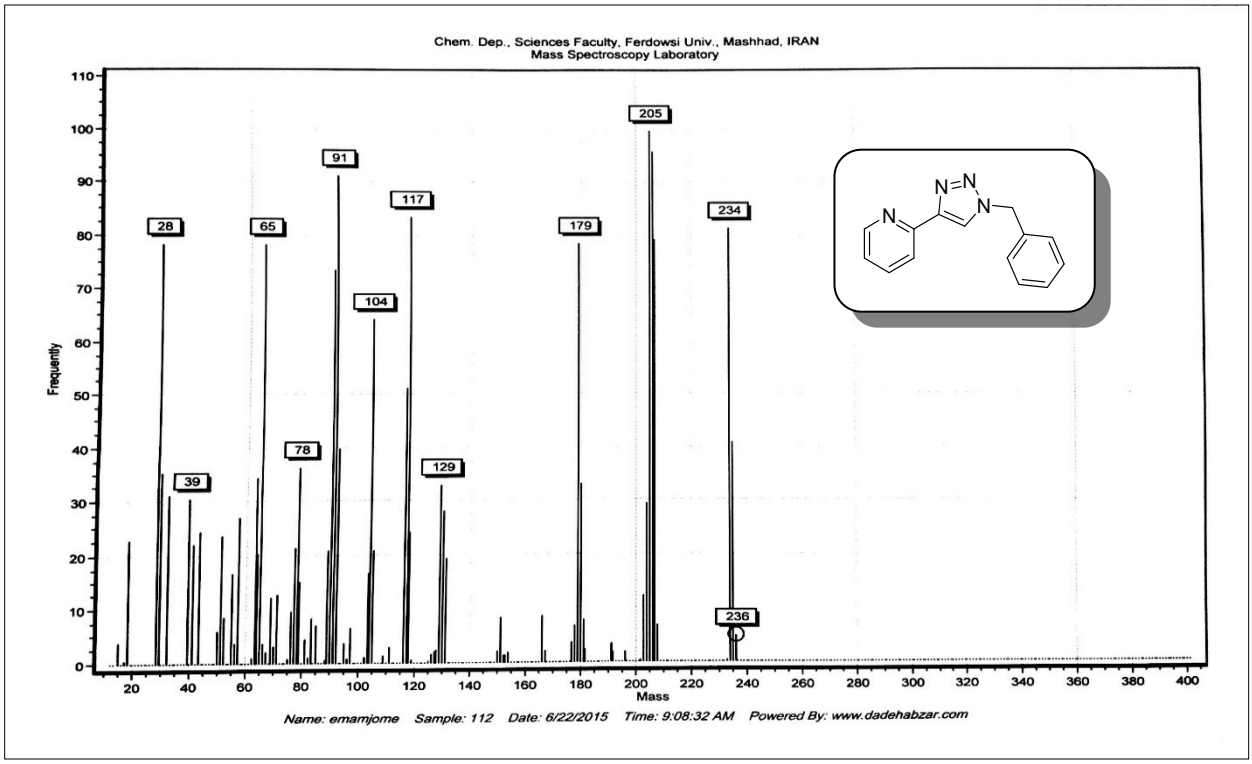

Figure 27: Mass spectrum of 2-(1-benzyl-1*H*-1,2,3-triazol-4-yl)pyridine (**4h**).

1-(4-chlorobenzyl)-4-phenyl-1*H*-1,2,3-triazole (4i) (0.25 g, 93%); white solid (crystals); mp 140–143 ºC (from EtOH) (Lit.[2] 142–145 ºC); FT-IR (KBr): ν_{max}/cm^{-1} 3113, 3083, 3064, 3035, 2933, 1491, 1462 (CH_2), 1411, 1356, 1220 (N–N=N–), 1139 (C–N), 1093, 1080, 1015, 972, 821 (=C–H oop, triazole ring), 805, 764, 688, 497; ^{1}H NMR: δH (300 MHz; $CDCl_3$; Me_4Si) 7.83 (2 H, d, *J* = 7.6 Hz, Ar-H), 7.69 (1 H, s, C=C<u>H</u>), 7.46–7.32 (5 H, m, Ar-H), 7.27 (2 H, d, *J* = 8.7 Hz, Ar-H), 5.58 (2 H, s, C<u>H</u>$_2$); MS, *m/z* 269 (M^+, 7%), 271 (2, M + 2), 268 (33, M – H), 266 (75, M – 3 H), 125 (80, M – $C_8H_6N_3$), 116 (92, M – $C_7H_6ClN_2$), 102 (66, M – $C_7H_6ClN_3$), 89 (87), 77 (65, M – $C_9H_7ClN_3$), 39 (75), 28 (62, M – $C_{15}H_{12}ClN$).

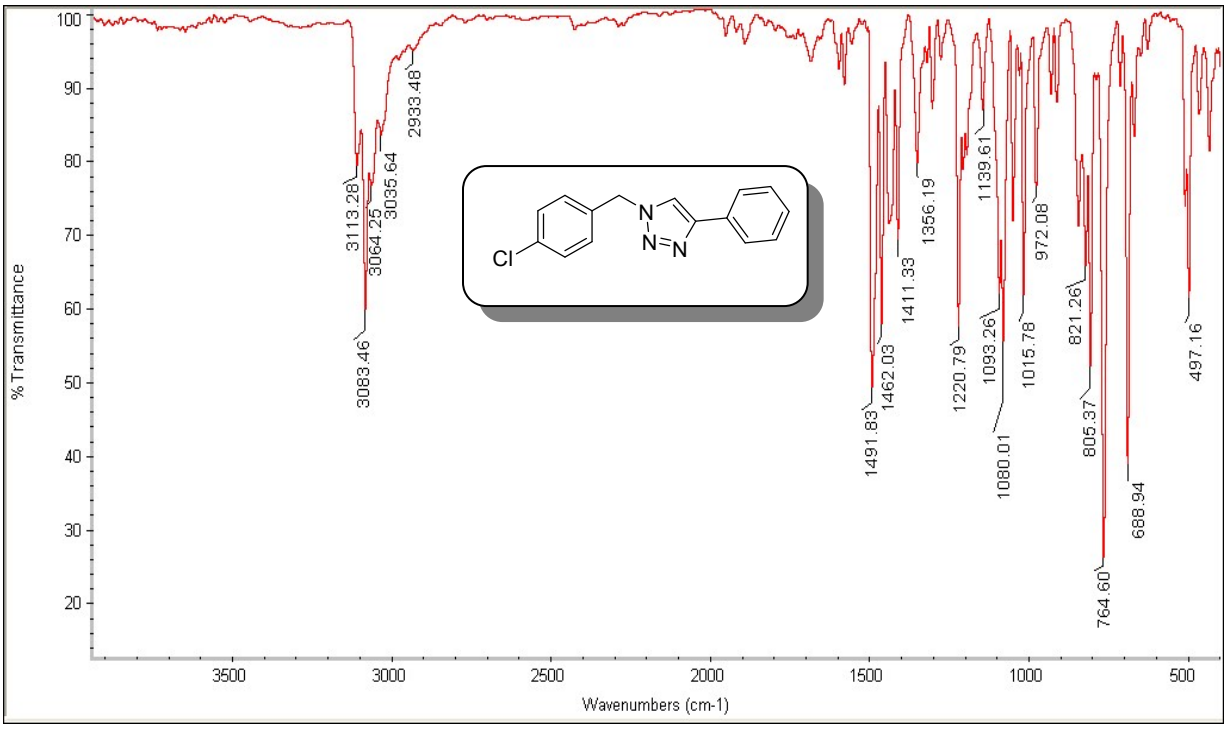

Figure 28: FT-IR (KBr) of 1-(4-chlorobenzyl)-4-phenyl-1*H*-1,2,3-triazole (**4i**).

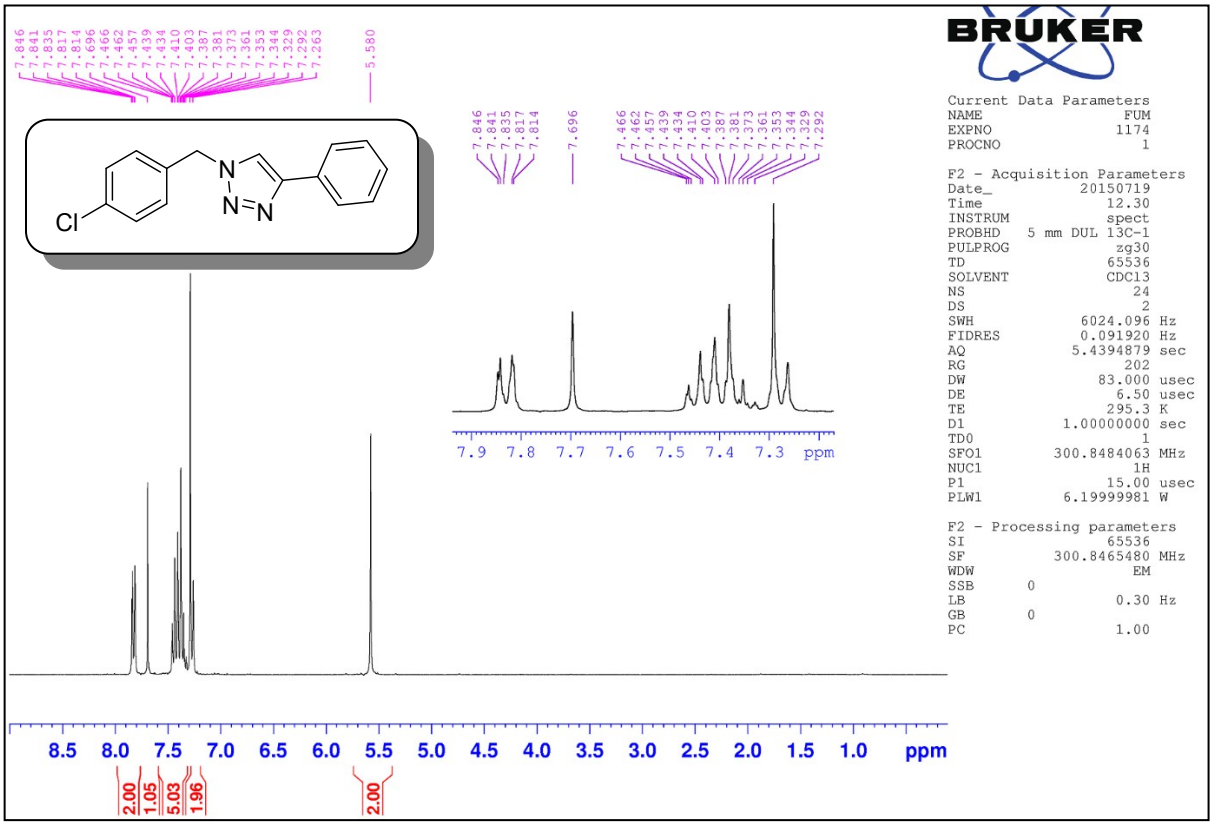

Figure 29: ^{1}H NMR (300 MHz, $CDCl_3$) of 1-(4-chlorobenzyl)-4-phenyl-1*H*-1,2,3-triazole (**4i**).

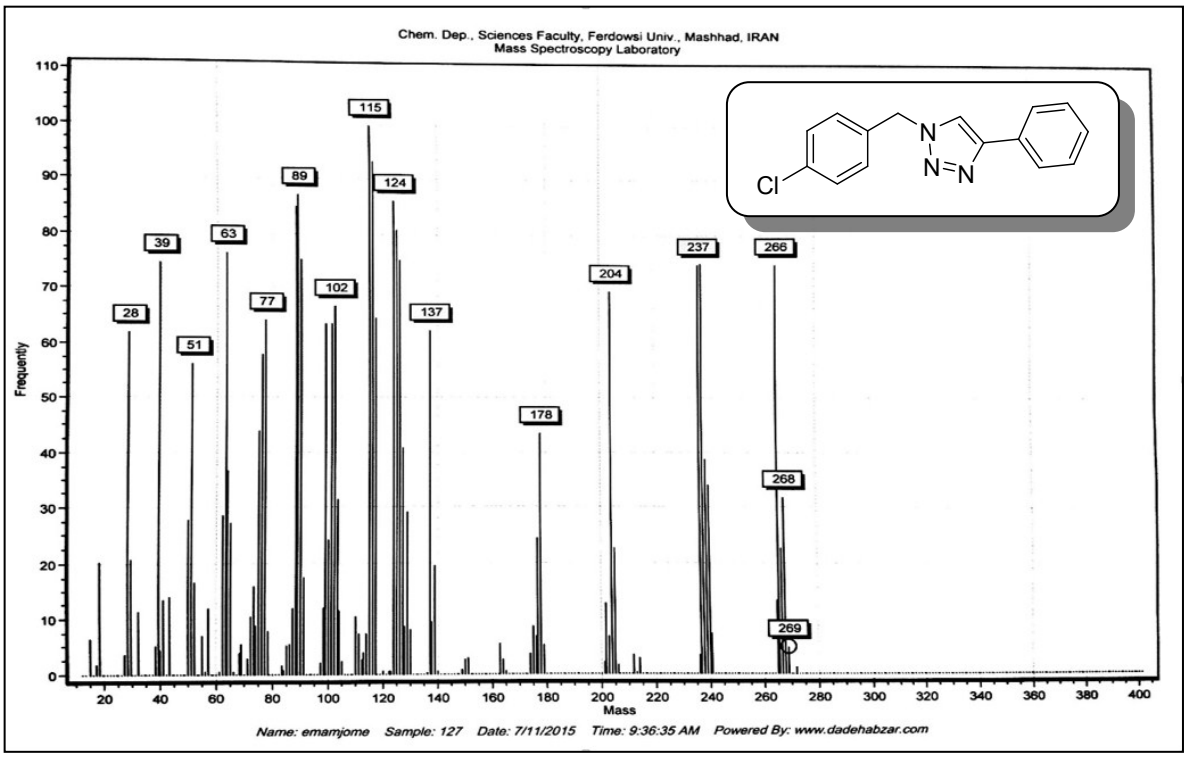

Figure 30: Mass spectrum of 1-(4-chlorobenzyl)-4-phenyl-1*H*-1,2,3-triazole (**4i**).

1-(4-chlorobenzyl)-4-(*p*-tolyl)-1*H*-1,2,3-triazole (4j) (0.26 g, 92%); white solid (crystals); mp 141–142 ºC (from EtOH) (Lit.[2] 140–143 ºC); FT-IR (KBr): ν_{max}/cm^{-1} 3117, 3090, 3047, 2921, 1492, 1454 (CH_2), 1410, 1356, 1220 (N–N=N–), 1170 (C–N), 1081, 1047, 1015, 976, 818 (=C–H oop, triazole ring), 767, 517; ^{1}H NMR: δH (300 MHz; $CDCl_3$; Me_4Si) 7.71 (2 H, d, J = 8.1 Hz, Ar-H), 7.65 (1 H, s, C=C<u>H</u>), 7.39 (2 H, d, J = 8.4 Hz, Ar-H), 7.29-7.23 (4 H, m, Ar-H), 5.56 (2 H, s, C<u>H</u>$_2$), 2.39 (3 H, s, C<u>H</u>$_3$); MS, *m/z* 283 (M^+, 25%), 285 (8, M + 2), 282 (40, M – H), 281 (85, M – 2 H), 125 (85, M – $C_9H_8N_3$), 116 (60, M – $C_7H_6ClN_3$), 89 (85), 77 (85, M – ($C_9H_7ClN_3$ + CH_3)), 28 (82, M – $C_{16}H_{14}ClN$), 15 (38, M – $C_{15}H_{11}ClN_3$).

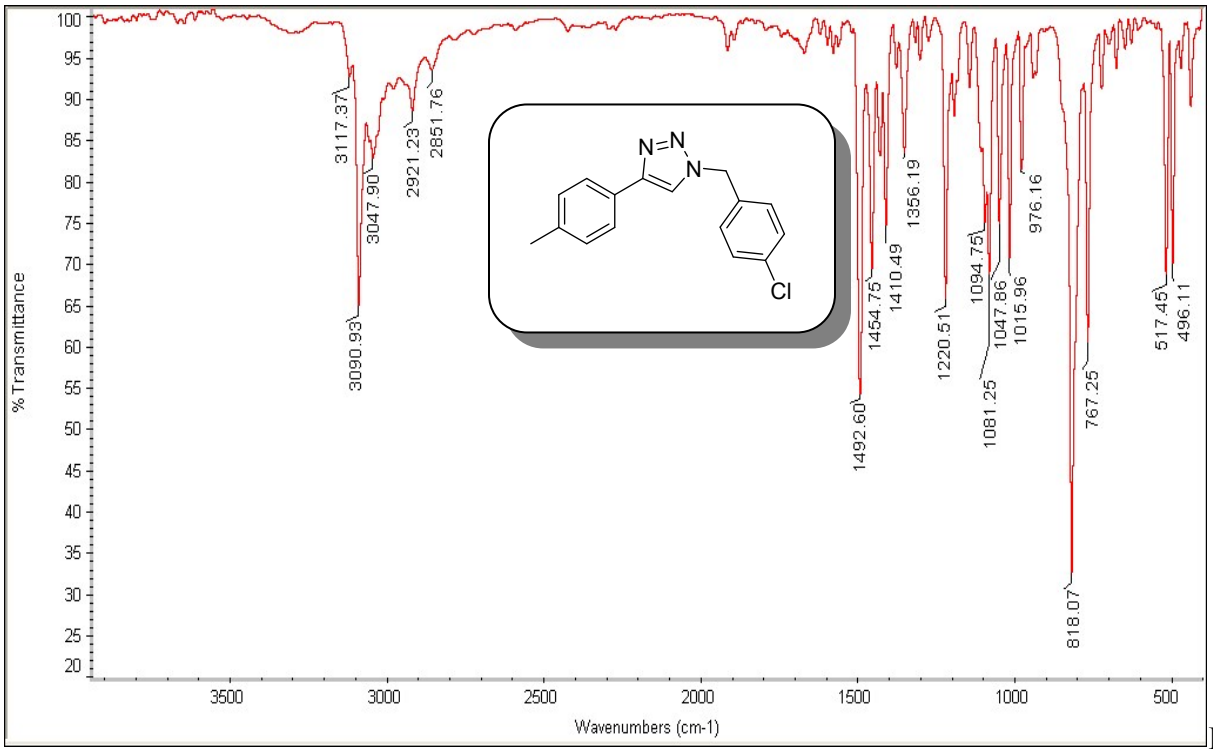

Figure 31: FT-IR (KBr) of 1-(4-chlorobenzyl)-4-(*p*-tolyl)-1*H*-1,2,3-triazole (**4j**).

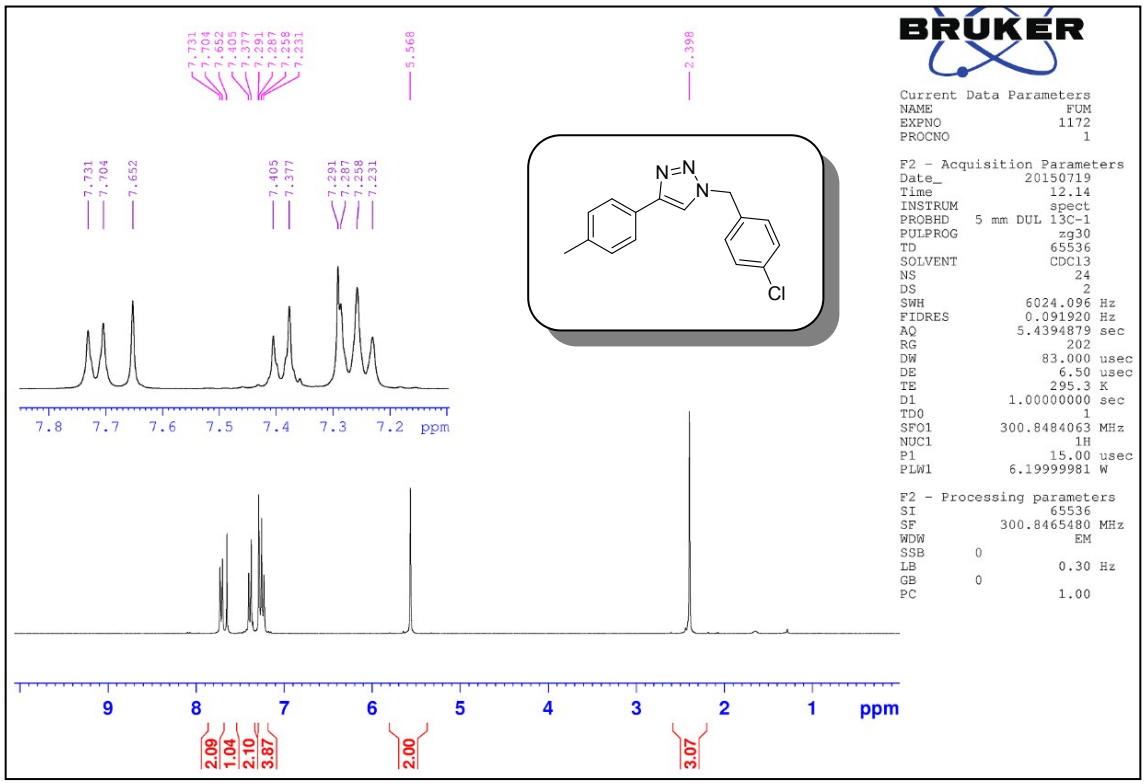

Figure 32: ^{1}H NMR (300 MHz, $CDCl_3$) of 1-(4-chlorobenzyl)-4-(*p*-tolyl)-1*H*-1,2,3-triazole (**4j**).

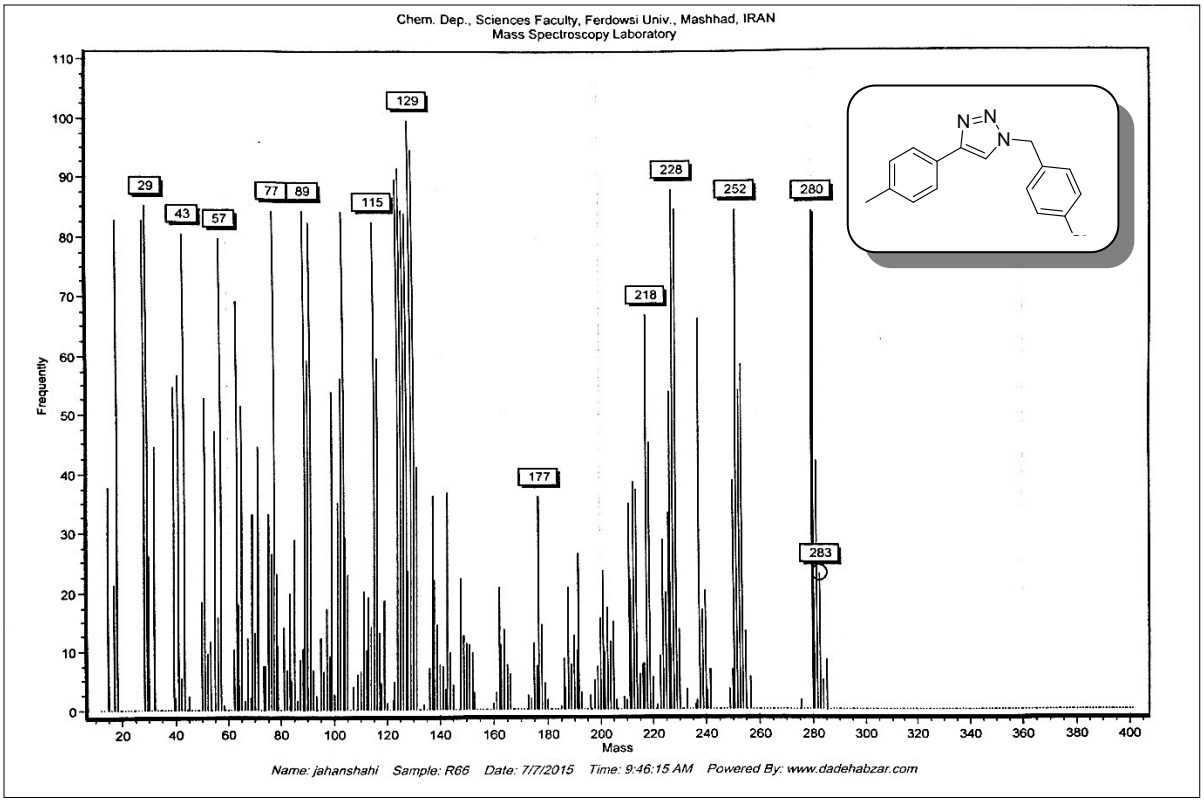

Figure 33: Mass spectrum of 1-(4-chlorobenzyl)-4-(*p*-tolyl)-1*H*-1,2,3-triazole (**4j**).

1-(4-chlorobenzyl)-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (4k) (0.27 g, 90%); white solid (crystals); mp 150–152 ºC (from EtOH); elemental analysis: Found: C, 63.99; H, 4.65; N, 13.92. Calc. for $C_{16}H_{14}ClN_3O$: C, 64.11; H, 4.71; N, 14.02%; FT-IR (KBr): ν_{max}/cm^{-1} 3121, 3091, 3019, 2958, 2933, 2835, 1616, 1561, 1493, 1453 (CH_2), 1434, 1351, 1302, 1255 (N–N=N–), 1218, 1175 (C–N), 1030, 1016, 976, 818 (=C–H oop, triazole ring), 765; ^{1}H NMR: δH (300 MHz; $CDCl_3$; Me_4Si) 7.76–7.28 (7 H, m, Ar-H, C=C<u>H</u>), 6.96 (2 H, d, *J* = 6.3 Hz, Ar-H), 5.55 (2 H, s, C<u>H</u>$_2$), 2.86 (3 H, s, C<u>H</u>$_3$); ^{13}C NMR: δC (75 MHz; $CDCl_3$; Me_4Si) 159, 148, 134, 133, 129, 127, 123, 118, 114, 55, 53; MS, *m/z* 299 (M^+, 5%), 301 (2, M + 2), 298 (43, M – H), 297 (95, M – 2 H), 267 (96, M – CH_3O), 146 (42, M – $C_7H_6ClN_2$), 125 (90, M – $C_9H_8N_3O$), 89 (95), 76 (91, M – (CH_3O + $C_9H_7ClN_3$)), 28 (55, M – $C_{16}H_{14}ClNO$).

Eager 300 Summarize Results

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Hydrogen%	4.657544765
Sulphur%	0

Calcd for $C_{16}H_{14}ClN_3O$

Nitrogen%	14.02
Carbon%	64.11
Hydrogen%	4.71
Sulphor%	0

1 Sample(s) in Group No : 1

Component Name	Average
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Carbon%	63.99537582
Hydrogen%	4.657544765
Sulphur%	0

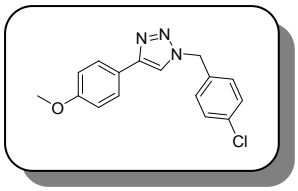


Figure 34: Elemental analysis of 1-(4-chlorobenzyl)-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (**4k**).

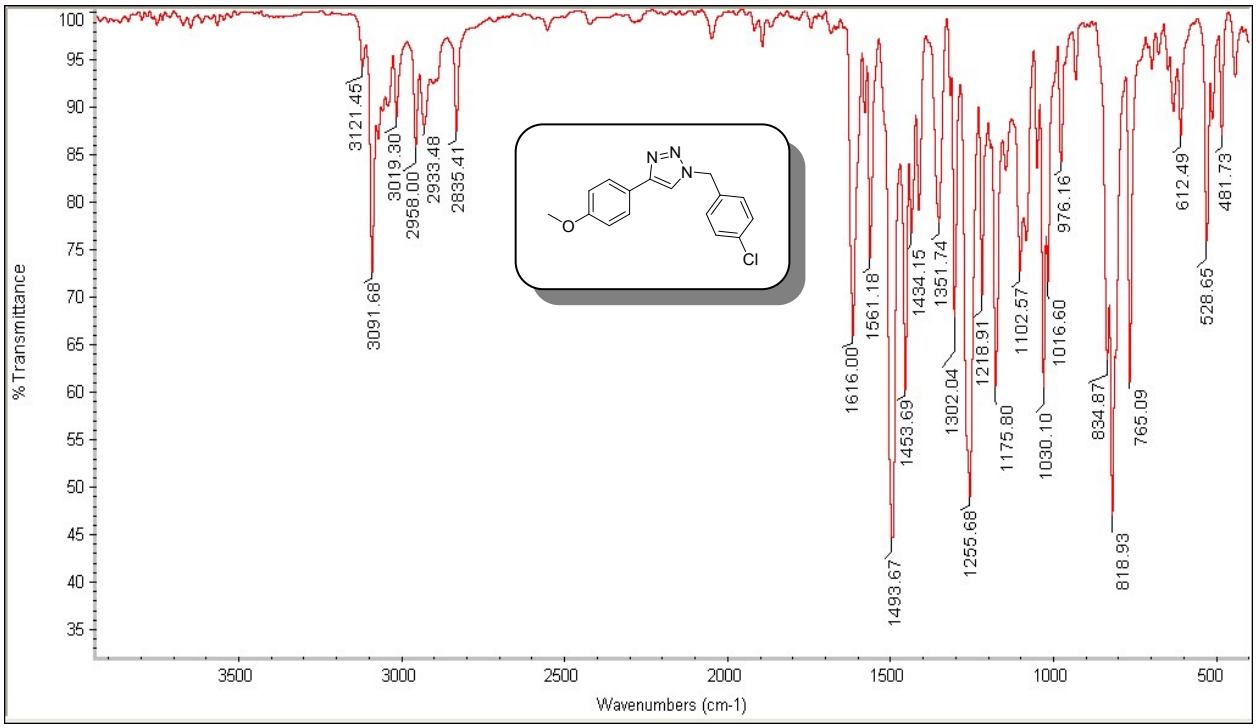


Figure 35: FT-IR (KBr) of 1-(4-chlorobenzyl)-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (**4k**).

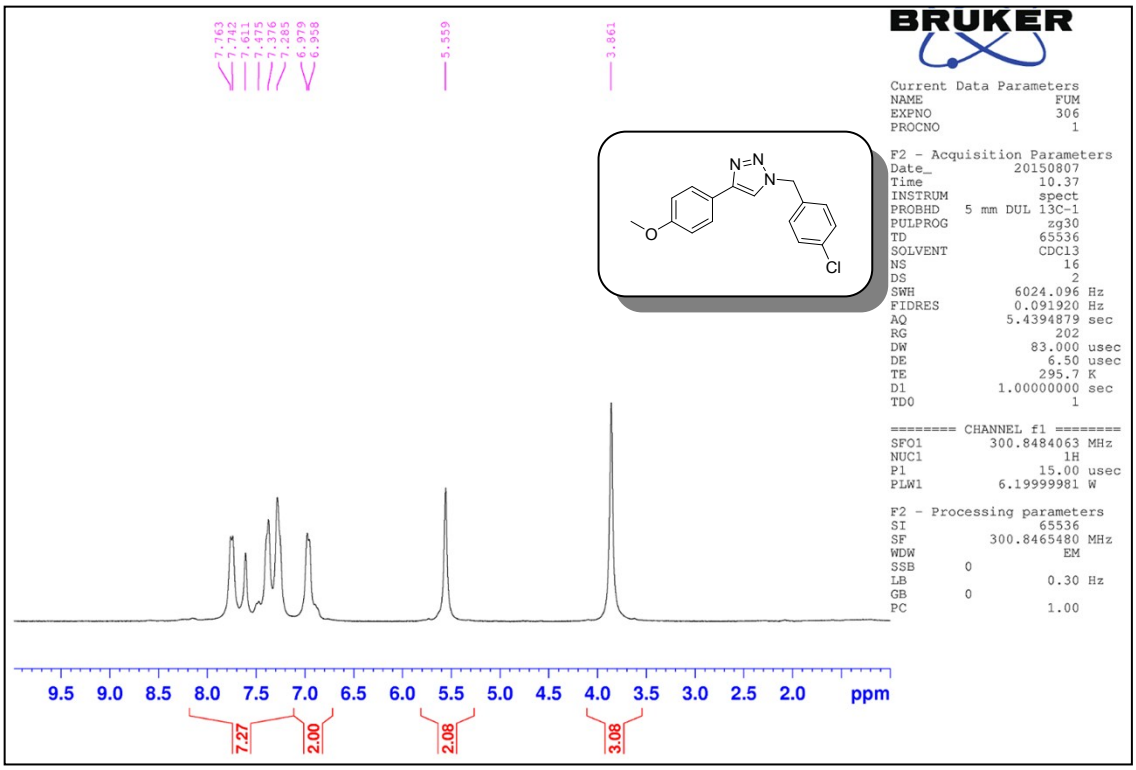


Figure 36: ^{1}H NMR (300 MHz, $CDCl_3$) of 1-(4-chlorobenzyl)-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (**4k**).

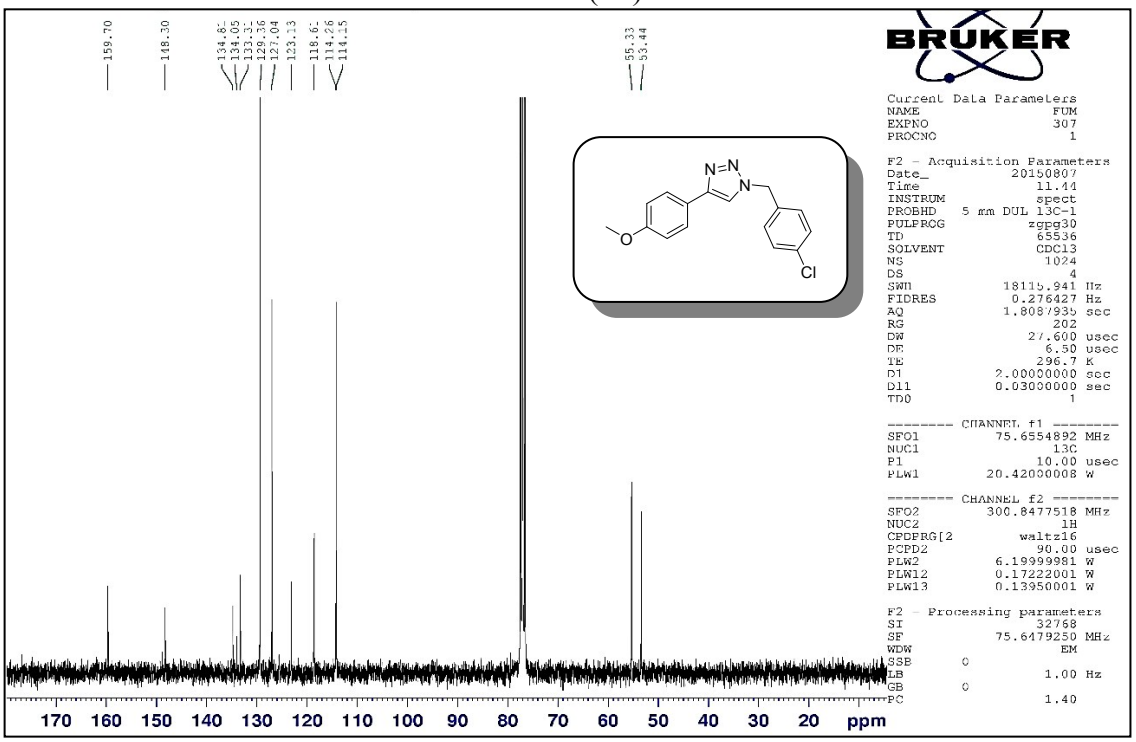


Figure 37: ^{13}C NMR (75MHz, $CDCl_3$) of 1-(4-chlorobenzyl)-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (**4k**).

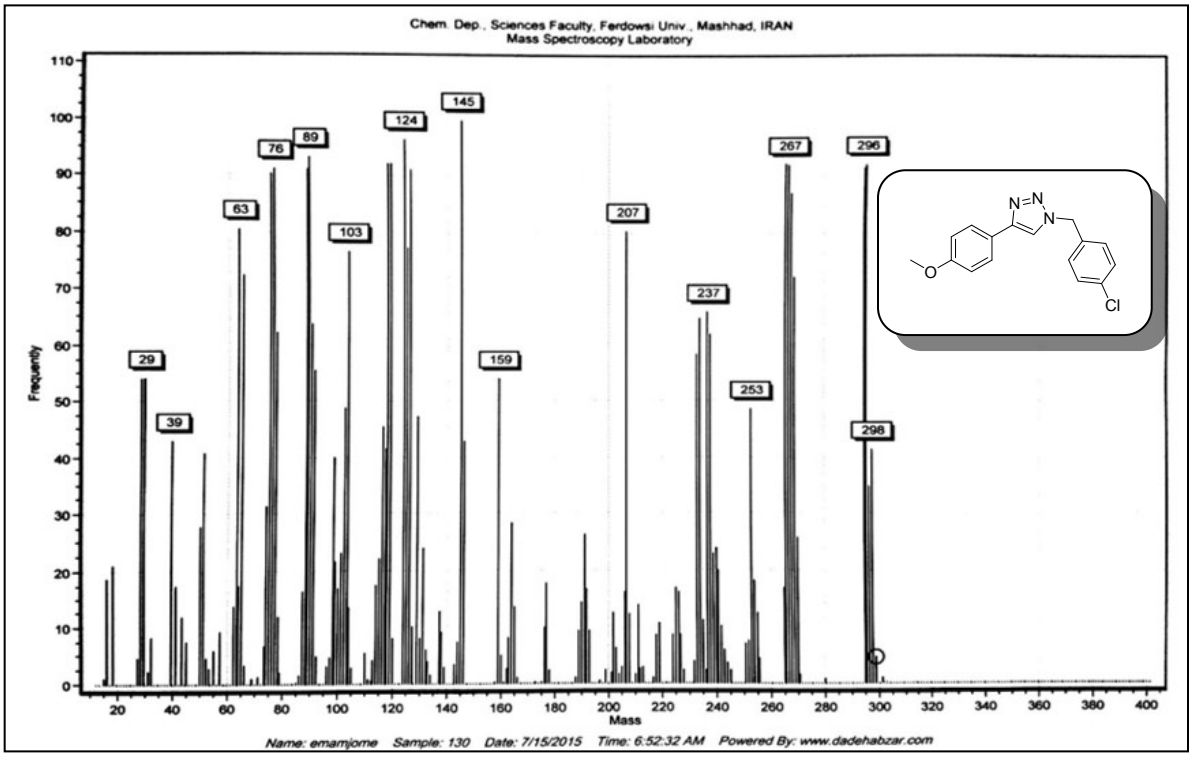
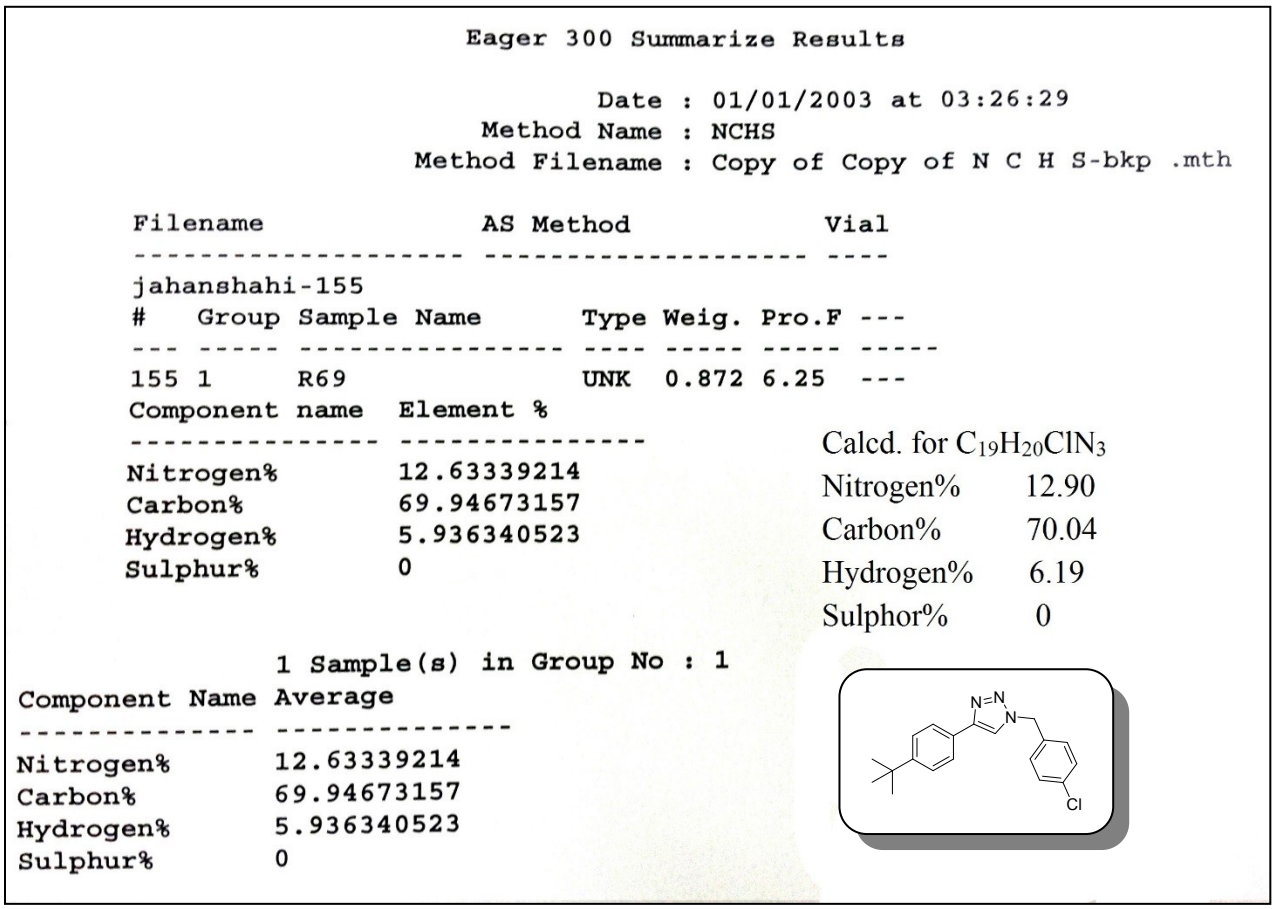


Figure 38: Mass spectrum of 1-(4-chlorobenzyl)-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (**4k**).

4-(4-(*tert*-butyl)phenyl)-1-(4-chlorobenzyl)-1*H*-1,2,3-triazole (4l) (0.28 g, 86%); white solid (crystals); mp 153–154 ºC (from EtOH); elemental analysis: Found: C, 69.94; H, 5.93; N, 12.63. Calc. for $C_{19}H_{20}ClN_3$: C, 70.04; H, 6.19; N, 12.90%; FT-IR (KBr): ν_{max}/cm^{-1} 3133, 2959, 2904, 2868, 1492, 1457 (CH_2), 1427, 1361, 1224 (N–N=N–), 1157 (C–N), 1049, 1014, 976, 833 (=C–H oop, triazole ring), 806, 776, 560; ^1H NMR: δH (300 MHz; $CDCl_3$; Me_4Si) 7.75 (2 H, d, J = 8.4 Hz, Ar-H), 7.67 (1 H, s, C=C<u>H</u>), 7.45 (2 H, d, J = 8.4 Hz, Ar-H), 7.37 (2 H, d, J = 8.4 Hz, Ar-H), 7.26 (2 H, t, J = 8.4 Hz, Ar-H), 5.55 (2 H, s, C<u>H</u>$_2$), 1.36 (9 H, s, 3 C<u>H</u>$_3$); ^{13}C NMR: δC (75 MHz; $CDCl_3$; Me_4Si) 151, 148, 134, 133, 129, 127, 125, 119, 53, 34, 31; MS, *m/z* 325 (M^+, 64%), 327 (19, M +

2), 324 (65, M – H), 323 (69, M – 2 H), 172 (91, M – $C_7H_6ClN_2$), 173 (61, M – C_8H_7ClN), 125 (92, M – $C_{12}H_{14}N_3$), 77 (63, M – ($C_{13}H_{16}N_3$ + Cl)), 57 (67, M – $C_{15}H_{11}ClN_3$), 28 (63, M – N_2).



Eager 300 Summarize Results

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Component name	Element %
Nitrogen%	12.63339214
Carbon%	69.94673157
Hydrogen%	5.936340523
Sulphur%	0

Calcd. for $C_{19}H_{20}ClN_3$

Nitrogen%	12.90
Carbon%	70.04
Hydrogen%	6.19
Sulphor%	0

1 Sample(s) in Group No : 1

Component Name	Average
Nitrogen%	12.63339214
Carbon%	69.94673157
Hydrogen%	5.936340523
Sulphur%	0

Figure 39: Elemental analysis of 4-(4-(*tert*-butyl)phenyl)-1-(4-chlorobenzyl)-1*H*-1,2,3-triazole (**4l**).

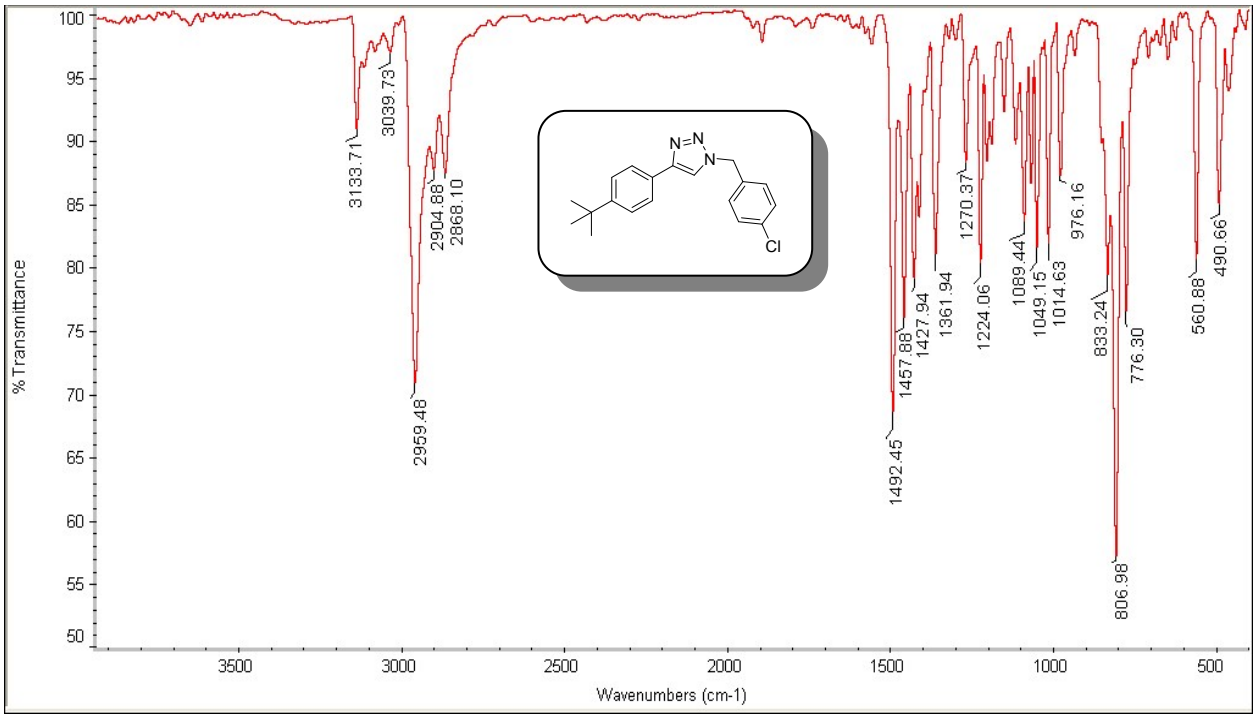


Figure 40: FT-IR (KBr) of 4-(4-(*tert*-butyl)phenyl)-1-(4-chlorobenzyl)-1*H*-1,2,3-triazole (**4l**).

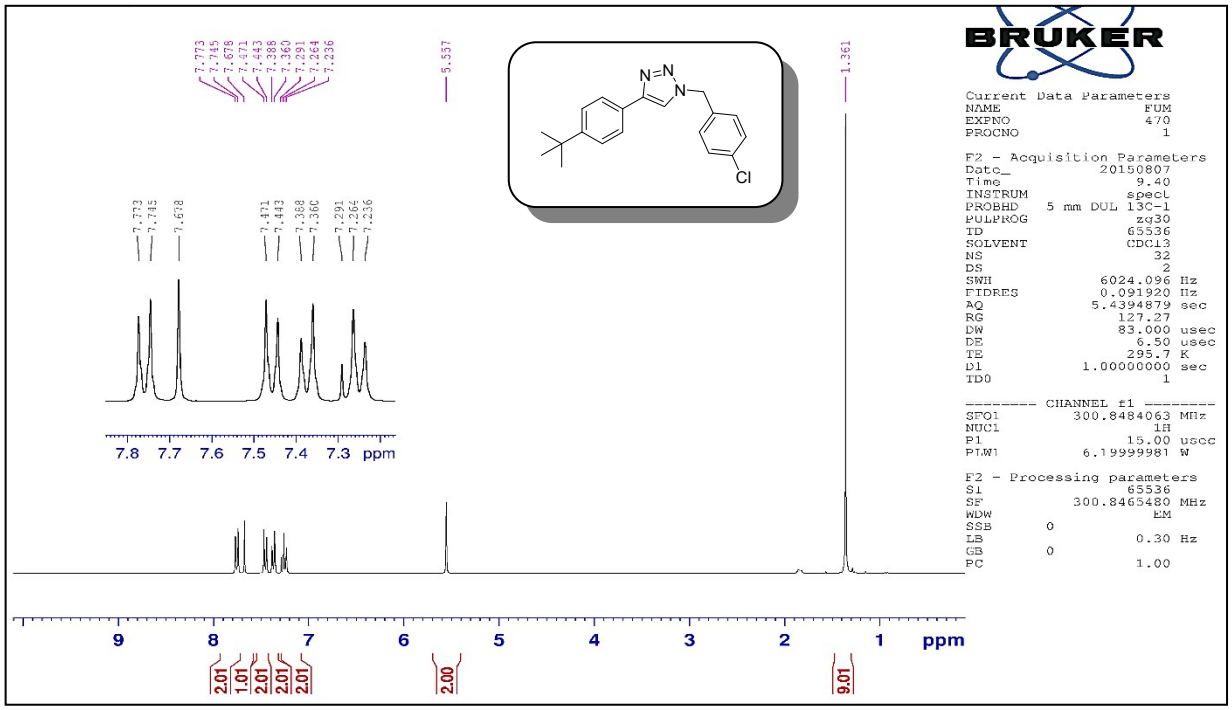


Figure 41: ^{1}H NMR (300 MHz, $CDCl_3$) of 4-(4-(*tert*-butyl)phenyl)-1-(4-chlorobenzyl)-1*H*-1,2,3-triazole (**4l**).

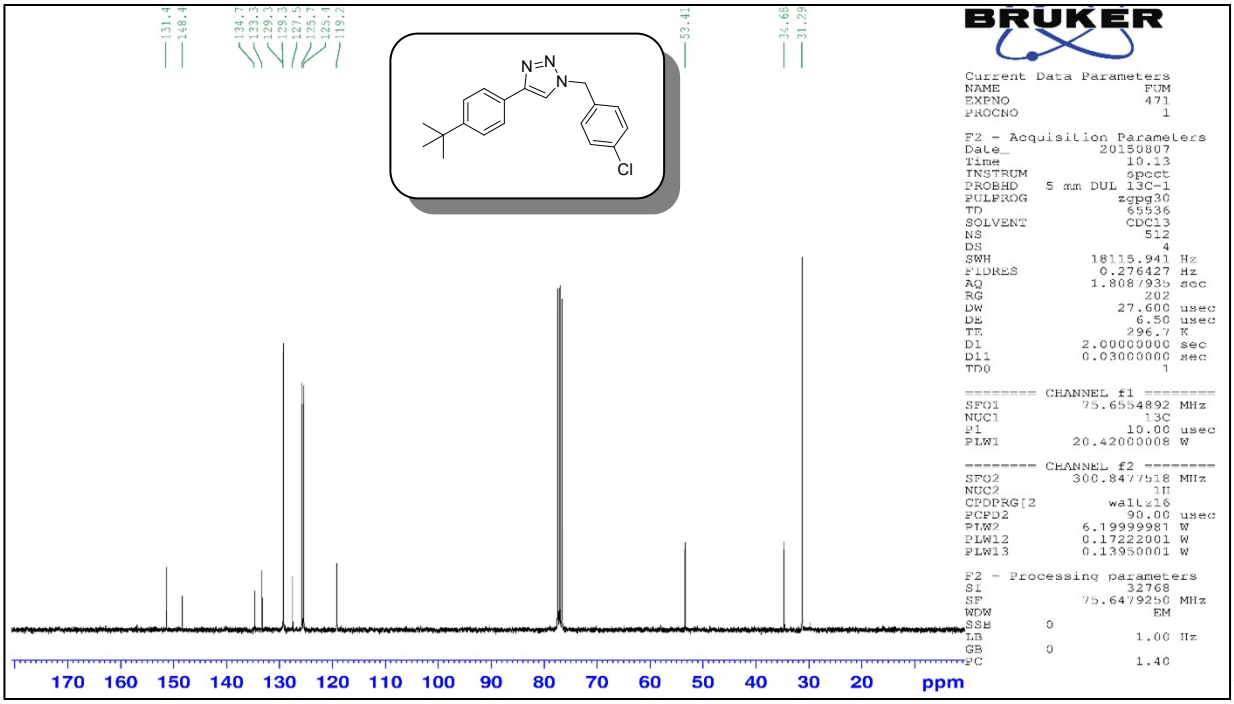


Figure 42: ^{13}C NMR (75MHz, $CDCl_3$) of 4-(4-(*tert*-butyl)phenyl)-1-(4-chlorobenzyl)-1*H*-1,2,3-triazole (**4l**).

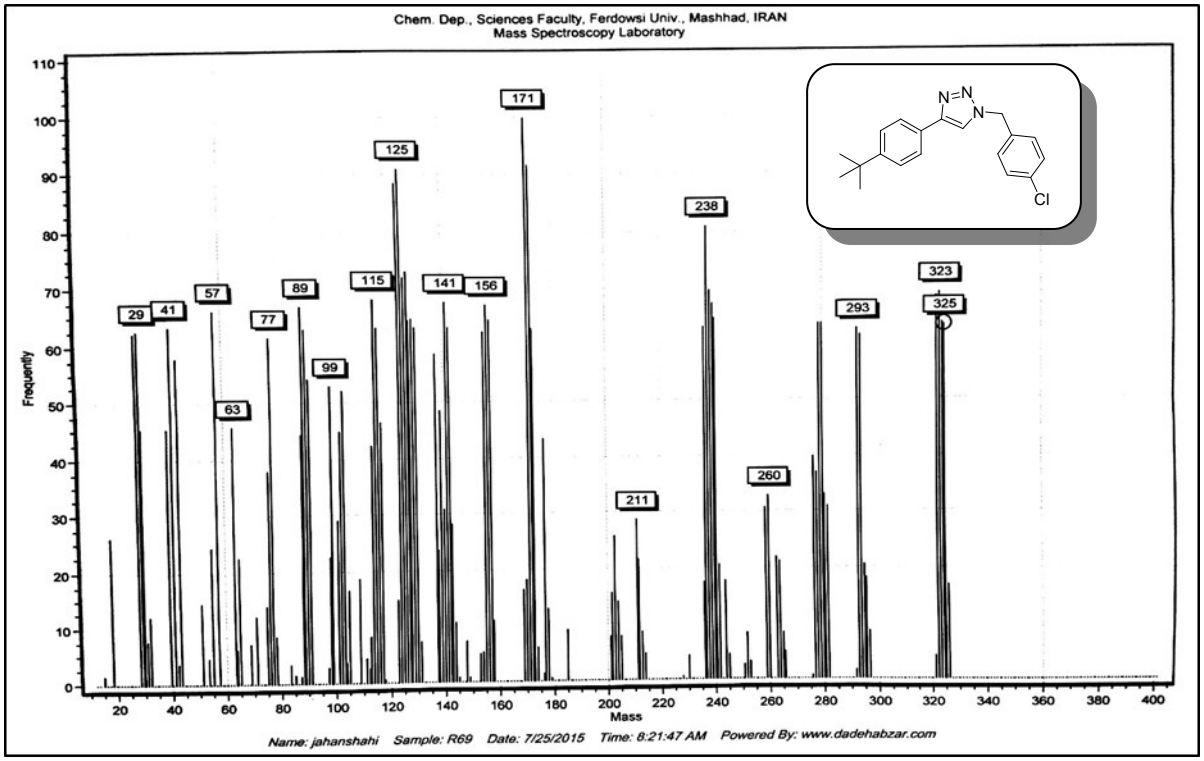


Figure 43: Mass spectrum of 4-(4-(*tert*-butyl)phenyl)-1-(4-chlorobenzyl)-1*H*-1,2,3-triazole (**4l**).

2-(1-(4-chlorobenzyl)-1*H*-1,2,3-triazol-4-yl)pyridine (4m) (0.24 g, 88%); yellow solid (crystals); mp 113–114 ºC (from EtOH) (Lit.[2] 115–117 ºC); FT-IR (KBr): ν_{max}/cm^{-1} 3113, 3088, 3060, 2925, 2855, 1595, 1568, 1491, 1469 (CH_2), 1419, 1325, 1224 (N–N=N–), 1147 (C–N), 1080, 1046, 1015, 994, 805 (=C–H oop, triazole ring), 784, 768, 739, 677; ^{1}H NMR: δH (300 MHz; $CDCl_3$; Me_4Si) 8.56 (1 H, d, *J* = 4.2 Hz, Py-H), 8.20 (1 H, d, *J* = 7.8 Hz, Py-H), 8.07 (1 H, s, C=C<u>H</u>), 7.79 (1 H, td, J_1= 7.65 Hz, J_2 = 1.8 Hz, Py-H), 7.39-7.22 (5 H, m, Ar-H), 5.58 (2 H, s, C<u>H</u>$_2$); ^{13}C NMR: δC (75 MHz; $CDCl_3$; Me_4Si) 150, 149, 148, 136, 134, 132, 129.61, 129.41, 122, 121, 120, 53; MS, *m/z* 270 (M^+, 40%), 272 (13, M + 2), 269 (43, M – H), 268 (55, M – 2 H), 242 (43, M – N_2), 125 (100, M – $C_7H_5N_4$), 117 (96, M – $C_7H_6ClN_2$), 99 (75, M – ($C_8H_7N_4$ + Cl)), 103 (50, M – $C_7H_6ClN_3$), 90 (88), 78 (75, M – $C_9H_7ClN_3$), 28 (50, M – $C_{14}H_{11}ClN_2$).

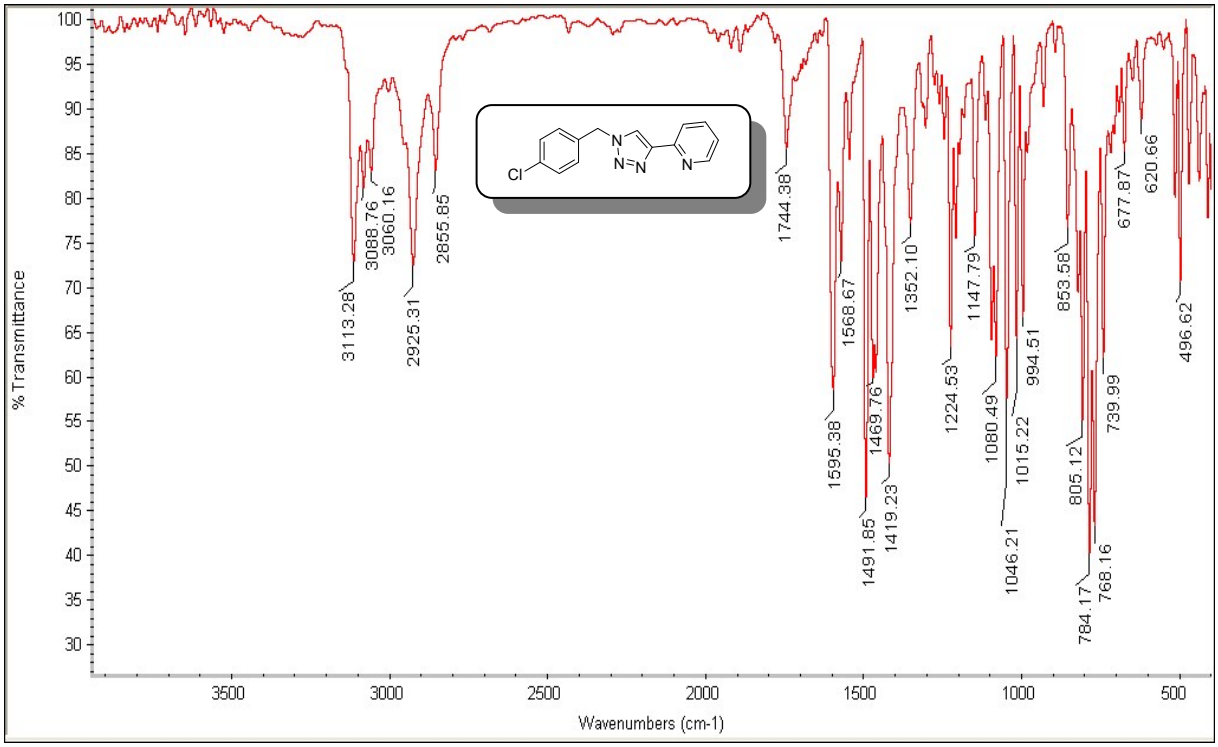


Figure 44: FT-IR (KBr) of 2-(1-(4-chlorobenzyl)-1*H*-1,2,3-triazol-4-yl)pyridine (**4m**).

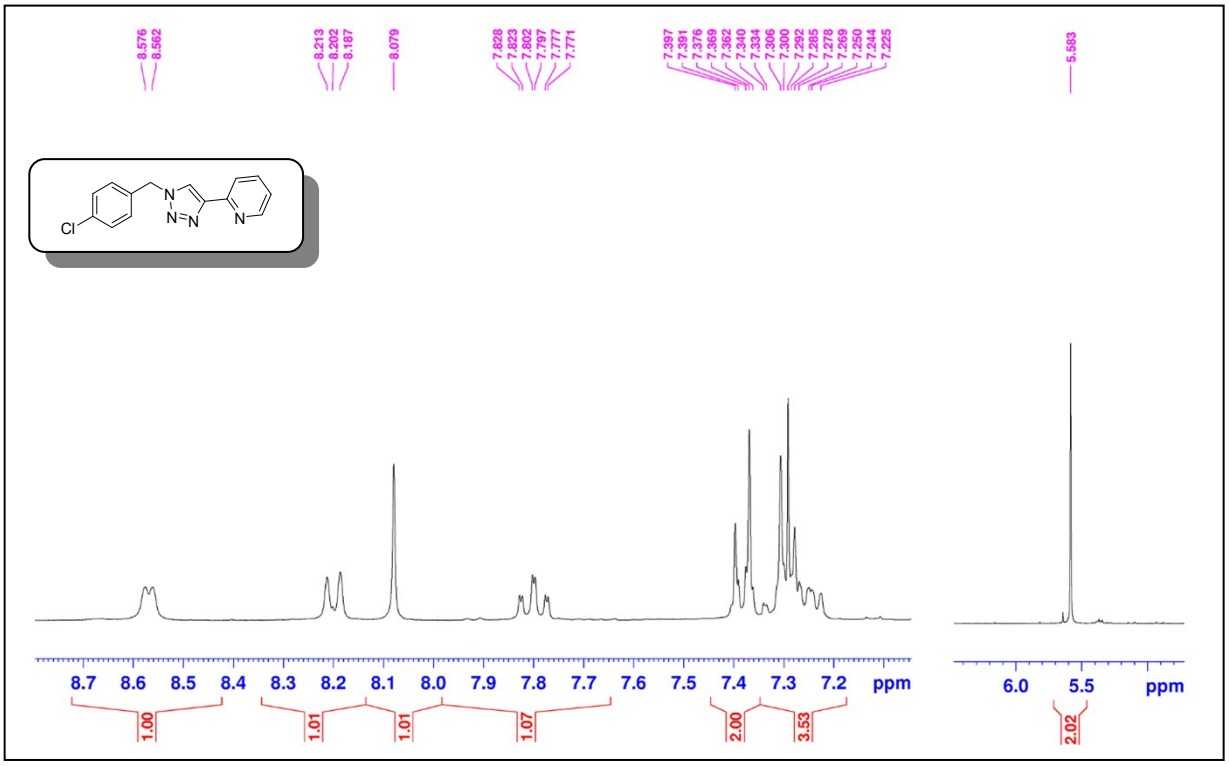


Figure 45: ^{1}H NMR (300 MHz, $CDCl_3$) of 2-(1-(4-chlorobenzyl)-1*H*-1,2,3-triazol-4-yl)pyridine (**4m**).

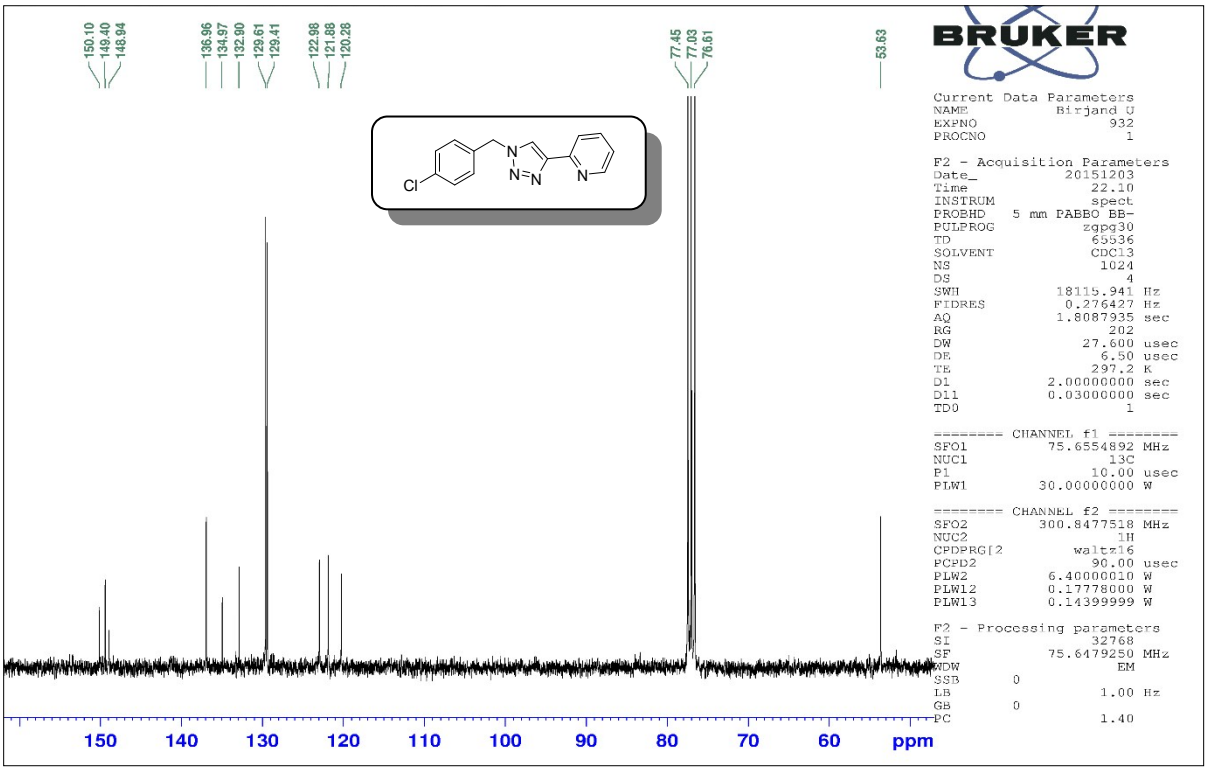


Figure 46: ^{13}C NMR (75MHz, $CDCl_3$) of 2-(1-(4-chlorobenzyl)-1*H*-1,2,3-triazol-4-yl)pyridine (**4m**).

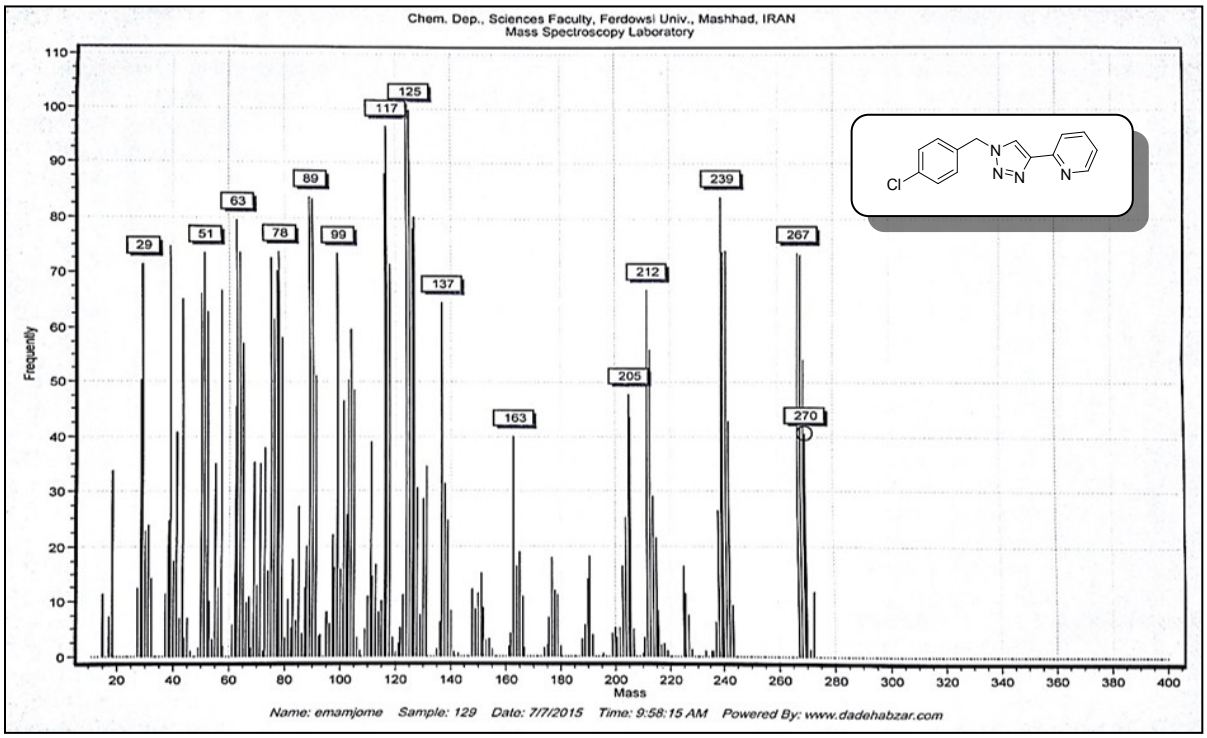


Figure 47: Mass spectrum of 2-(1-(4-chlorobenzyl)-1*H*-1,2,3-triazol-4-yl)pyridine (**4m**).

1-(4-nitrobenzyl)-4-phenyl-1*H*-1,2,3-triazole (4n) (0.25 g, 91%); white solid (crystals); mp 157–158 ºC (from EtOH) (Lit.[8] 156–157 ºC); FT-IR (KBr): ν_{max}/cm^{-1} 3126, 3080, 2962, 2855, 1607, 1517, 1462 (CH_2), 1443, 1348, 1218 (N–N=N–), 1186 (C–N), 1071, 1046, 1016, 972, 861, 806 (=C–H oop, triazole ring), 764, 726, 693, 513; ^1H NMR: δH (300 MHz; $CDCl_3$; Me_4Si) 8.25 (2 H, d, *J* = 8.7 Hz, Ar-H), 7.84 (2 H, d, *J* = 8.7 Hz, Ar-H), 7.79 (1 H, s, C=C<u>H</u>), 7.48-7.29 (5 H, m, Ar-H), 5.72 (2 H, s, C<u>H</u>$_2$); MS, *m/z* 280 (M^+, 5%), 279 (21, M – H), 278 (86, M – 2 H), 204 (40, M – C_6H_5), 177 (18, M – C_7H_5N), 135 (41, M – $C_8H_6N_3$), 116 (100, M – $C_7H_6N_3O_2$), 78 (85, M – $C_9H_7N_4O_2$), 29 (72, M – $C_{15}H_{12}N_2O_2$).

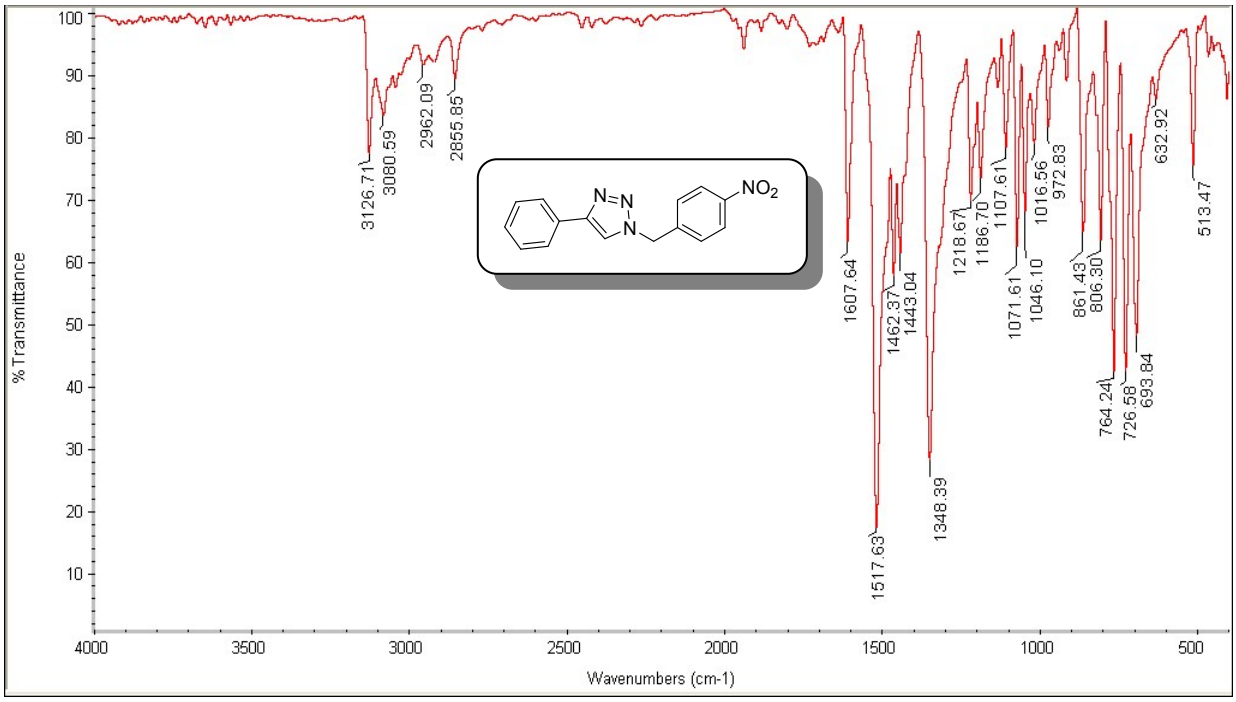


Figure 48: FT-IR (KBr) of 1-(4-nitrobenzyl)-4-phenyl-1*H*-1,2,3-triazole (**4n**).

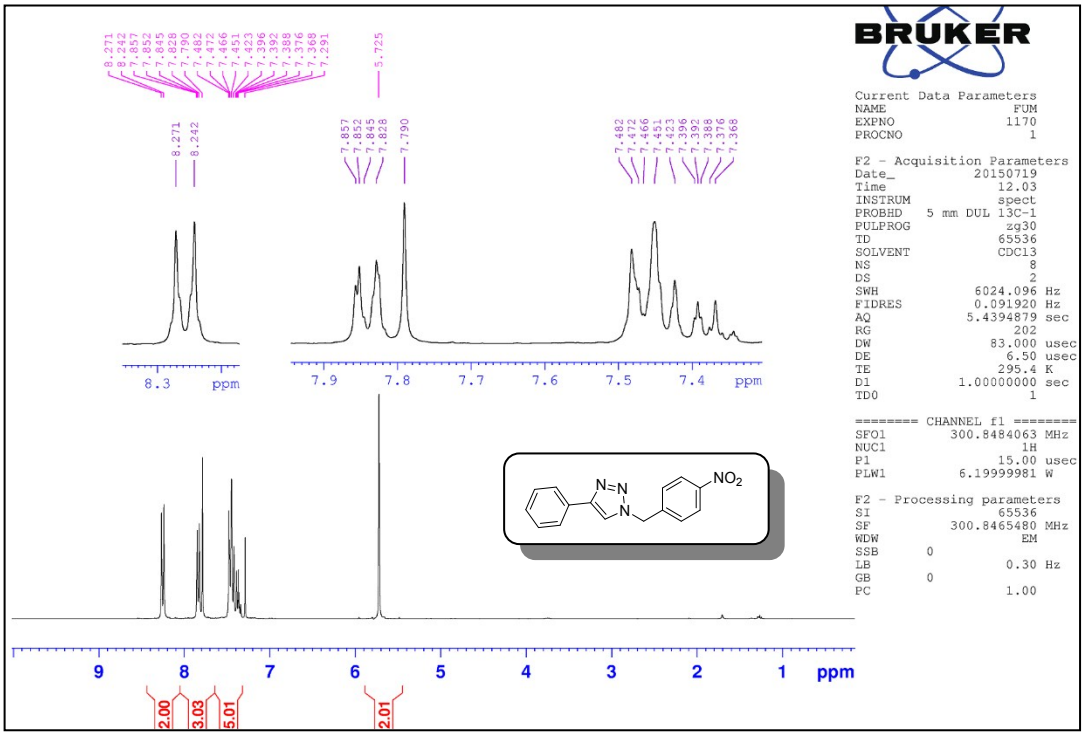


Figure 49: ^{1}H NMR (300 MHz, $CDCl_3$) of 1-(4-nitrobenzyl)-4-phenyl-1*H*-1,2,3-triazole (**4n**).

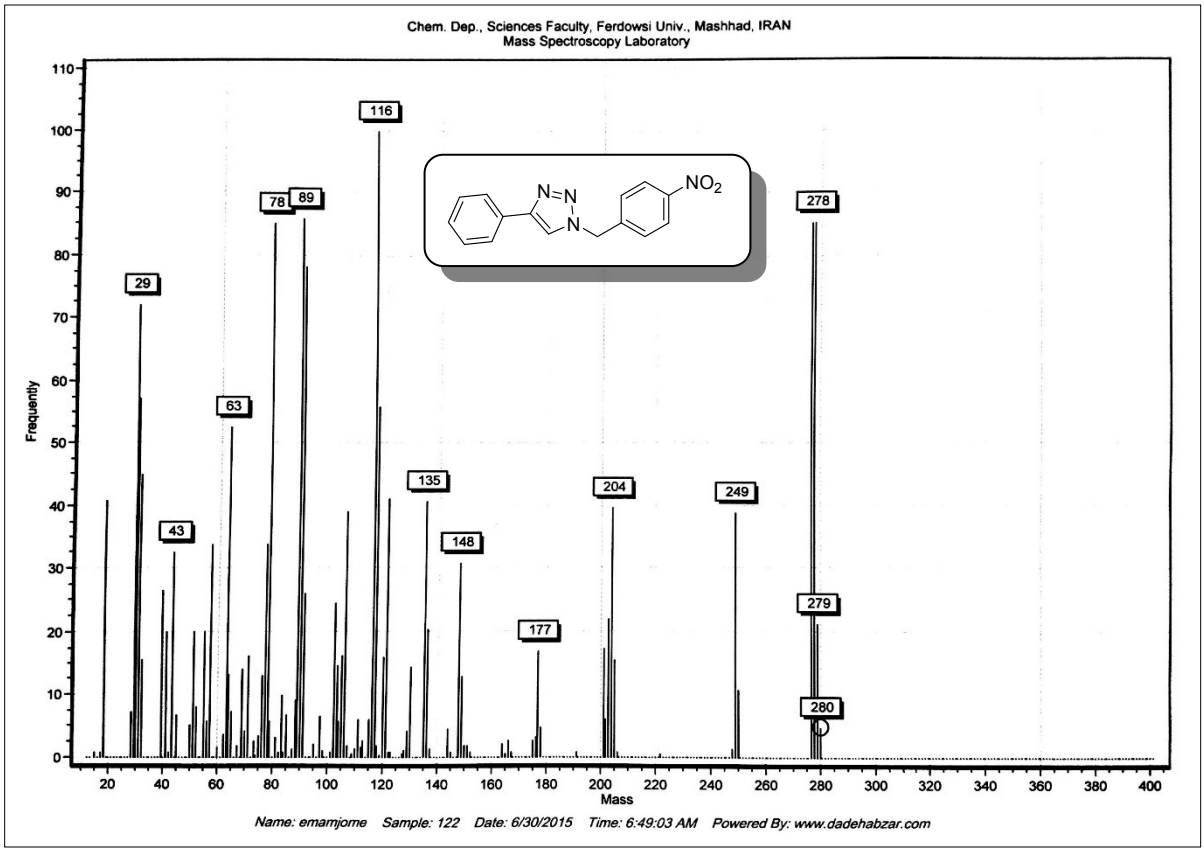


Figure 50: Mass spectrum of 1-(4-nitrobenzyl)-4-phenyl-1*H*-1,2,3-triazole (**4n**).

1-(4-nitrobenzyl)-4-(*p*-tolyl)-1*H*-1,2,3-triazole (4o) (0.26 g, 89%); white solid (crystals); mp 145–146 ºC (from EtOH) (Lit.[9] 145–147 ºC); FT-IR (KBr): ν_{max}/cm^{-1} 3094, 3051, 2925, 2855, 1603, 1515, 1455 (CH_2), 1429, 1348, 1287, 1222 (N–N=N–), 1110 (C–N), 1043, 980, 845, 818 (=C–H oop, triazole ring), 801, 730, 514; MS, *m/z* 294 (M^+, 5%), 293 (20, M – H), 292 (78, M – 2 H), 249 (43, M – NO_2), 204 (29, M – C_7H_7), 177 (55, M – C_8H_7N), 135 (77, M – $C_9H_8N_3$), 130 (100, M – $C_7H_6N_3O_2$), 103 (83, M – $C_8H_7N_4O_2$), 91 (68, M – $C_9H_7N_4O_2$), 77 (93, M – (NO_2 + $C_{10}H_{10}N_3$)), 29 (81, M – $C_{16}H_{14}N_2O_2$).

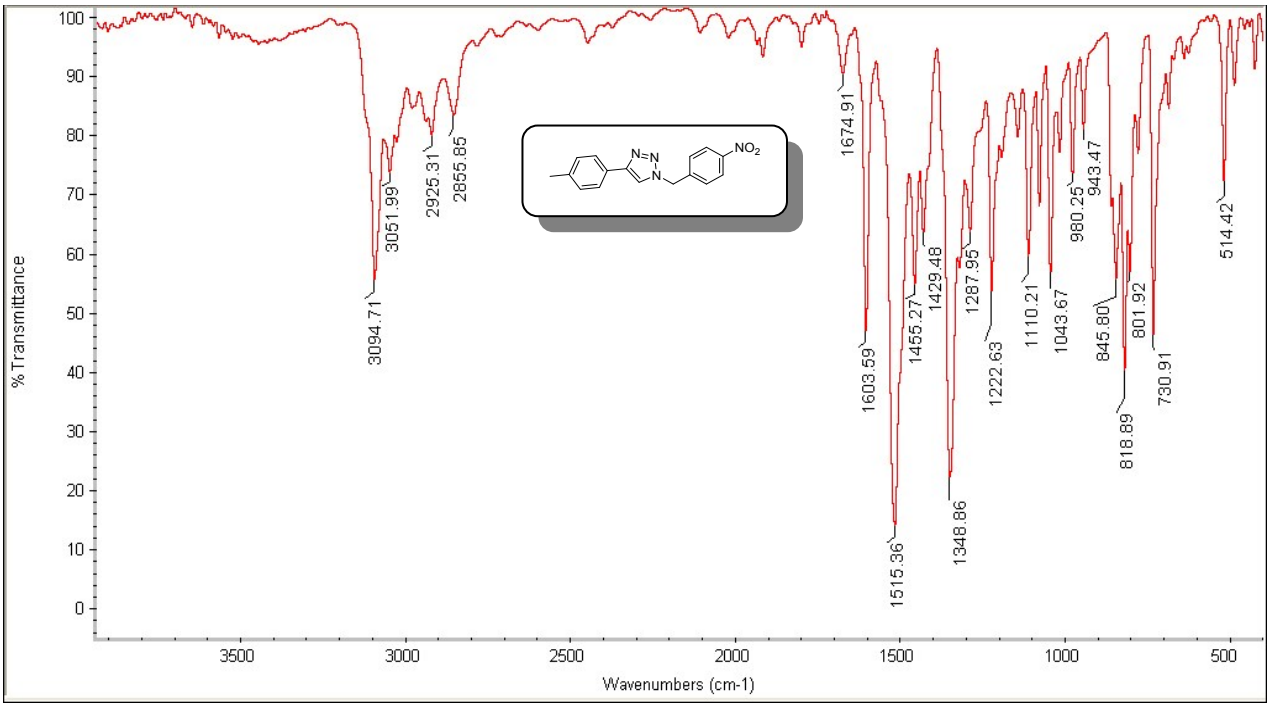


Figure 51: FT-IR (KBr) of 1-(4-nitrobenzyl)-4-(*p*-tolyl)-1*H*-1,2,3-triazole (**4o**).

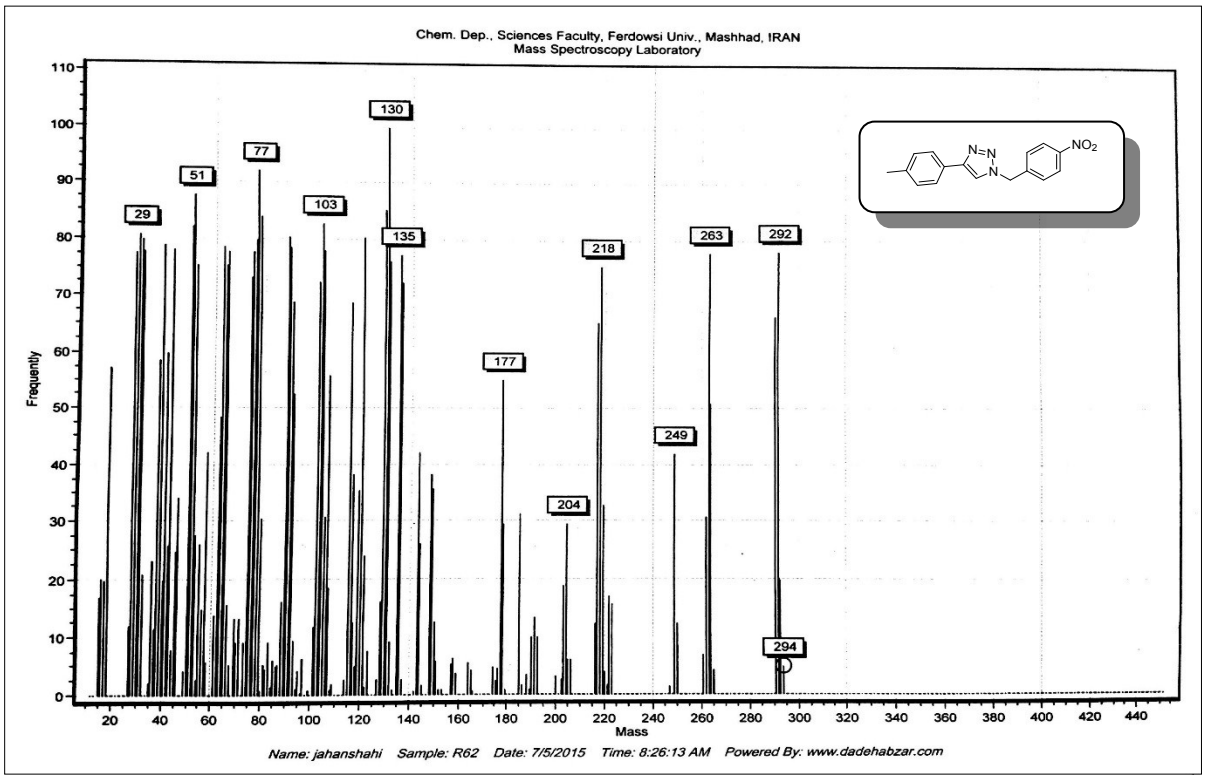


Figure 52: Mass spectrum of 1-(4-nitrobenzyl)-4-(*p*-tolyl)-1*H*-1,2,3-triazole (**4o**).

4-(4-methoxyphenyl)-1-(4-nitrobenzyl)-1*H*-1,2,3-triazole (4p) (0.26 g, 86%); white solid (crystals); mp 94–96 ºC (from EtOH) (Lit.[10] 95–98 ºC); FT-IR (KBr): ν_{max}/cm^{-1} 3125, 3092, 3002, 2941, 2839, 1611, 1556, 1530, 1502, 1452 (CH_2), 1343, 1248 (N–N=N–), 1222, 1174 (C–N), 1107, 1027, 980, 819 (=C–H oop, triazole ring), 845, 727, 608, 538; ^{1}H NMR: δH (300 MHz; $CDCl_3$; Me_4Si) 8.21 (2 H, d, *J* = 8.4 Hz, Ar-H), 7.84 (1 H, s, C=C<u>H</u>), 7.73 (2 H, d, *J* = 8.7 Hz, Ar-H), 7.43 (2 H, d, *J* = 8.4 Hz, Ar-H), 6.94 (2 H, d, *J* = 8.4 Hz, Ar-H), 5.68 (2 H, s, C<u>H</u>$_2$), 3.83 (3 H, s, OC<u>H</u>$_3$); MS, *m/z* 310 (M^+, 5%), 309 (21, M – H), 308 (86, M – 2 H), 279 (95, M – CH_3O), 265 (23, M – NO_2), 146 (97, M – $C_7H_6N_3O_2$), 119 (44, M – $C_8H_7N_4O_2$), 77 (34, M – (NO_2 + $C_{10}H_{10}N_3O$)), 29 (97, M – $C_{16}H_{14}N_2O_3$).

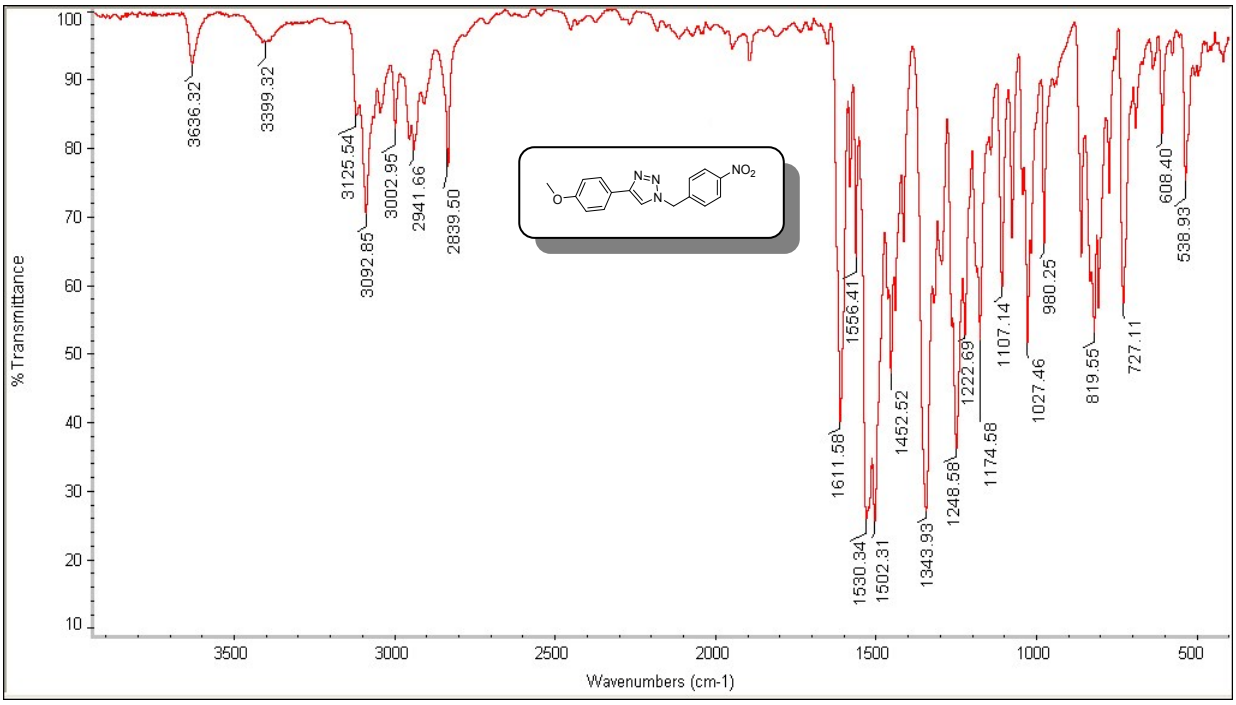


Figure 53: FT-IR (KBr) of 4-(4-methoxyphenyl)-1-(4-nitrobenzyl)-1*H*-1,2,3-triazole (**4p**).

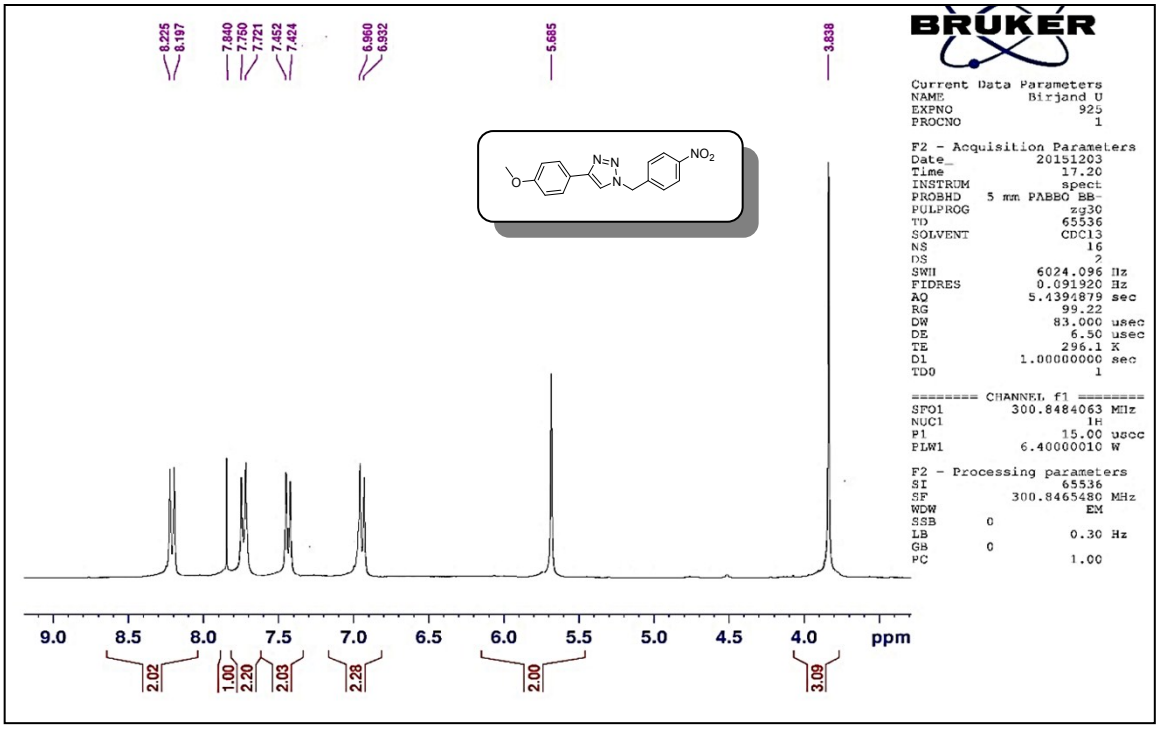


Figure 54: ^{1}H NMR (300 MHz, $CDCl_3$) of 4-(4-methoxyphenyl)-1-(4-nitrobenzyl)-1*H*-1,2,3-triazole (**4p**).

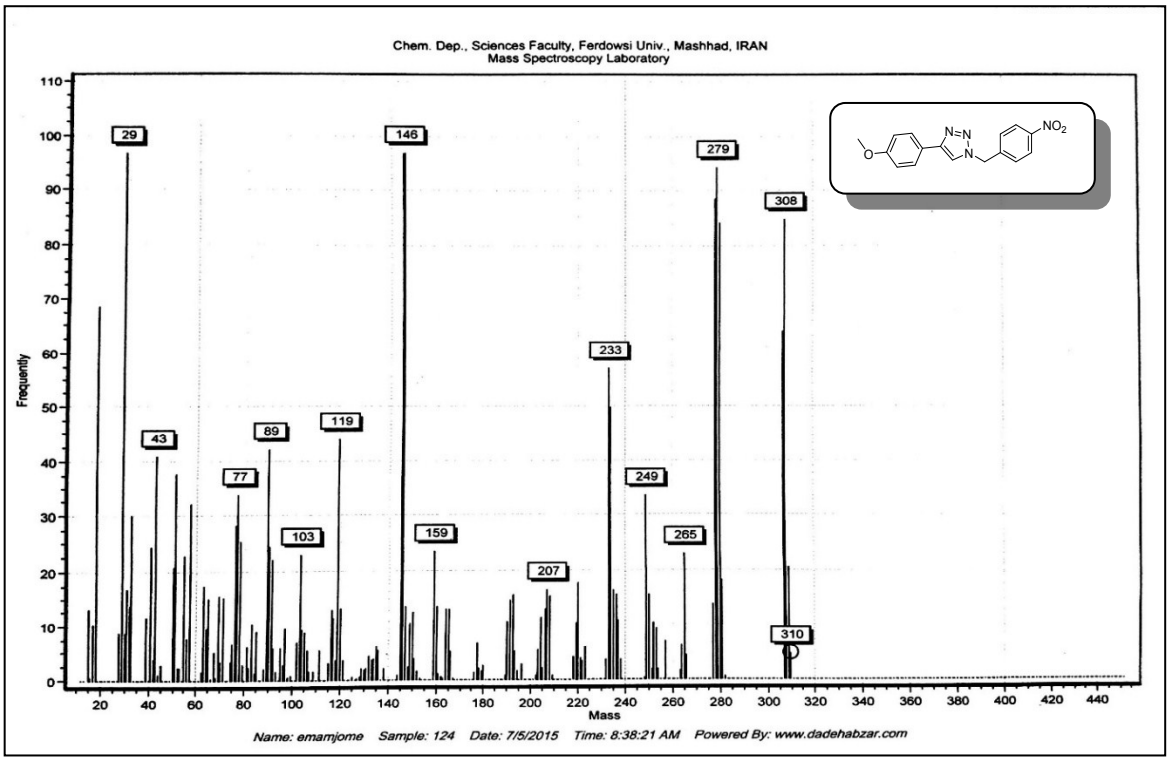


Figure 55: Mass spectrum of 4-(4-methoxyphenyl)-1-(4-nitrobenzyl)-1*H*-1,2,3-triazole (**4p**).

4-(4-(*tert*-butyl)phenyl)-1-(4-nitrobenzyl)-1*H*-1,2,3-triazole (4q) (0.29 g, 86%); white solid (crystals); mp 145–147 ºC (from EtOH); elemental analysis Found: C, 67.67; H, 5.67; N, 16.92. Calc. for $C_{19}H_{20}N_4O_2$: C, 67.84; H, 5.99; N, 16.66%; FT-IR (KBr): ν_{max}/cm^{-1} 3117, 3084, 2962, 2900, 2865,1604, 1516, 1495, 1457 (CH_2), 1346, 1220 (N–N=N–), 1109 (C–N), 1072, 1044, 976, 835 (=C–H oop, triazole ring), 782, 739, 723, 559; ^{1}H NMR: δH (300 MHz; $CDCl_3$; Me_4Si) 8.25 (2 H, d, *J* = 8.7 Hz, Ar-H), 7.77 (3 H, d, *J* = 7.8 Hz, Ar-H, C=C<u>H</u>), 7.48-7.43 (4 H, m, Ar-H), 5.72 (2 H, s, C<u>H</u>$_2$), 1.36 (9 H, s, 3 C<u>H</u>$_3$); ^{13}C NMR: δC (75 MHz; $CDCl_3$; Me_4Si) 151, 148.74, 148.08, 141, 128, 127, 125.64, 125.50, 124, 119, 53, 34, 31; MS, *m/z* 336 (M^+, 5%), 335 (10, M – H), 334 (28, M – 2 H), 333 (48, M – 3 H), 332 (40, M – 4 H), 290 (20, M – NO_2), 203 (17, M – $C_{10}H_{13}$), 171 (100, M – $C_7H_6N_3O_2$), 57 (83, M – $C_{15}H_{11}N_4O_2$), 28 (37, M – $C_{19}H_{20}N_2O_2$).

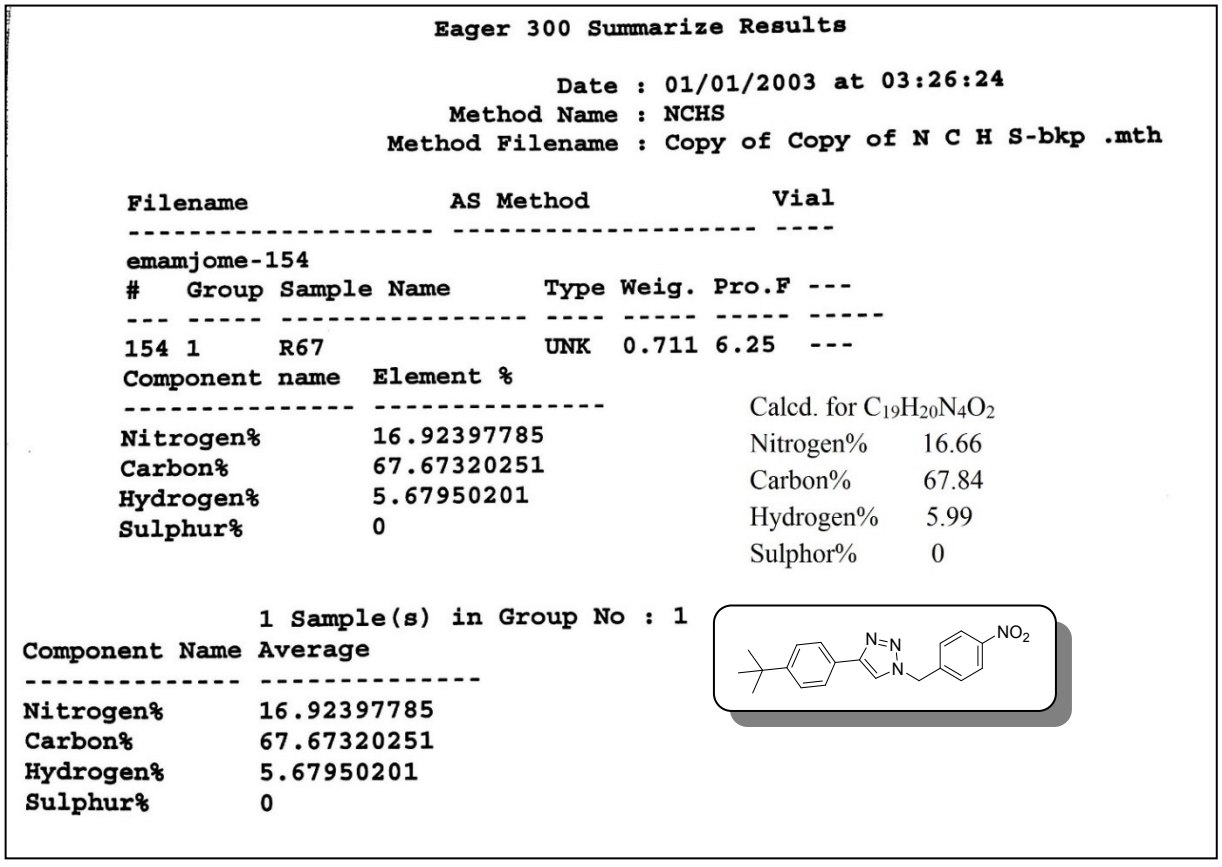


Figure 56: Elemental analysis of 4-(4-(*tert*-butyl)phenyl)-1-(4-nitrobenzyl)-1*H*-1,2,3-triazole (**4q**).

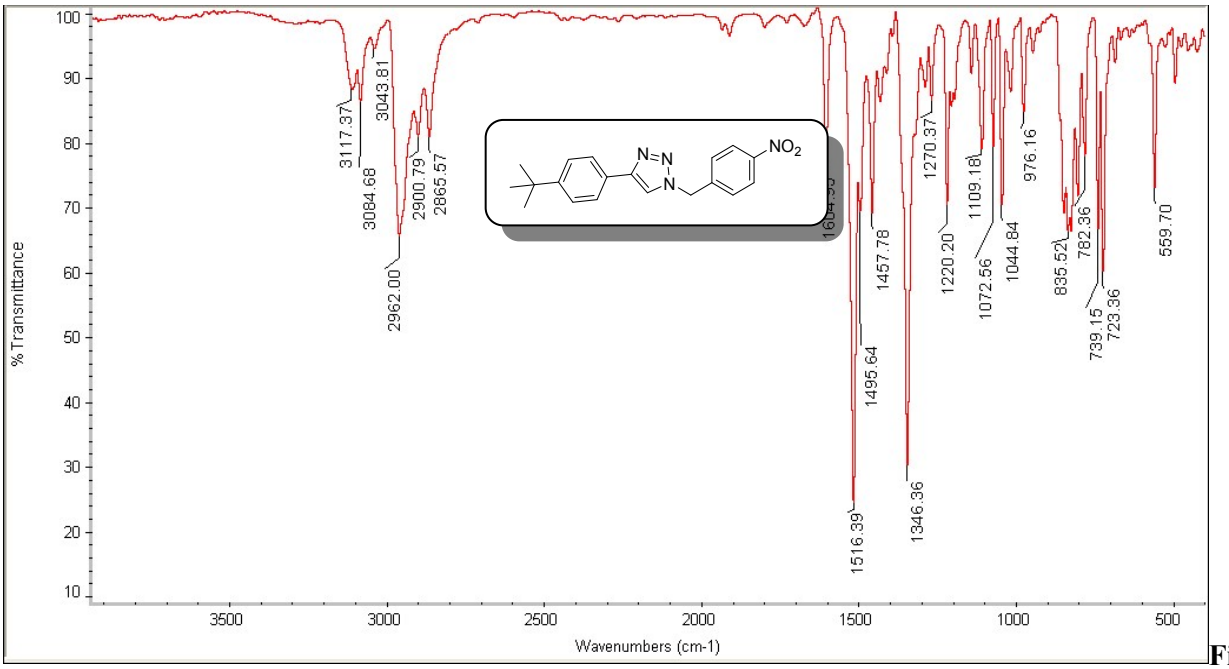


Figure 57: FT-IR (KBr) of 4-(4-(*tert*-butyl)phenyl)-1-(4-nitrobenzyl)-1*H*-1,2,3-triazole (**4q**).

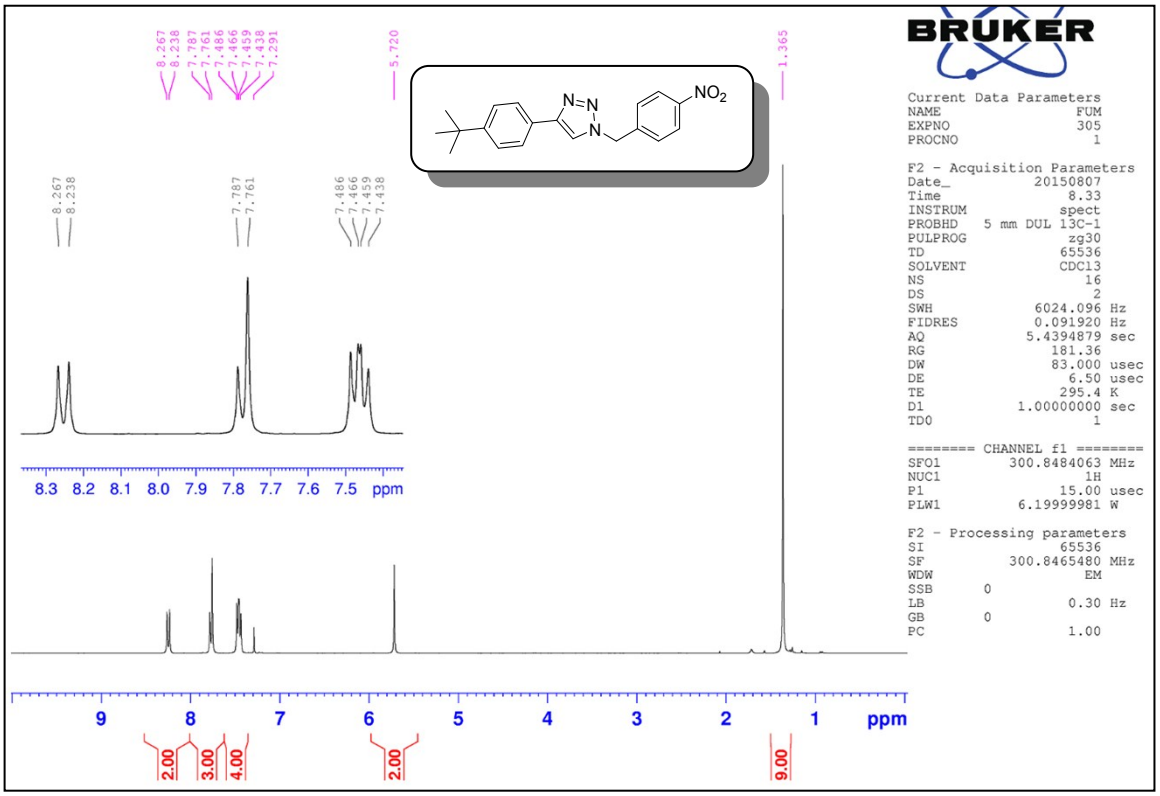


Figure 58: ^{1}H NMR (300 MHz, $CDCl_3$) of 4-(4-(*tert*-butyl)phenyl)-1-(4-nitrobenzyl)-1*H*-1,2,3-triazole (**4q**).

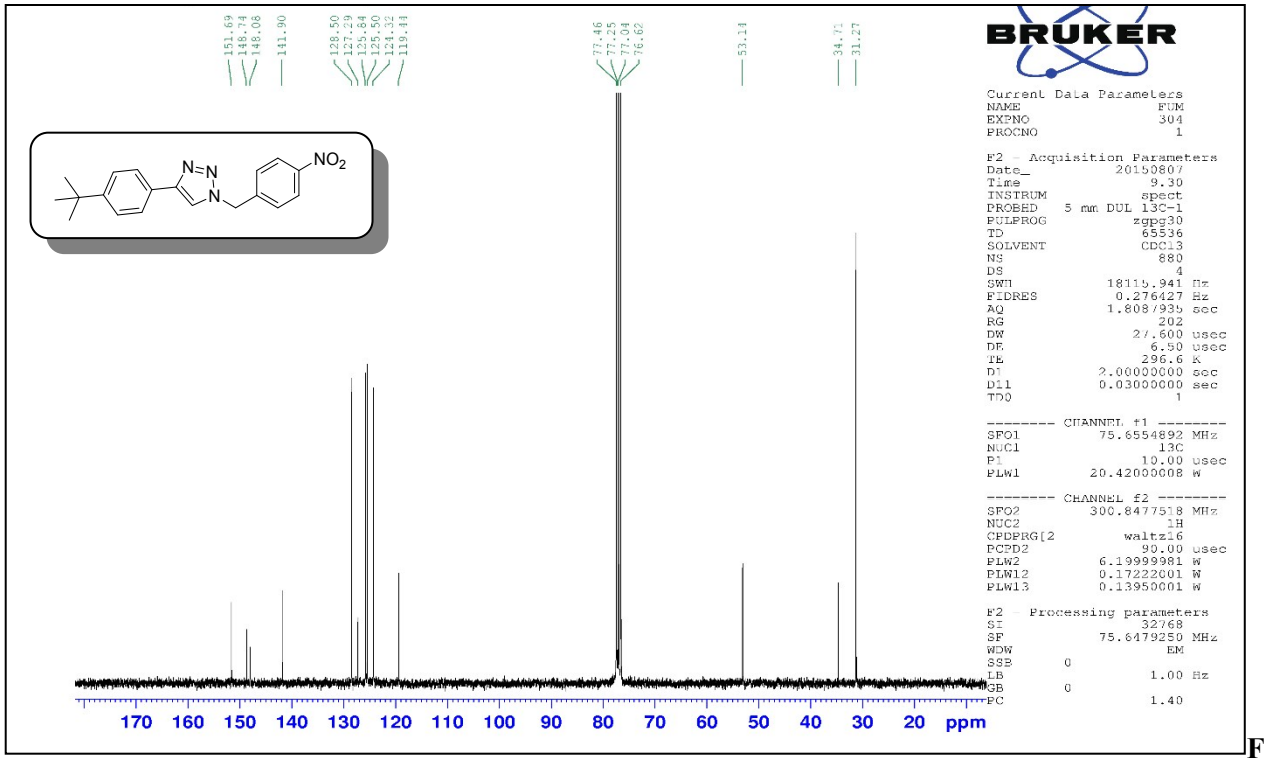


Figure 59: ^{13}C NMR (75 MHz, $CDCl_3$) of 4-(4-(*tert*-butyl)phenyl)-1-(4-nitrobenzyl)-1*H*-1,2,3-triazole (**4q**).

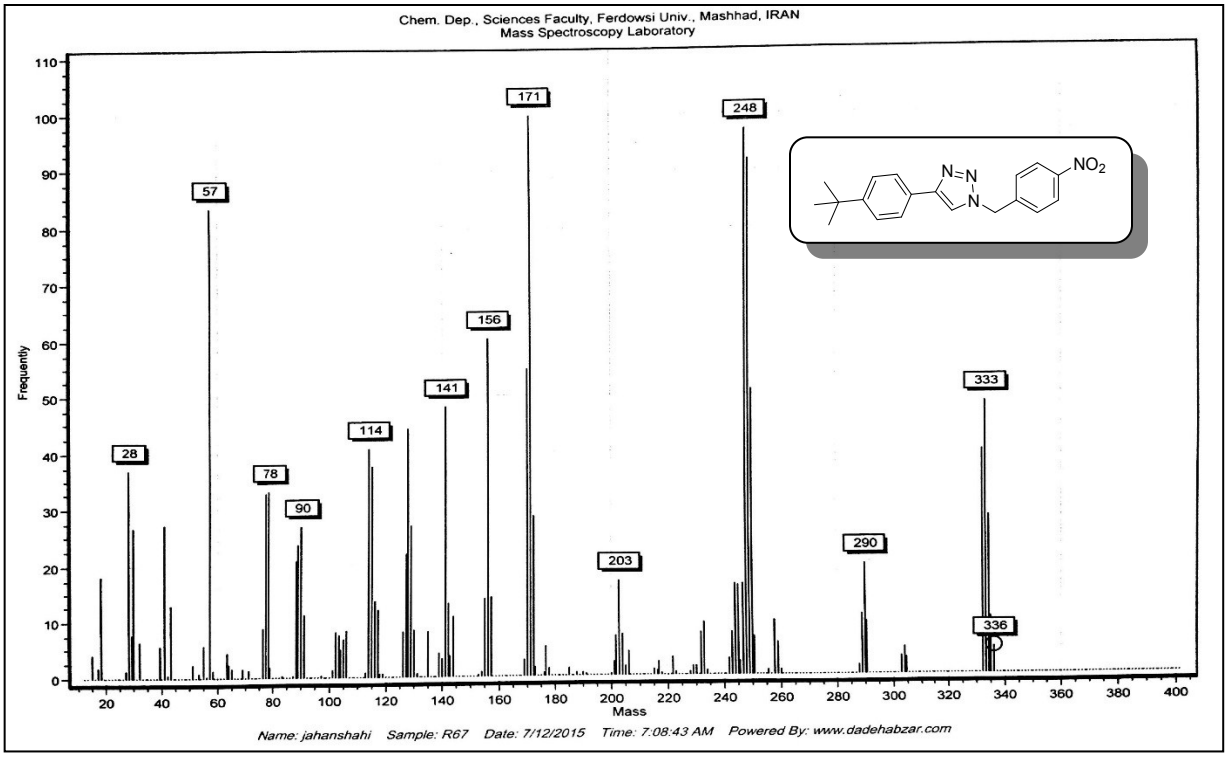


Figure 60: Mass spectrum of 4-(4-(*tert*-butyl)phenyl)-1-(4-nitrobenzyl)-1*H*-1,2,3-triazole (**4q**).

2-(1-(4-nitrobenzyl)-1*H*-1,2,3-triazol-4-yl)pyridine (4r) (0.23 g, 84%); yellow solid (crystals); mp 175–177 ºC (from EtOH) (Lit.[10] 176–179 ºC); 3114, 3088, 3056, 3007, 2851, 1603, 1511, 1469 (CH_2), 1418, 1348, 1229 (N–N=N–), 1200, 1147 (C–N), 1078, 1046, 995, 859, 808 (=C–H oop, triazole ring), 786, 729, 510; MS, *m/z* 281 (M^+, 5%), 280 (27, M – H), 278 (20, M – 3 H), 177 (10, M – $C_6H_4N_2$), 130 (99, M – $C_7H_6N_2O_2$), 117 (100, M – $C_7H_6N_3O_2$), 103 (68, M – $C_7H_6N_4O_2$), 90 (96, M – (NO_2 + $C_7H_5N_4$)), 78 (98, M – $C_9H_7N_4O_2$), 28 (74, M – $C_{14}H_{11}N_3O_2$).

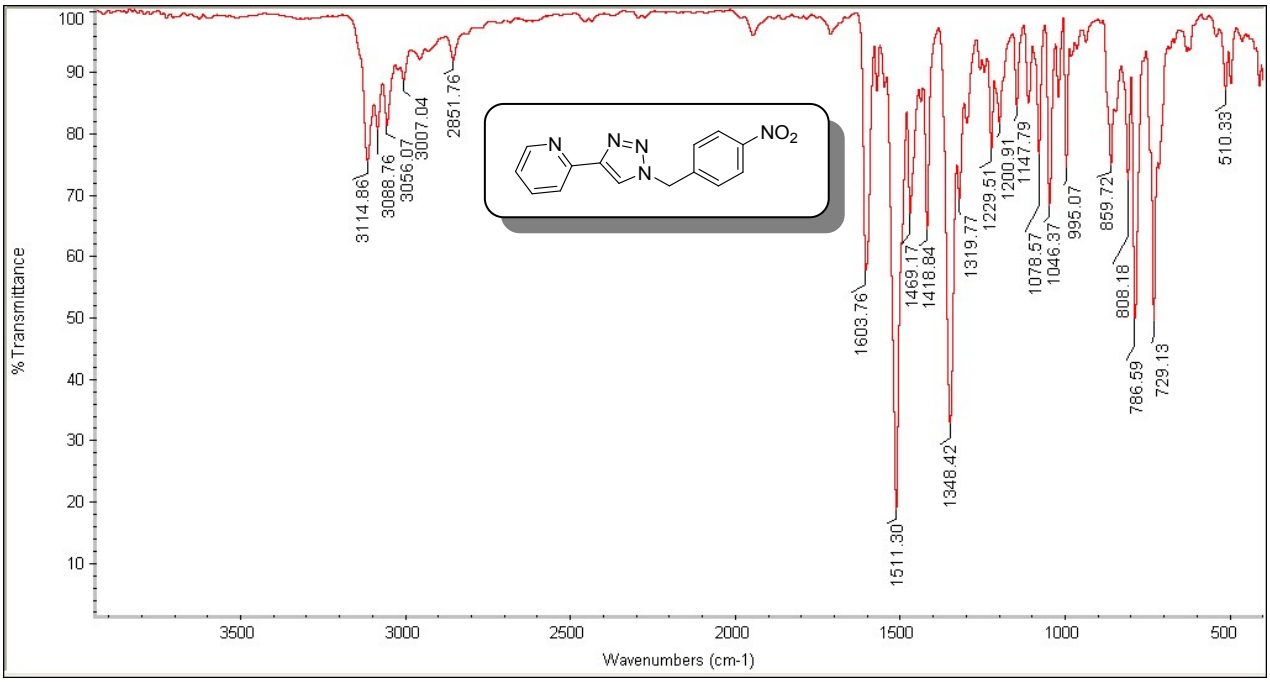


Figure 61: FT-IR (KBr) of 2-(1-(4-nitrobenzyl)-1*H*-1,2,3-triazol-4-yl)pyridine (**4r**).

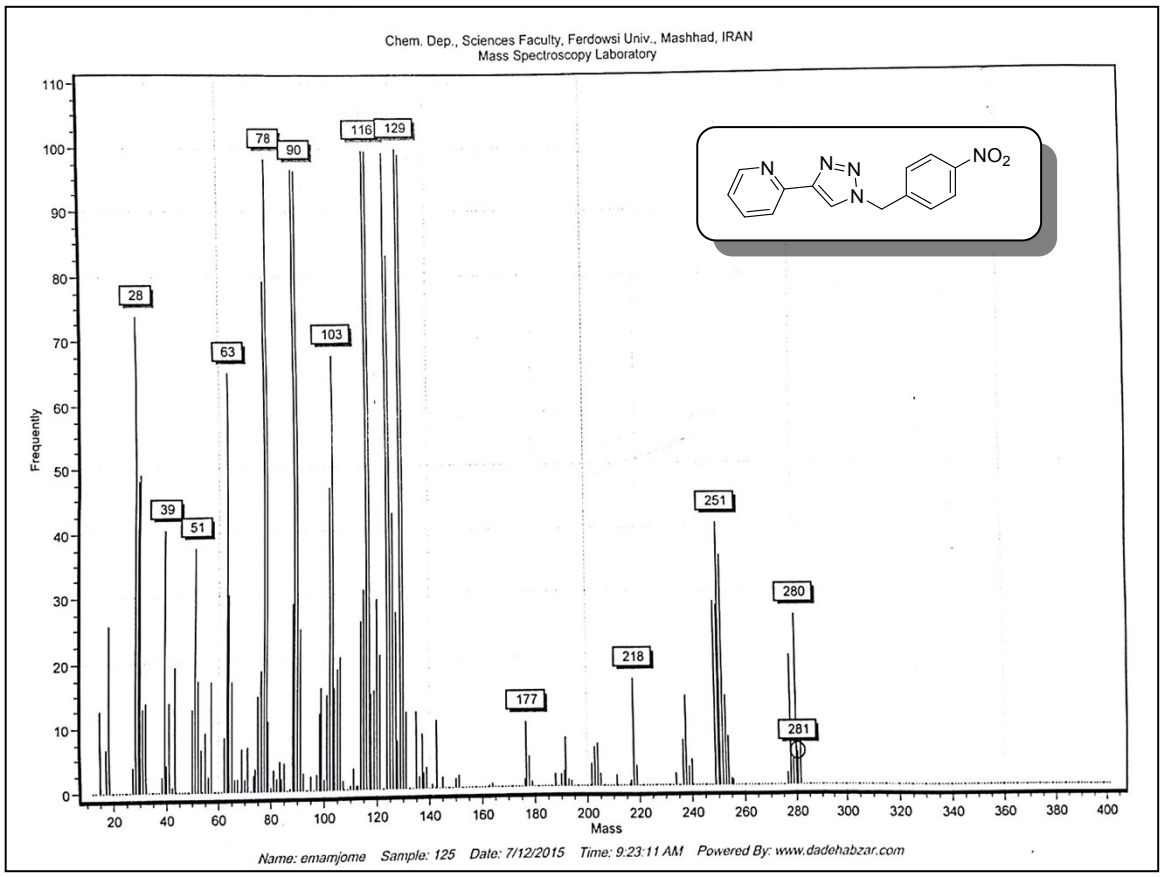


Figure 62: Mass spectrum of 2-(1-(4-nitrobenzyl)-1*H*-1,2,3-triazol-4-yl)pyridine (**4r**).

1-allyl-4-phenyl-1*H*-1,2,3-triazole (4s) (0.16 g, 90%); yellow (crystals); mp 40 ºC (from EtOH) (Lit.[11] 40–41 ºC); FT-IR (KBr): ν_{max}/cm^{-1} 3131, 3084, 3035, 2953, 2924, 2853, 1642, 1609, 1485, 1464 (CH_2), 1359, 1225 (N–N=N–), 1171 (C–N), 1045, 990, 913, 810 (=C–H oop, triazole ring), 763, 693, 517; MS, *m/z* 185 (M^+, 5%), 184 (38, M – H), 183 (27, M – 2 H), 116 (78, M – $C_3H_5N_2$), 83 (75, M – C_8H_6), 69 (76, M – C_8H_6N), 55 (100, M – $C_8H_6N_2$), 41 (77, M – $C_8H_6N_3$), 28 (72, M – $C_{11}H_{11}N$).

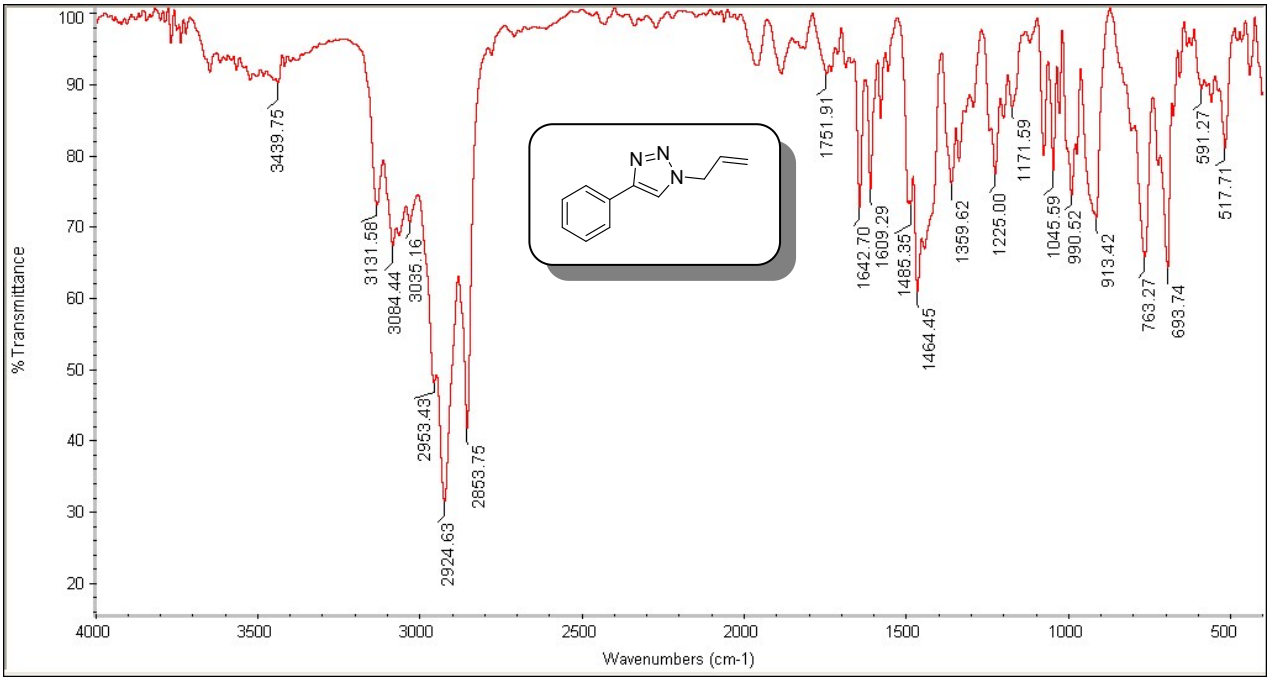


Figure 63: FT-IR (KBr) of 1-allyl-4-phenyl-1H-1,2,3-triazole (**4s**).

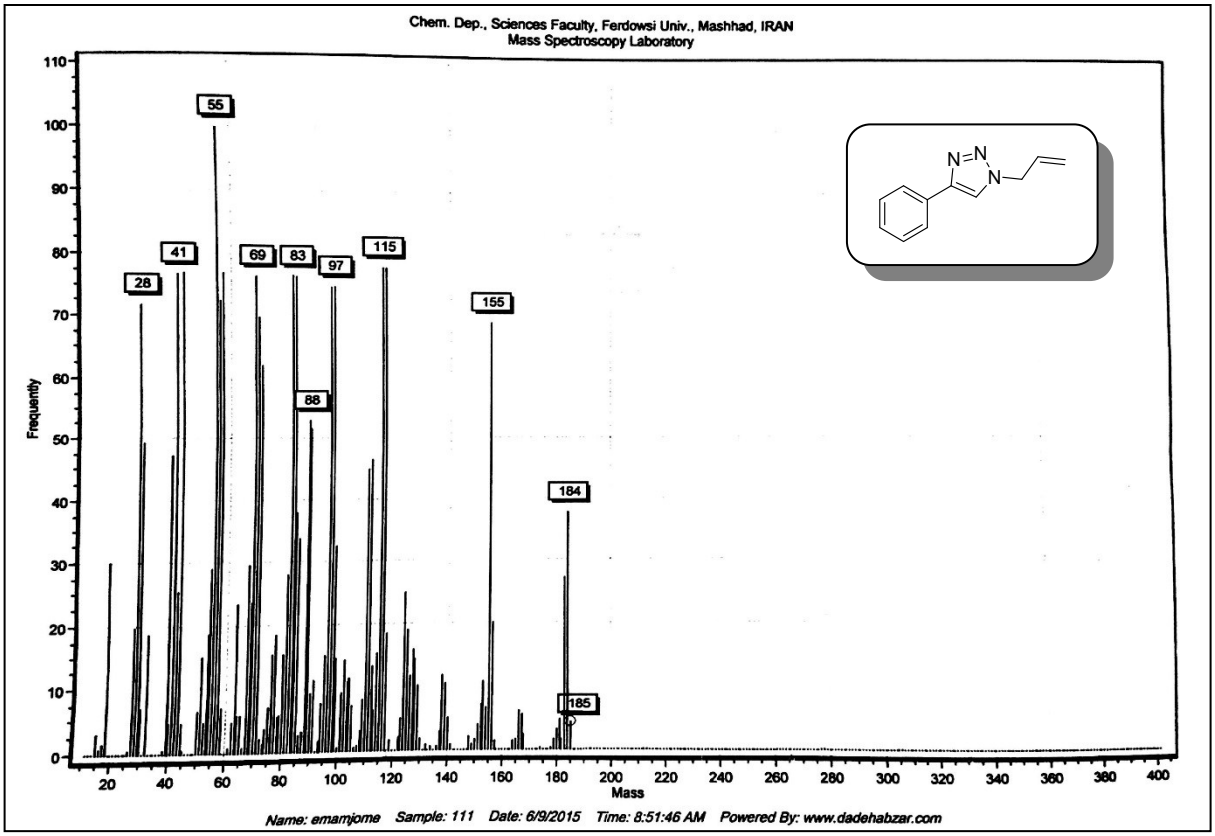


Figure 64: Mass spectrum of 1-allyl-4-phenyl-1H-1,2,3-triazole (**4s**).

1-allyl-4-(*p*-tolyl)-1*H*-1,2,3-triazole[12] **(4t)** (0.17 g, 87%); white solid (crystals); mp 82-83 ºC (from EtOH); FT-IR (KBr): ν_{max}/cm^{-1} 3125, 3106, 3027, 2978, 2917, 2859, 1642, 1497, 1451 (CH_2), 1339, 1217 (N–N=N–), 1171 (C–N), 1071, 1048, 988, 933, 817 (=C–H oop, triazole ring), 768, 726, 519; ^{1}H NMR: δH (400 MHz; $CDCl_3$; Me_4Si) 7.73-7.67 (2 H, m, Ar-H, C=C<u>H</u>), 7.26-7.16 (3 H, m, Ar-H), 6.06-6.04 (1 H, m, C=C<u>H</u>), 5.40-5.33 (2 H, m, <u>H$_2$</u>C=CH), 5.03-4.97 (2 H, m, C<u>H$_2$</u>), 2.35 (3 H, d, J = 9.6 Hz, C<u>H$_3$</u>); MS, *m/z* 199 (M^+, 36%), 198 (76, M – H), 197 (75, M – 2 H), 170 (56, M – N_2), 143 (36, M – C_3H_5N), 130 (87, M – $C_3H_5N_2$), 103 (77, M – $C_4H_6N_3$), 91 (39, M – $C_5H_6N_3$), 77 (78, M – (CH_3 + $C_5H_6N_3$)), 41 (73, M – $C_9H_8N_3$), 28 (44, M – $C_{12}H_{13}N$).

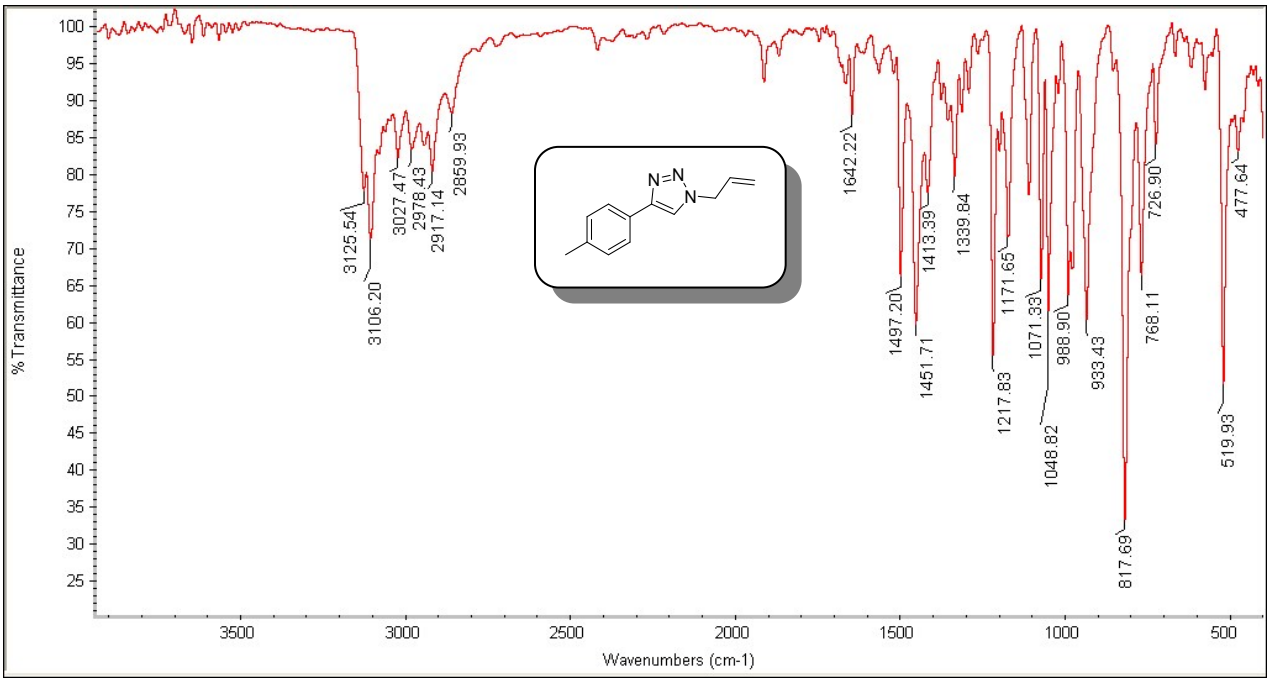


Figure 65: FT-IR (KBr) of 1-allyl-4-(*p*-tolyl)-1*H*-1,2,3-triazole (**4t**).

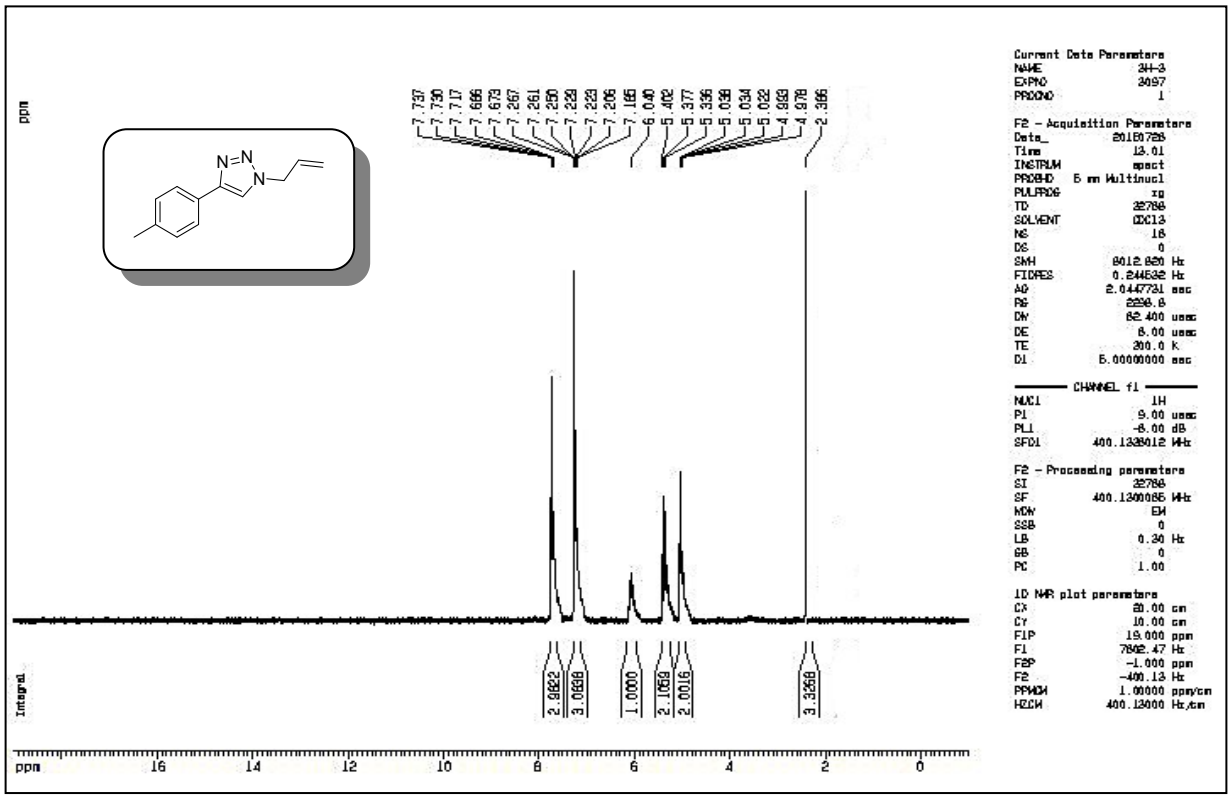
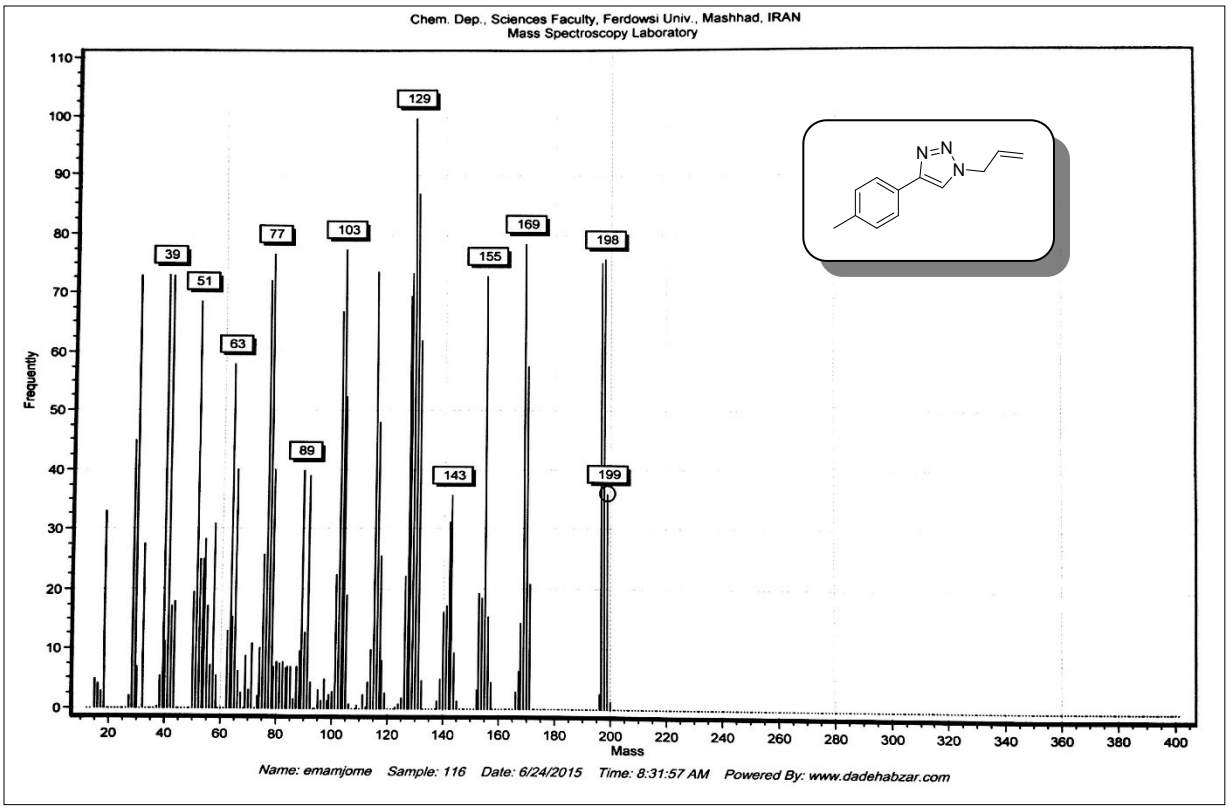


Figure 66: ^{1}H NMR (400 MHz, $CDCl_3$) of 1-allyl-4-(*p*-tolyl)-1*H*-1,2,3-triazole (**4t**).



1-allyl-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (4u) (0.18 g, 84%); white solid (crystals); mp 90–91 ºC (from EtOH) (Lit.[13] 88–89 ºC); FT-IR (KBr): ν_{max}/cm^{-1} 3121, 3101, 3051, 2949, 2835, 1618, 1562, 1501, 1455 (CH_2), 1303, 1250 (N–N=N–), 1218, 1175 (C–N), 1078, 1031, 976, 913, 823 (=C–H oop, triazole ring), 775, 620, 538; ^{1}H NMR: δH (300 MHz; $CDCl_3$; Me_4Si) 7.77 (2 H, d, J = 8.7 Hz, Ar-H), 7.0 (1 H, s, C=C<u>H</u>), 6.97 (2 H, d, J = 8.7 Hz, Ar-H), 6.14-6.01 (1 H, m, H_2C=C<u>H</u>), 5.40-5.33 (2 H, m, <u>H_2</u>C=CH), 5.02 (2 H, d, J = 6 Hz, C<u>H_2</u>), 3.85 (3 H, s, C<u>H_3</u>); ^{13}C NMR: δC (75 MHz; $CDCl_3$; Me_4Si) 159, 147, 131, 127, 123, 120, 118, 114, 55, 52; MS, *m/z* 215 (M^+, 4%), 214 (50, M – H), 213 (96, M – 2 H), 171 (68, M – CH_2), 145 (100, M – C_3H_5), 131 (41, M – C_3H_5N), 117 (41, M – C_4H_6N), 103 (33, M – $C_3H_5N_3$), 76 (38, M – $C_5H_6N_3$), 41 (51, M – $C_8H_6N_3$), 28 (100, M – $C_{11}H_{11}N$).

Figure 67: Mass spectrum of 1-allyl-4-(*p*-tolyl)-1*H*-1,2,3-triazole (**4t**).

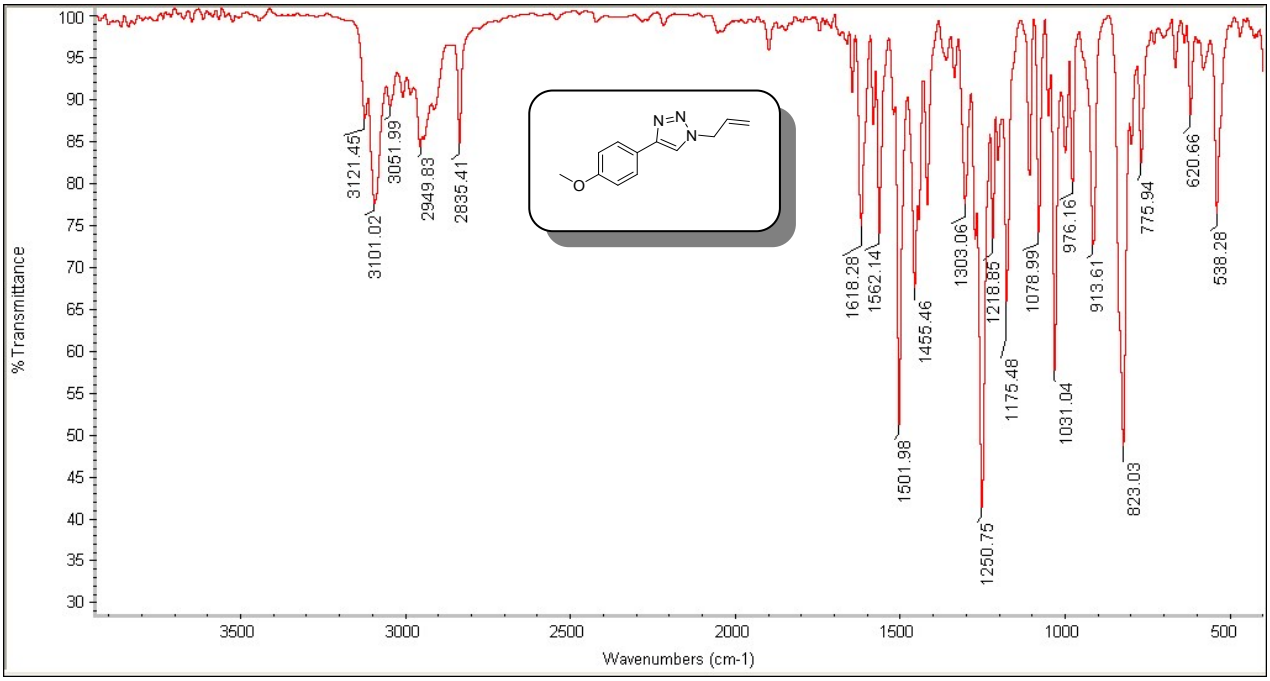


Figure 68: FT-IR (KBr) of 1-allyl-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (**4u**).

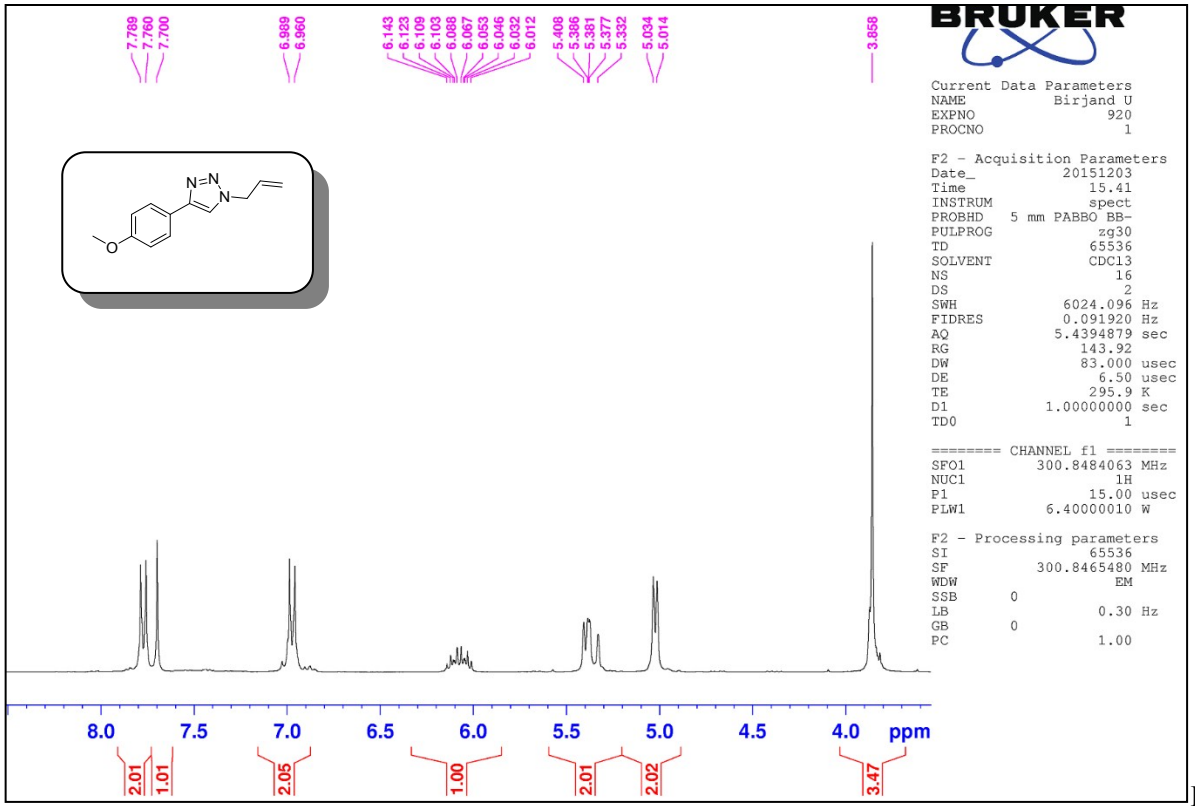


Figure 69: ^{1}H NMR (300 MHz, $CDCl_3$) of 1-allyl-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (**4u**).

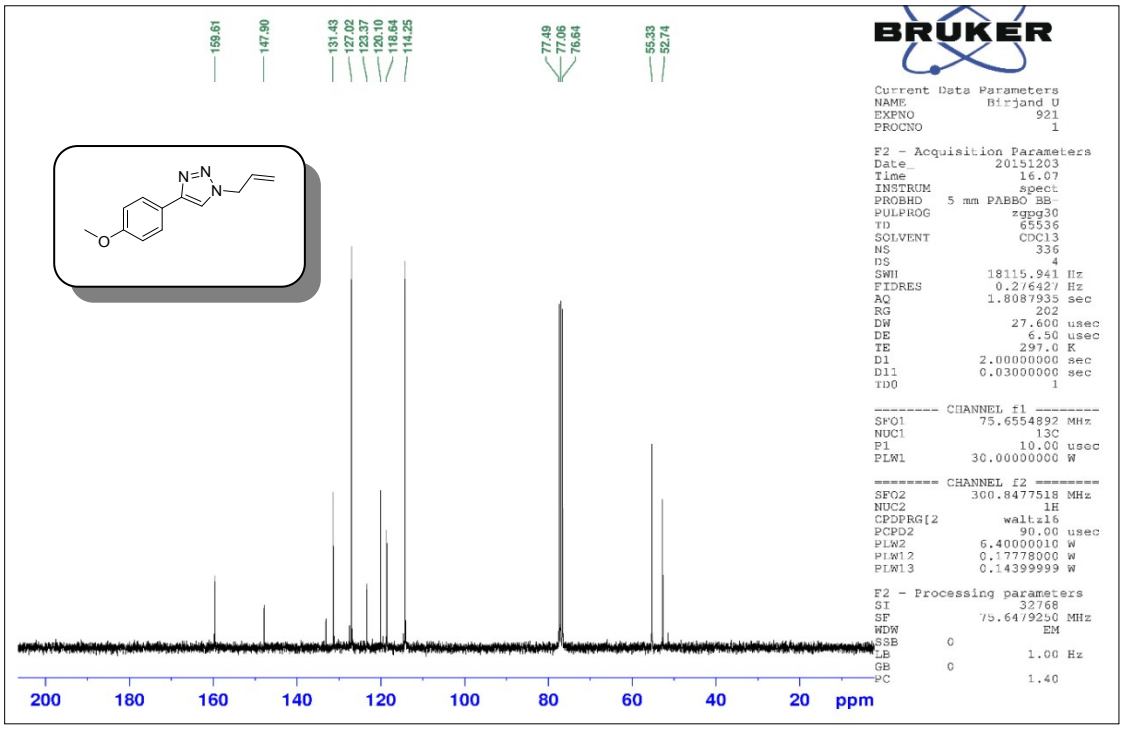


Figure 70: ^{13}C NMR (75 MHz, $CDCl_3$) of 1-allyl-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (**4u**).

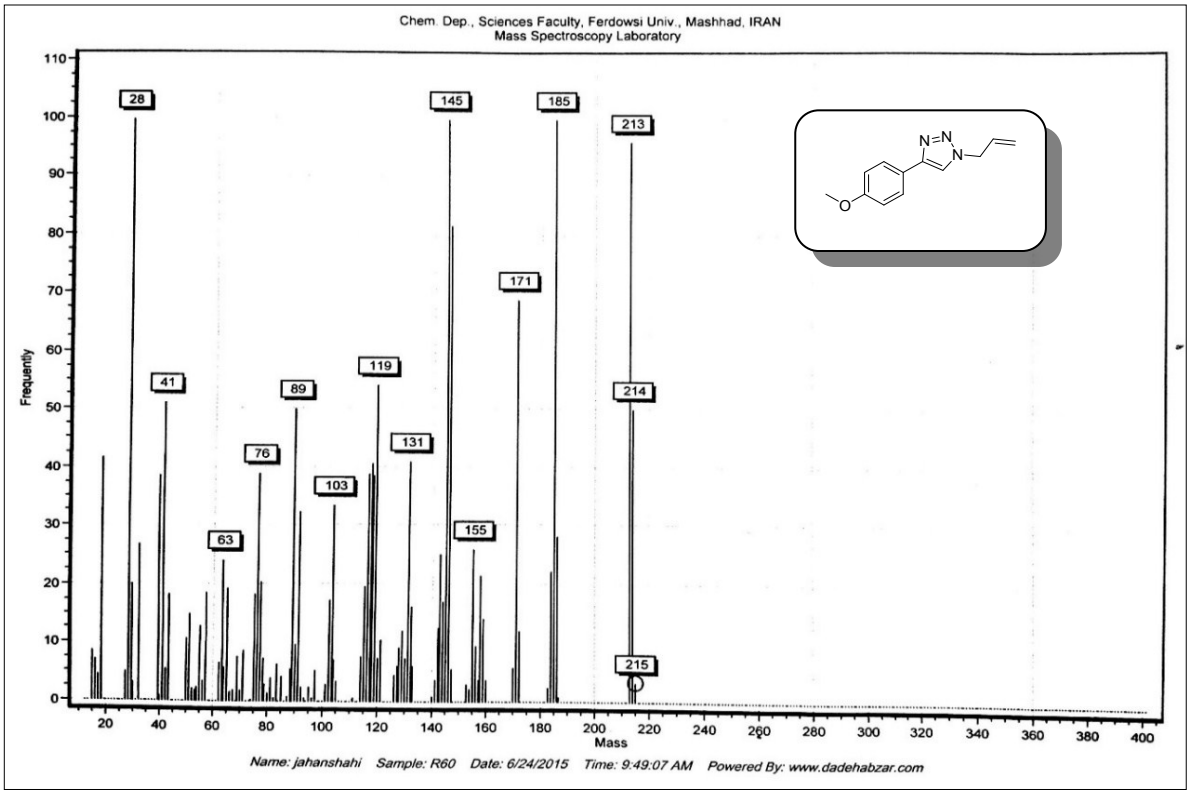


Figure 71: Mass spectrum of 1-allyl-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (**4u**).

1-allyl-4-(4-(*tert*-butyl)phenyl)-1*H*-1,2,3-triazole[12] **(4v)** (0.19 g, 82%); yellow (Oil); FT-IR (KBr): ν_{max}/cm^{-1} 2960, 2903, 2866, 1486, 1459 (CH_2), 1362, 1267 (N–N=N–), 1116 (C–N), 1021, 986, 834 (=C–H oop, triazole ring), 616, 561; MS, *m/z* 241 (M^+, 4%), 239 (16, M – 2 H), 172 (32, M – $C_3H_5N_2$), 142 (46, M – (C_3H_5 + C_4H_9)), 57 (41, M – $C_{11}H_{10}N_3$), 41 (44, M – $C_{12}H_{14}N_3$), 28 (51, M – $C_{15}H_{19}N$).

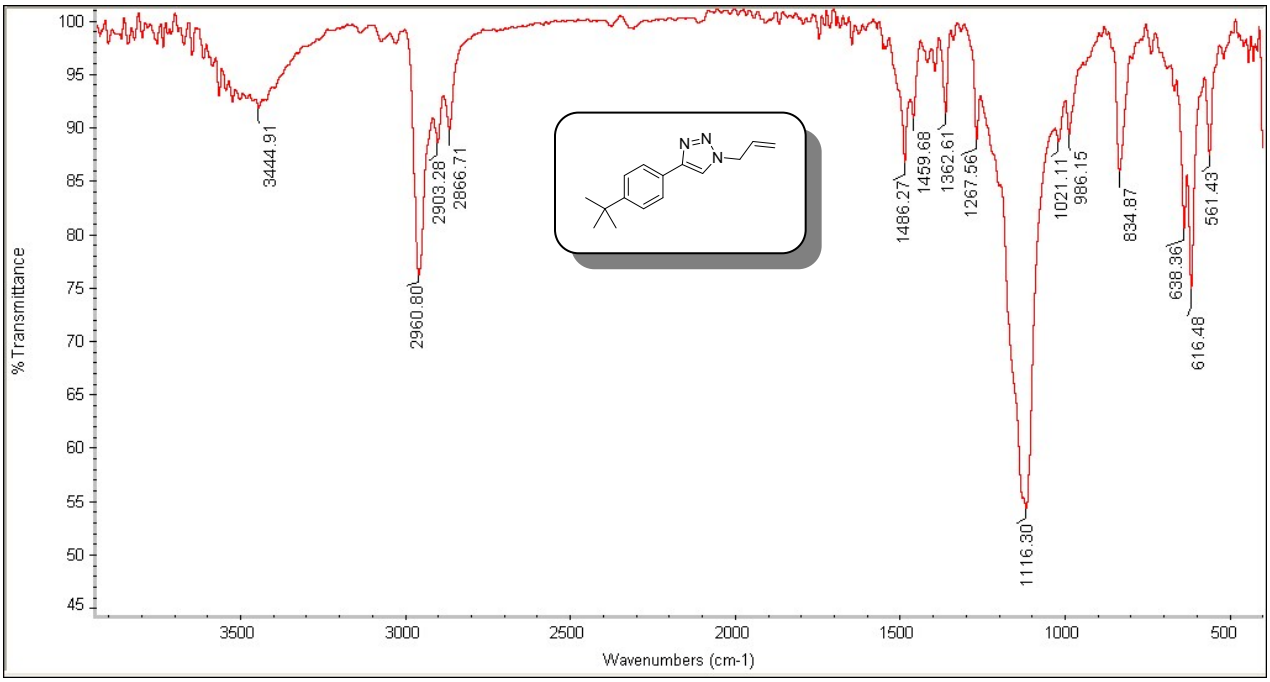


Figure 72: FT-IR (KBr) of 1-allyl-4-(4-(*tert*-butyl)phenyl)-1*H*-1,2,3-triazole (**4v**).

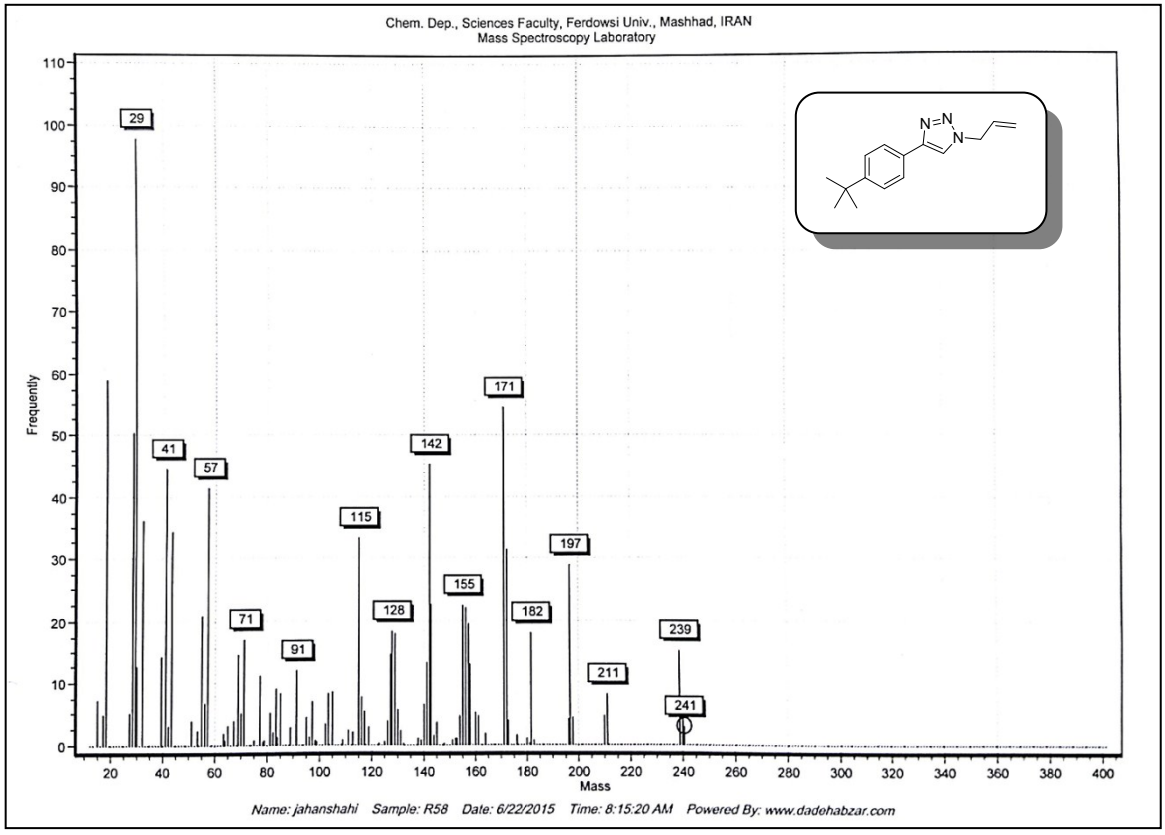


Figure 73: Mass spectrum of 1-allyl-4-(4-(*tert*-butyl)phenyl)-1*H*-1,2,3-triazole (**4v**).

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