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Supplementary Information

Direct access to stabilized Cu^{I} using cuttlebone as a natural-reducing support for efficient CuAAC click reactions 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 FT-IR 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 %). Elemental compositions were determined with an SC7620 Energy-dispersive X-ray analysis (EDX) presenting a 133 eV resolution at 20 kV. Surface analysis spectroscopy of the catalyst was performed in an ESCA/AES system. This system was equipped with a concentric hemispherical (CHA) electron energy analyzer (Specs model EA10 plus) suitable for X-ray photoelectron spectroscopy (XPS). Inductively coupled plasma (ICP) was carried out on a Varian, VISTA-PRO, CCD, Australia and 76004555 SPECTRO ARCOS ICP-OES analyzer. All yields refer to isolated products after purification by recrystallization.

1-Benzyl-4-phenyl-1*H*-1,2,3-triazole (Table 3, Entry 1) (0.22 g, 95%); 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=CH), 7.44-7.38 (5 H, m, Ar-H), 7.36-7.29 (3 H, m, Ar-H), 5.58 (2 H, s, CH_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 – $C_{15}H_{13}N$).

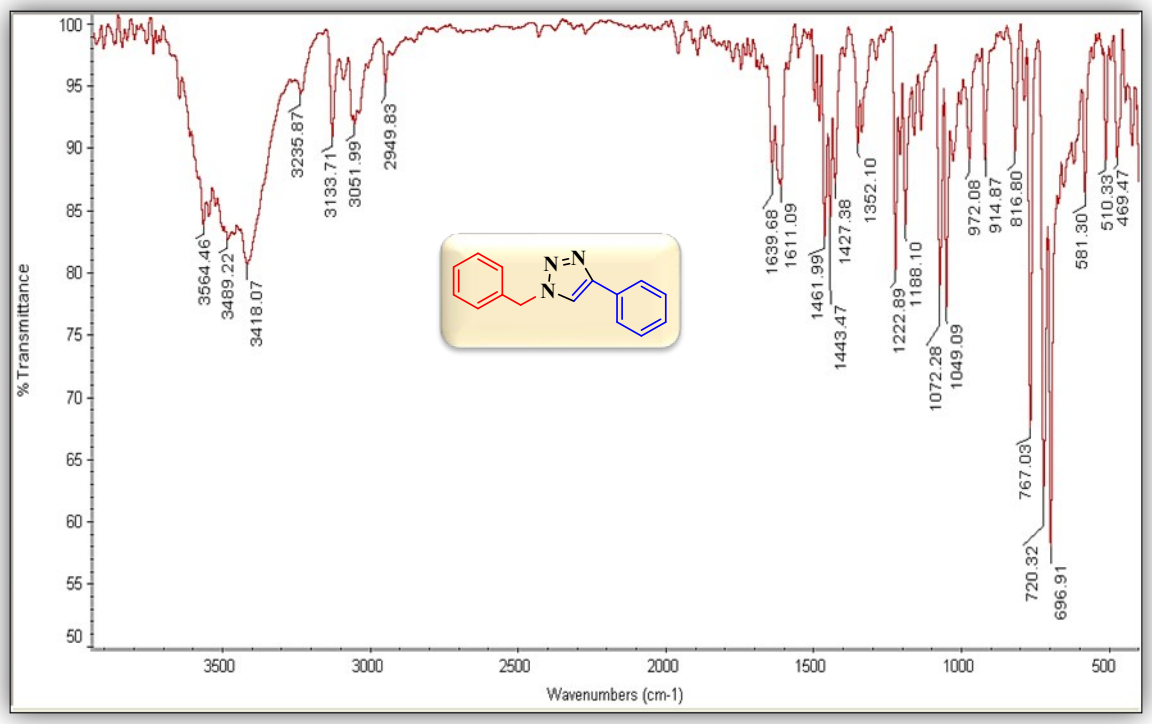


Figure 1: FT-IR (KBr) of 1-Benzyl-4-phenyl-1*H*-1,2,3-triazole (**Table 3, Entry 1**).

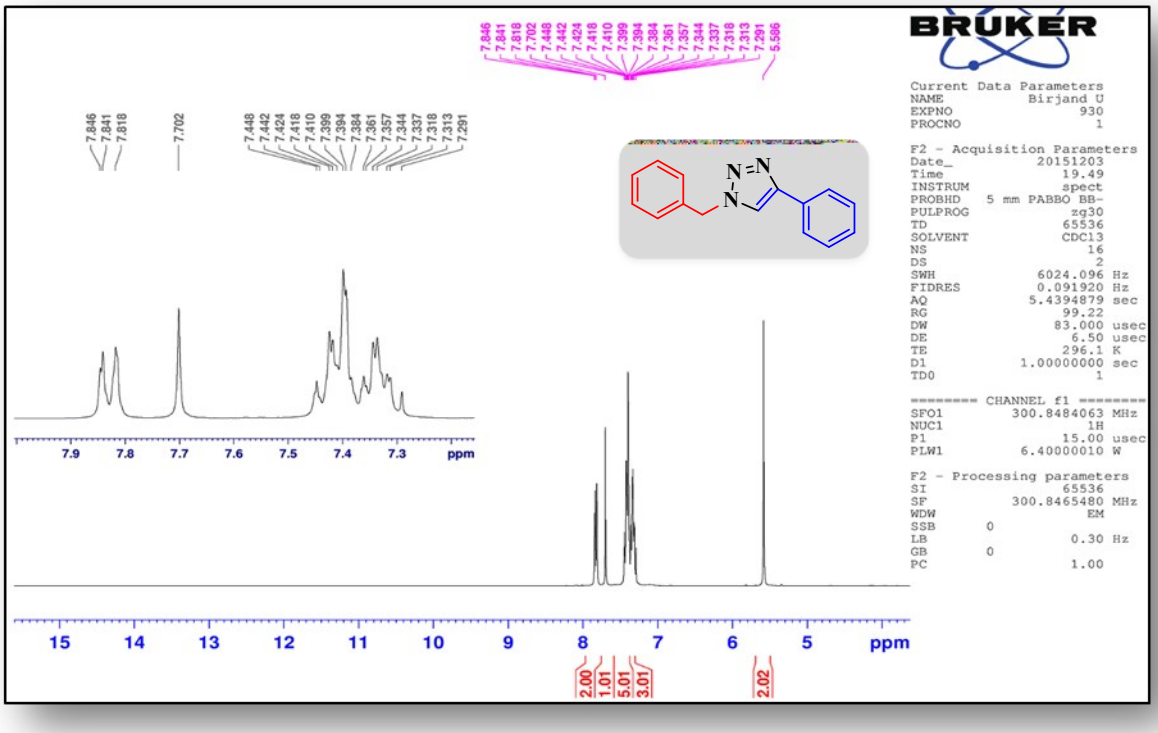


Figure 2: ^{1}H NMR (300 MHz, $CDCl_3$) of 1-Benzyl-4-phenyl-1*H*-1,2,3-triazole (**Table 3, Entry 1**).

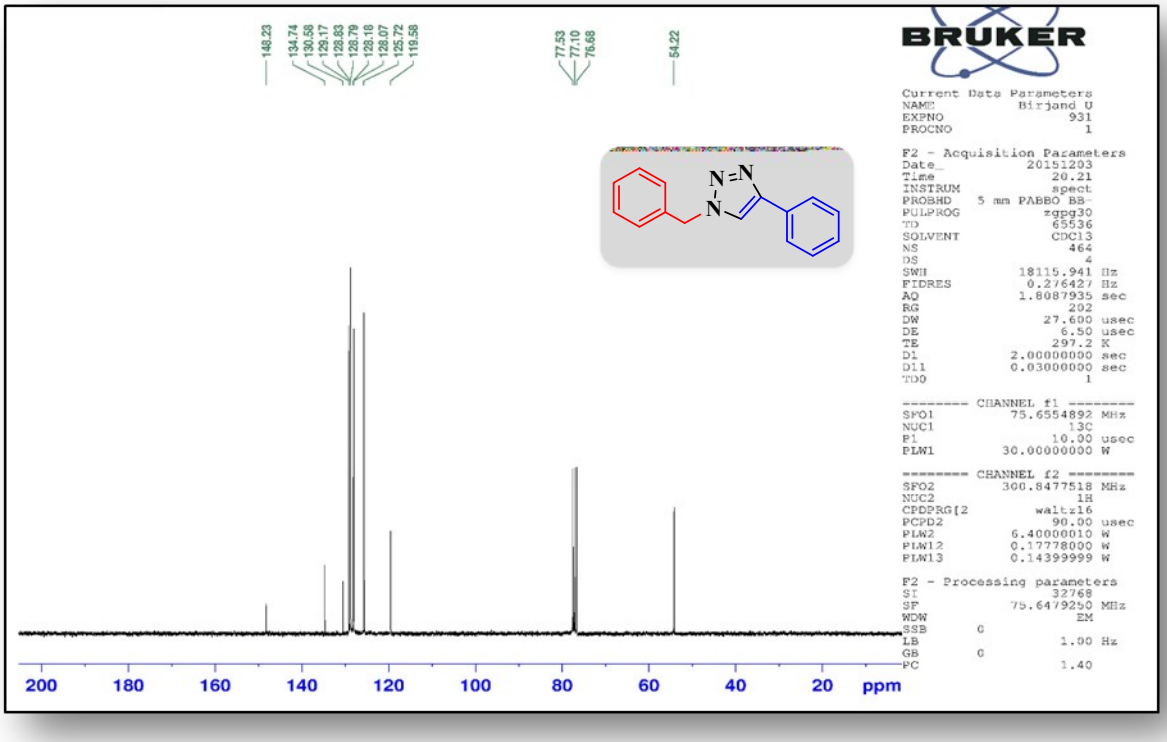


Figure 3: ^{13}C NMR (75MHz, $CDCl_3$) of 1-Benzyl-4-phenyl-1*H*-1,2,3-triazole (**Table 3, Entry 1**).

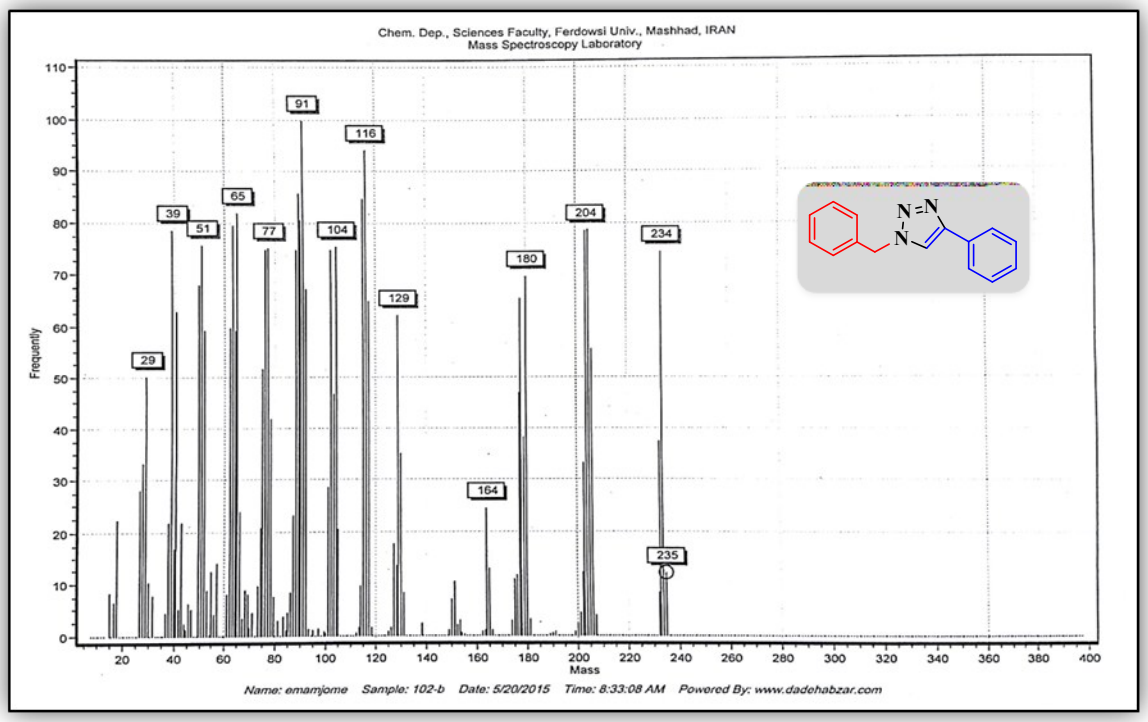


Figure 4: Mass spectrum of 1-Benzyl-4-phenyl-1*H*-1,2,3-triazole (**Table 3, Entry 1**).

1-Benzyl-4-(*p*-tolyl)-1*H*-1,2,3-triazole (**Table 3, Entry 2**) (0.23 g, 93%); 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=CH), 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, CH_2), 2.39 (3 H, s, CH_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 – $C_{16}H_{15}N$).

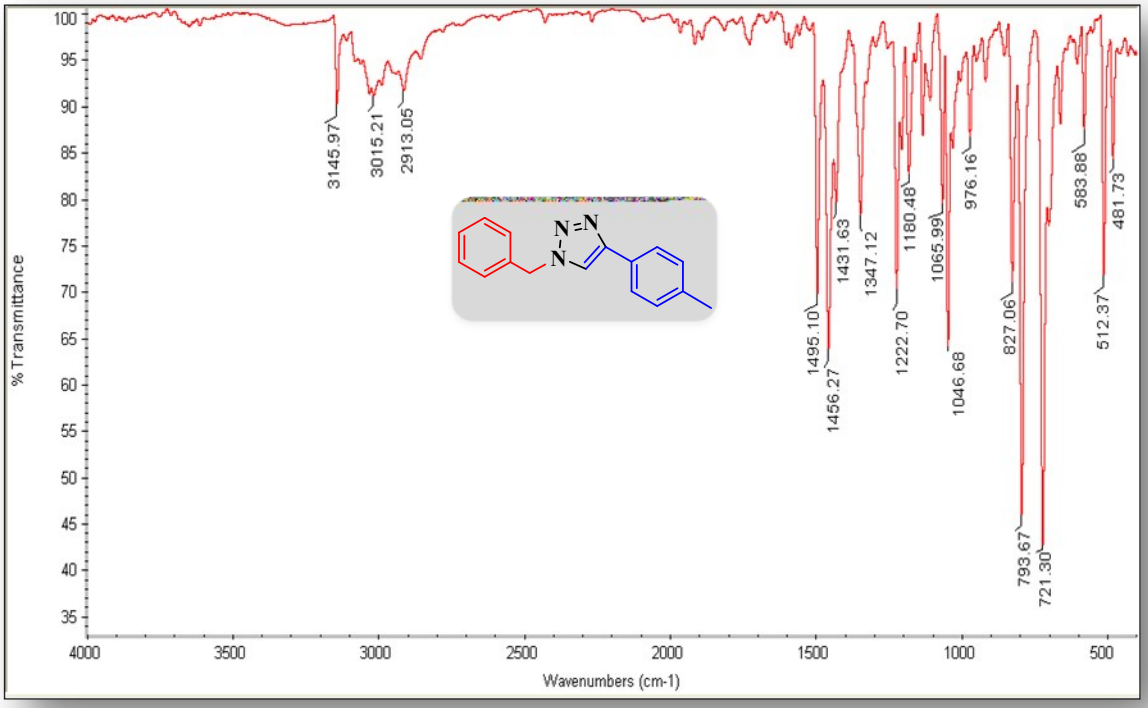


Figure 5: FT-IR (KBr) of 1-Benzyl-4-(*p*-tolyl)-1*H*-1,2,3-triazole (**Table 3, Entry 2**).

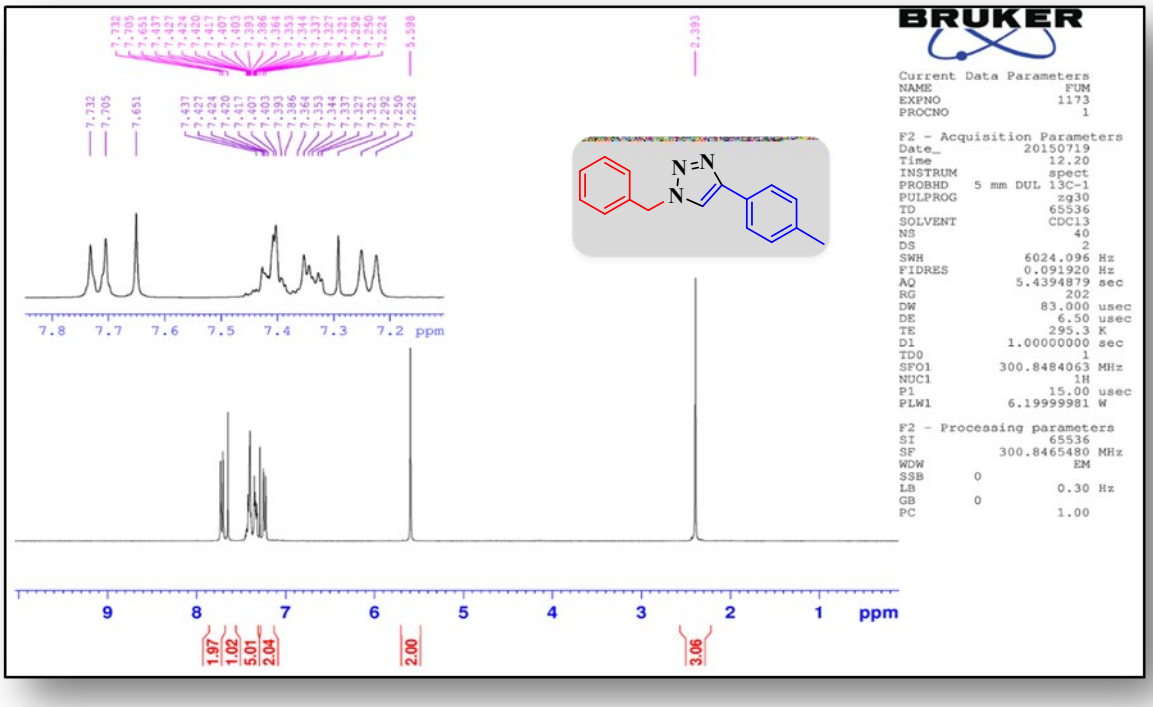


Figure 6: ^{1}H NMR (300 MHz, $CDCl_3$) of 1-Benzyl-4-(*p*-tolyl)-1*H*-1,2,3-triazole (**Table 3, Entry 2**).

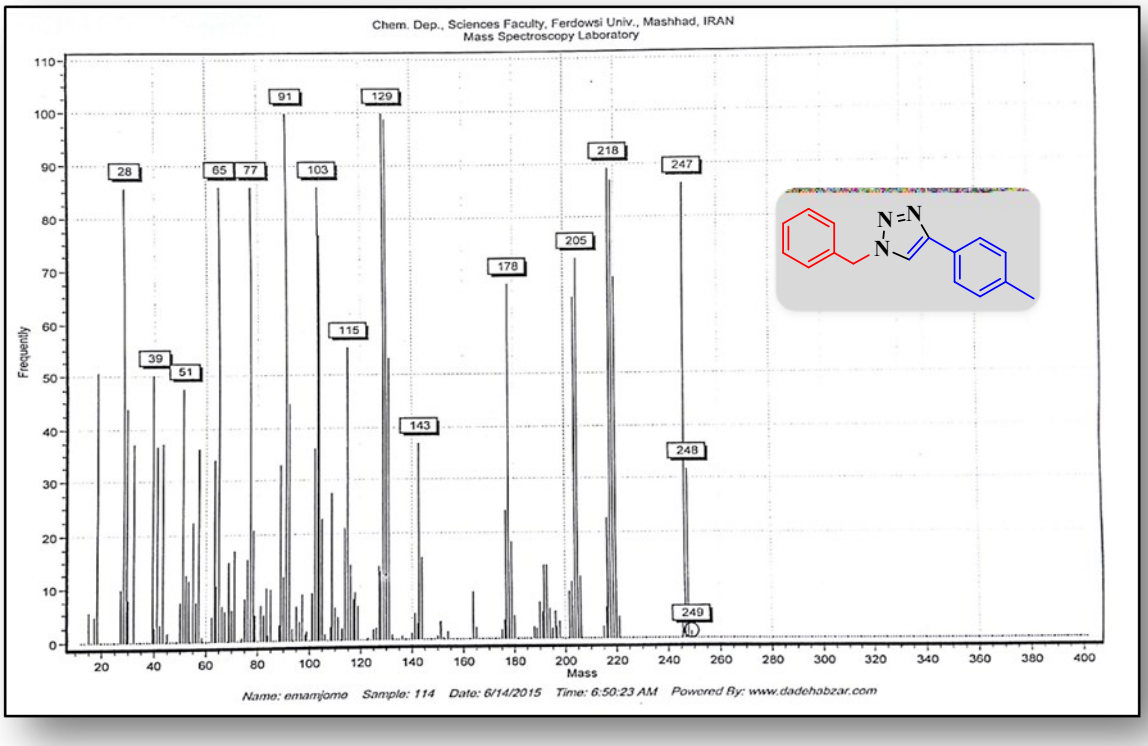


Figure 7: Mass spectrum of 1-Benzyl-4-(*p*-tolyl)-1*H*-1,2,3-triazole **(Table 3, Entry 2).**

1-Benzyl-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (**Table 3, Entry 3**) (0.22 g, 85%); 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=CH), 6.96 (2 H, d, *J* = 7.2 Hz, Ar-H), 5.58 (2 H, s, CH_2), 3.85 (3 H, s, OCH_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 – $C_{16}H_{15}NO$).

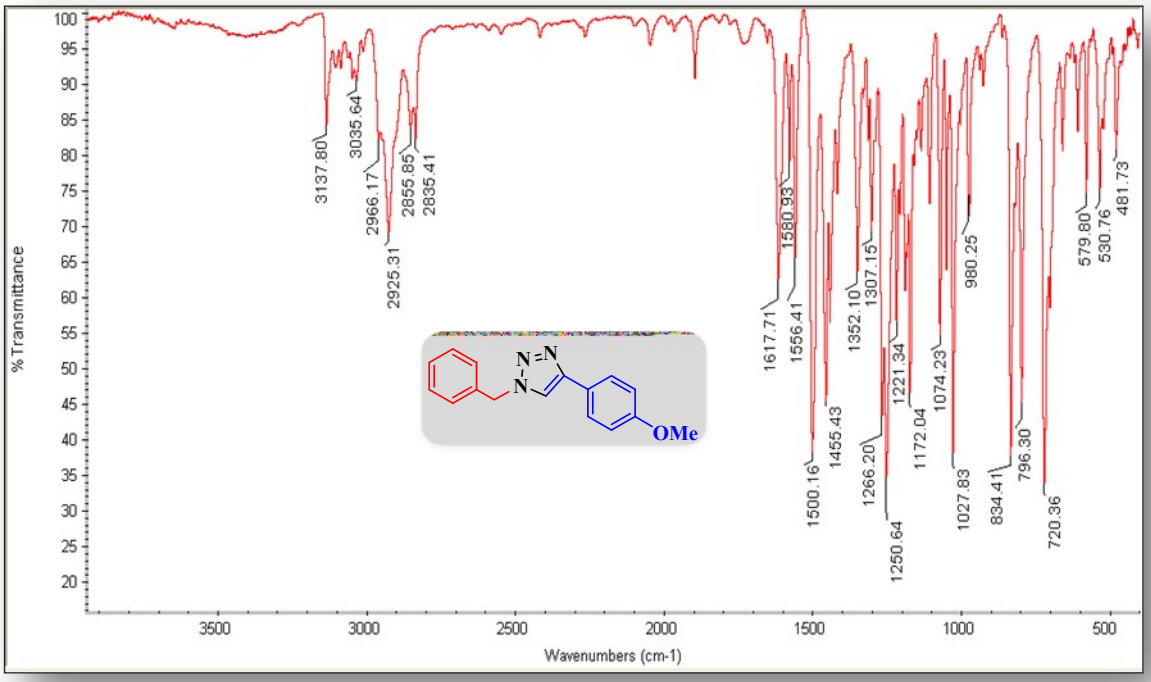


Figure 8: FT-IR (KBr) of 1-Benzyl-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (**Table 3, Entry 3**).

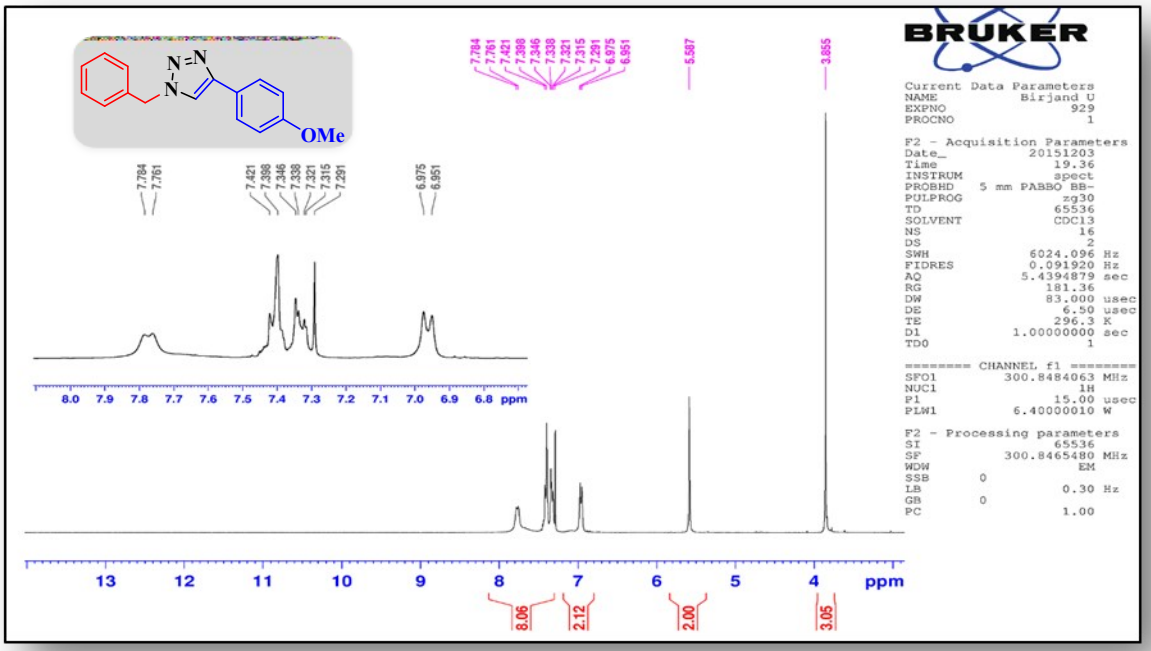


Figure 9: ^{1}H NMR (300 MHz, $CDCl_3$) of 1-Benzyl-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (**Table 3, Entry 3**).

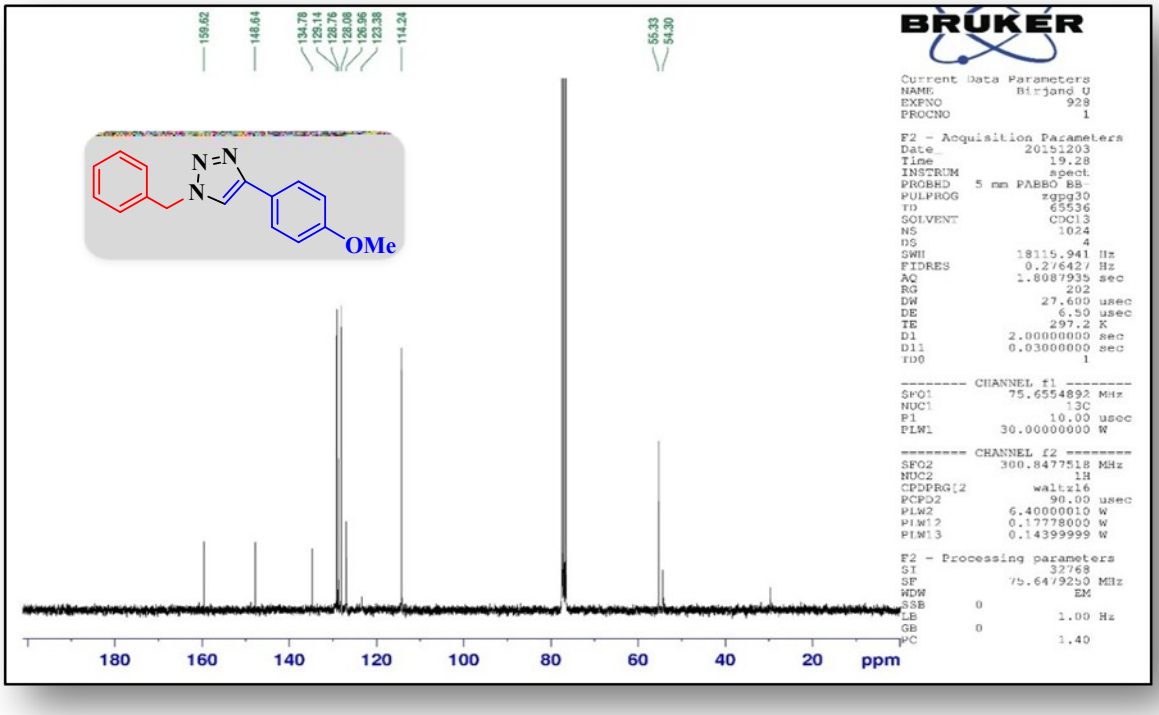


Figure 10: ^{13}C NMR (75MHz, $CDCl_3$) of 1-Benzyl-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (**Table 3, Entry 3**).

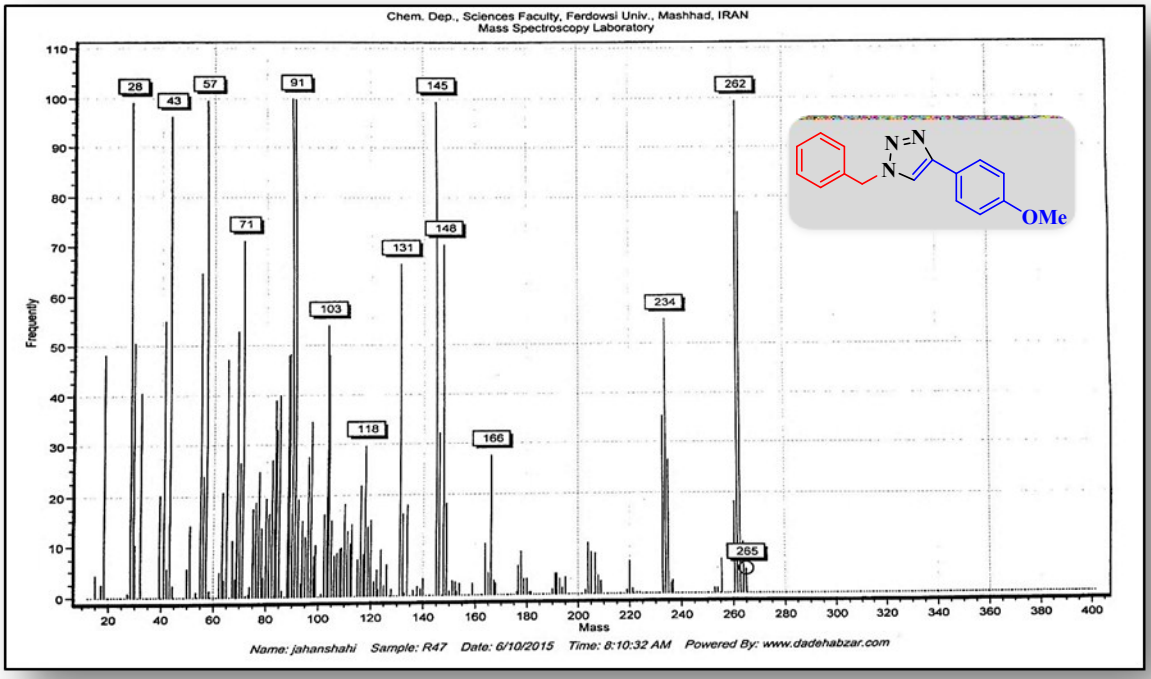


Figure 11: Mass spectrum of 1-Benzyl-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (**Table 3, Entry 3**).

1-benzyl-4-(4-(*tert*-butyl)phenyl)-1*H*-1,2,3-triazole (Table 3, Entry 4) (0.26 g, 90%); 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=CH), 7.43-7.21 (7 H, m, Ar-H,), 5.58 (2 H, s, CH_2), 1.37 (9 H, s, 3 CH_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 – $C_{19}H_{21}N$).

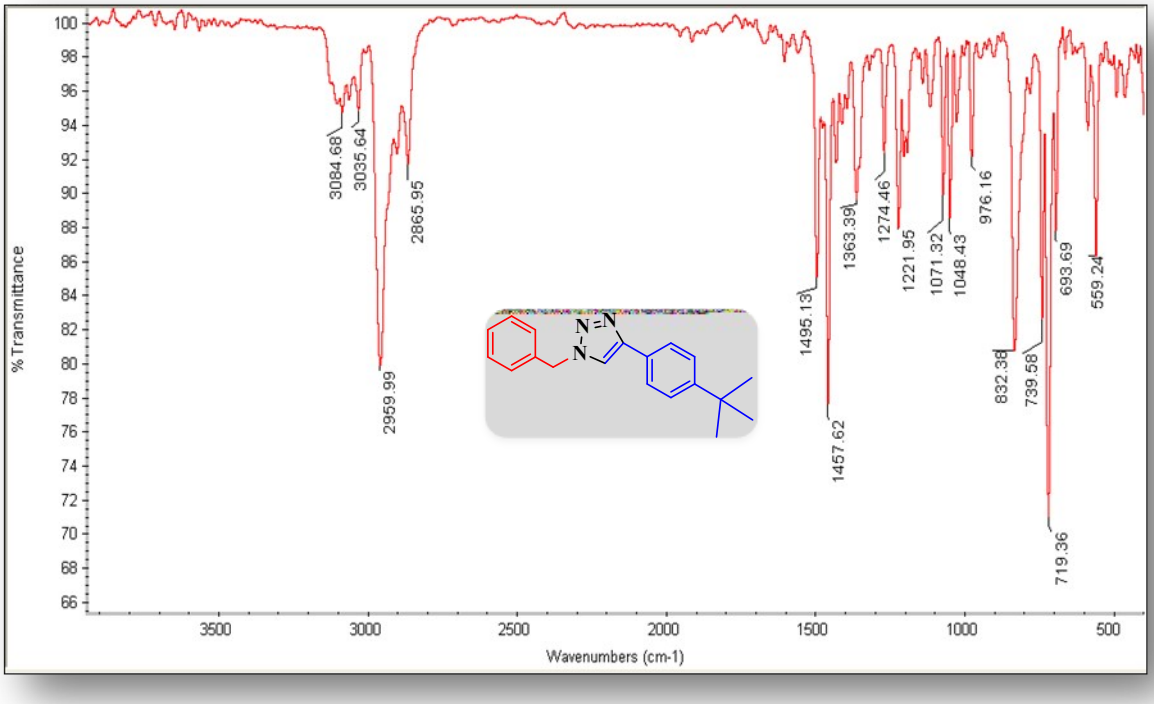


Figure 12: FT-IR (KBr) of 1-benzyl-4-(4-(*tert*-butyl)phenyl)-1*H*-1,2,3-triazole (**Table 3, Entry 4**).

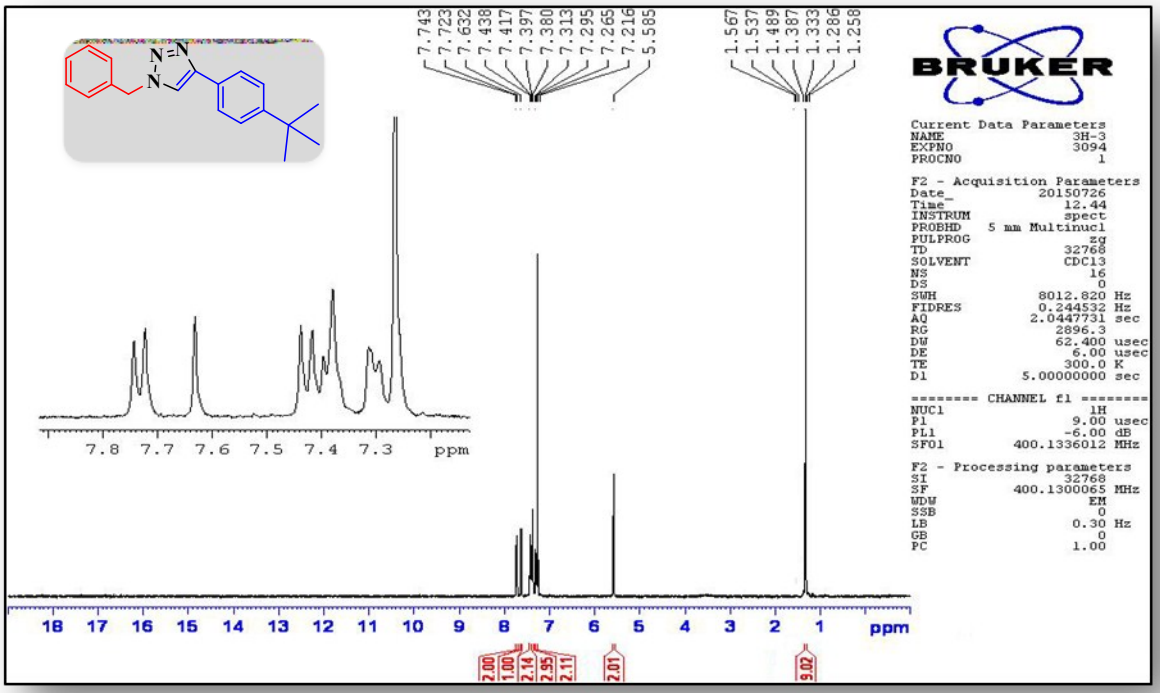


Figure 13: ^{1}H NMR (400 MHz, $CDCl_3$) of 1-benzyl-4-(4-(*tert*-butyl)phenyl)-1*H*-1,2,3-triazole (**Table 3, Entry 4**).

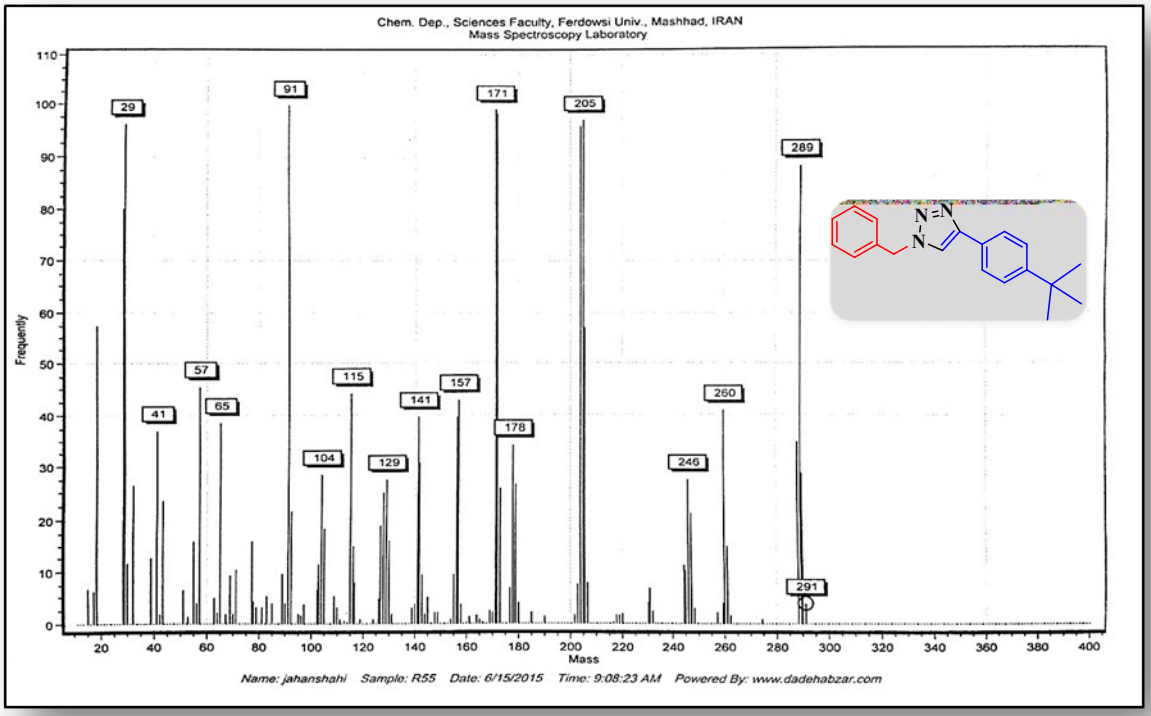


Figure 14: Mass spectrum of 1-benzyl-4-(4-(*tert*-butyl)phenyl)-1*H*-1,2,3-triazole (**Table 3, Entry 4**).

2-(1-benzyl-1*H*-1,2,3-triazol-4-yl)pyridine (Table 3, Entry 5) (0.19 g, 82%); white solid (crystals); mp 112–113 ºC (from EtOH) (Lit.[5] 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=CH), 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, CH_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 – $C_7H_5N_4$).

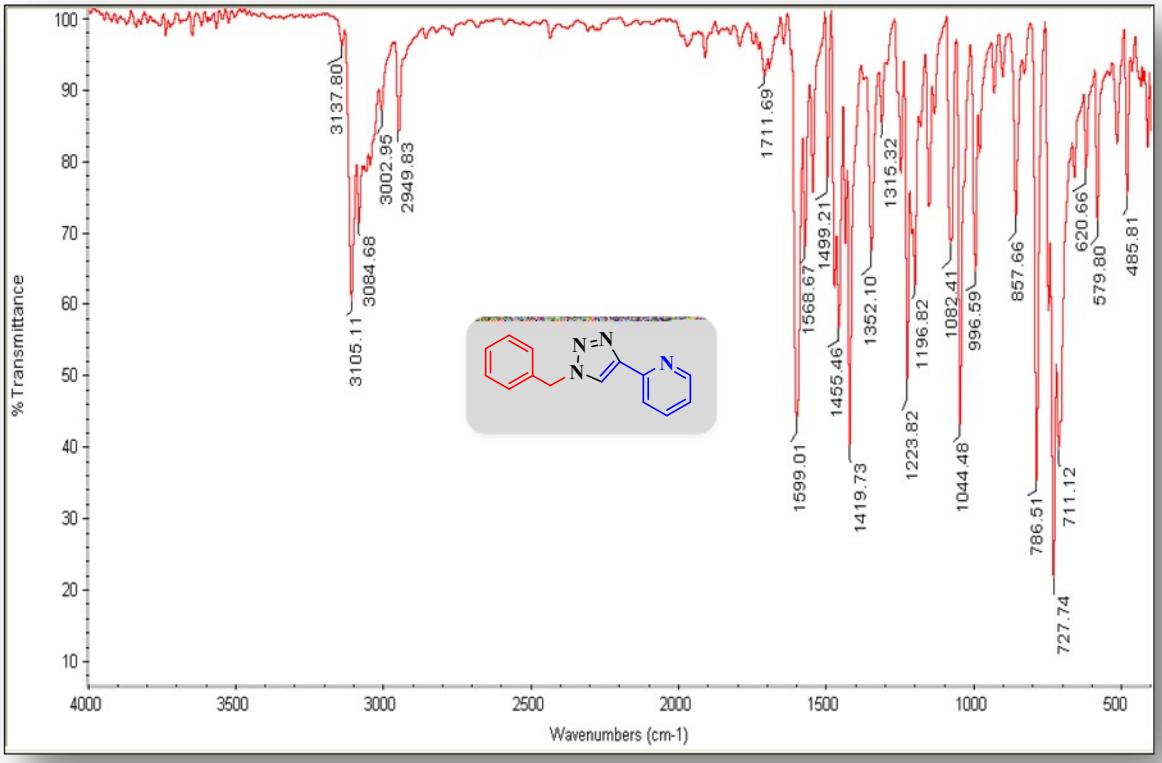


Figure 15: FT-IR (KBr) of 2-(1-benzyl-1*H*-1,2,3-triazol-4-yl)pyridine **(Table 3, Entry 5**

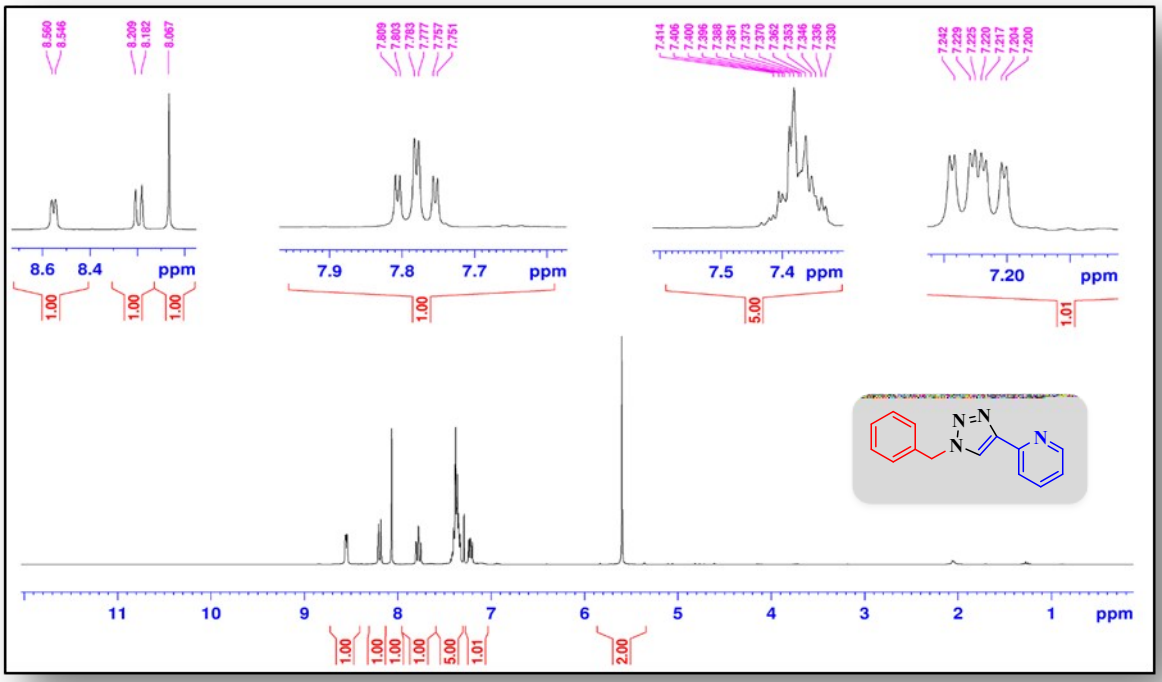


Figure 16: ^{1}H NMR (300 MHz, $CDCl_3$) of 2-(1-benzyl-1*H*-1,2,3-triazol-4-yl)pyridine **(Table 3, Entry 5).**

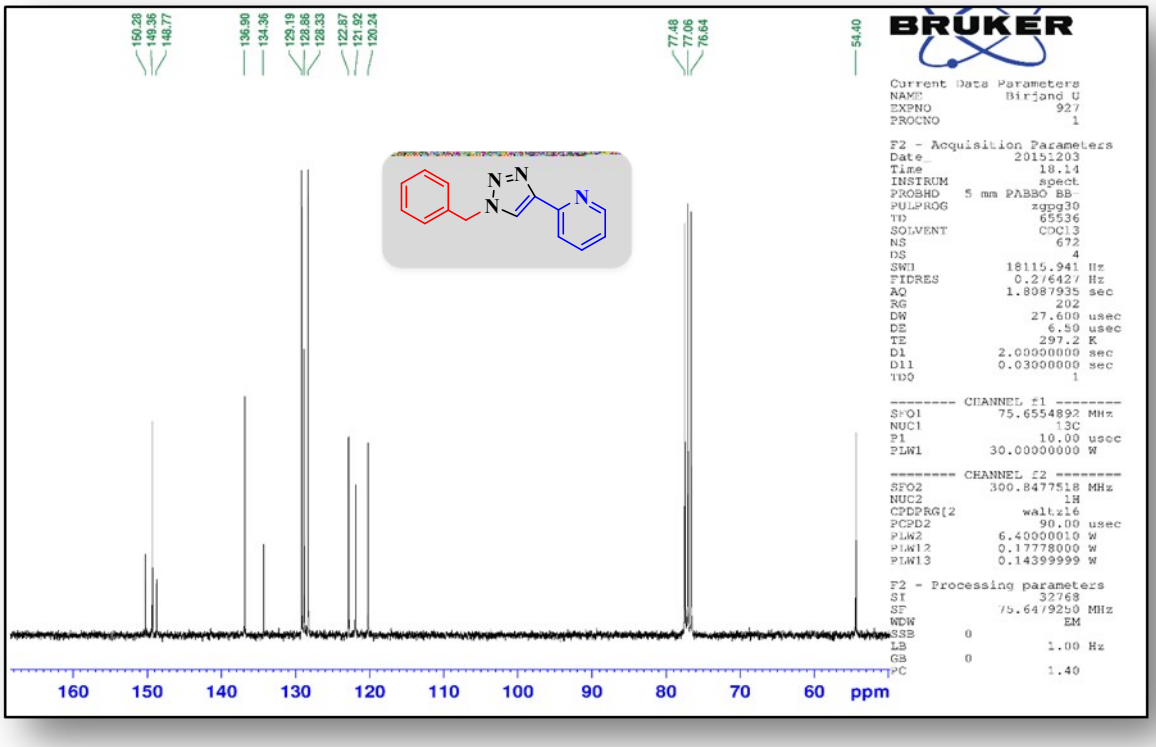


Figure 17: ^{13}C NMR (75MHz, $CDCl_3$) of 2-(1-benzyl-1*H*-1,2,3-triazol-4-yl)pyridine **(Table 3, Entry 5)**.

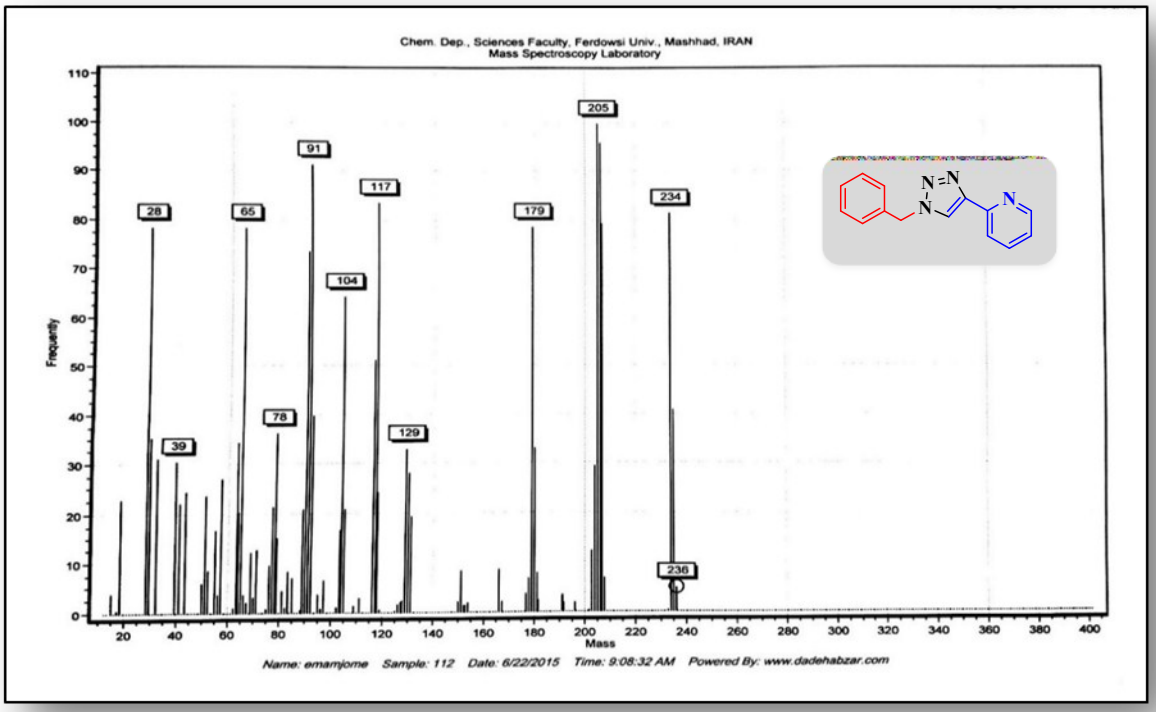


Figure 18: Mass spectrum of 2-(1-benzyl-1*H*-1,2,3-triazol-4-yl)pyridine **(Table 3, Entry 5)**.

1-benzyl-4-(4-chlorophenyl)-1*H*-1,2,3-triazole (Table 3, Entry 6) (0.24 g, 90%); white solid (crystals); mp 125–126 ºC (from EtOH) (Lit.[6] 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=CH), 7.40-7.29 (7 H, m, Ar-H), 5.57 (2 H, s, CH_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 – $C_{15}H_{12}ClN$).

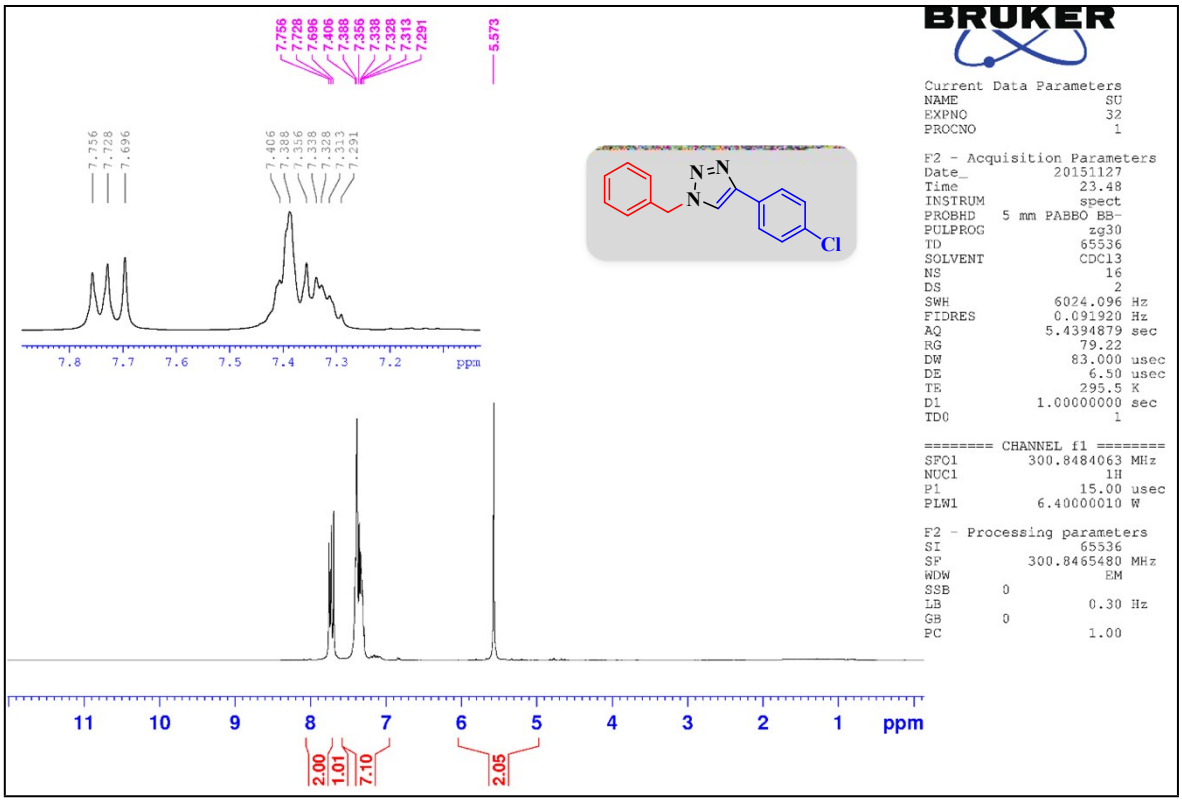


Figure 19: ^{1}H NMR (300 MHz, $CDCl_3$) of 1-(4-chlorobenzyl)-4-phenyl-1*H*-1,2,3-triazole **(Table 3, Entry 6)**.

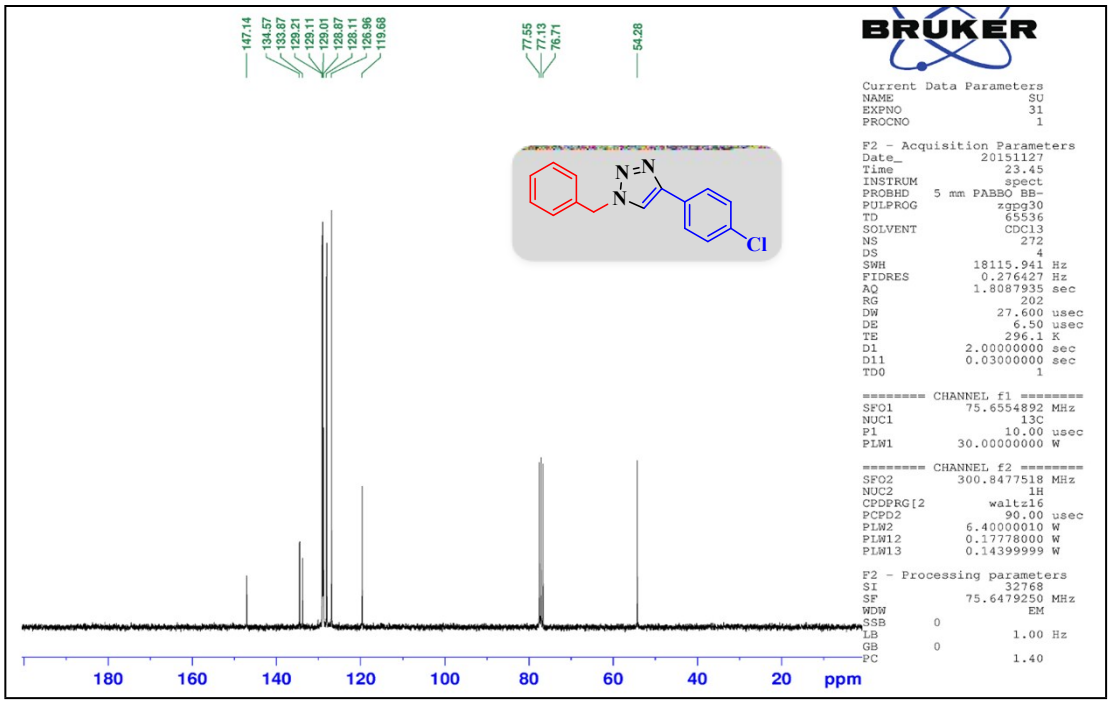


Figure 20: ^{13}C NMR (75MHz, $CDCl_3$) of 1-benzyl-4-(4-chlorophenyl)-1*H*-1,2,3-triazole **(Table 3, Entry 6)**.

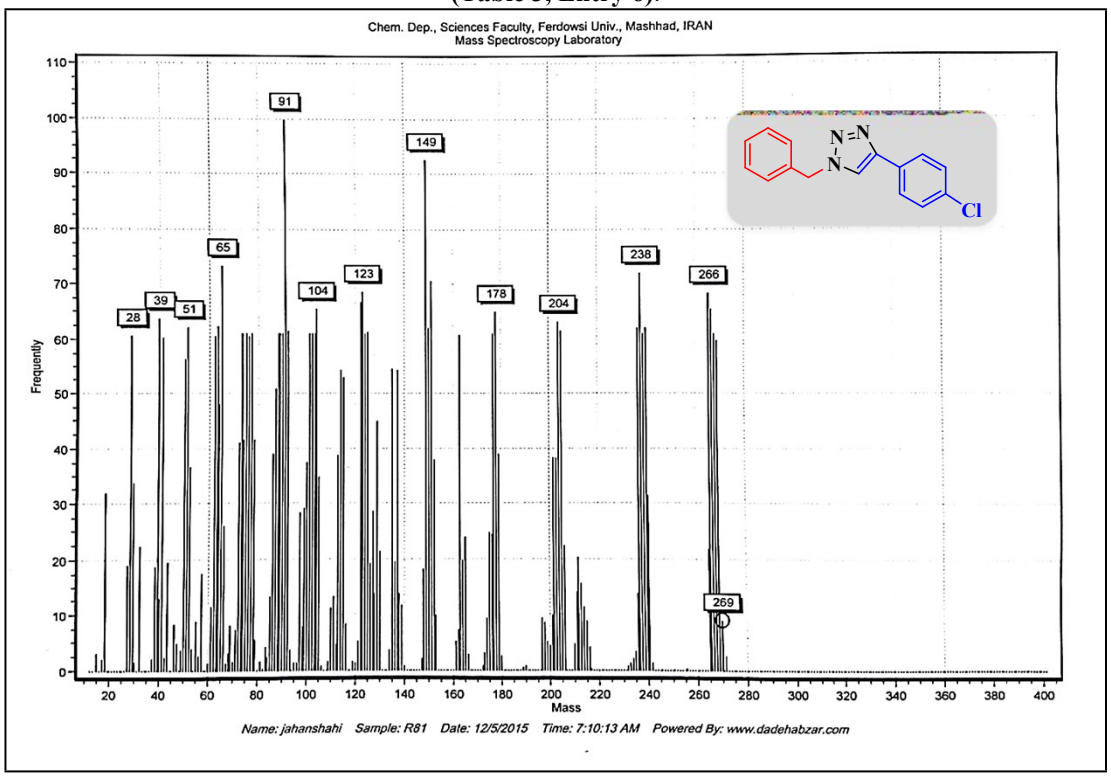


Figure 21: Mass spectrum of 1-benzyl-4-(4-chlorophenyl)-1*H*-1,2,3-triazole **(Table 3, Entry 6)**.

1-benzyl-4-(4-bromophenyl)-1*H*-1,2,3-triazole (Table 3, Entry 7) (0.27 g, 87%); white solid (crystals); mp 144 ºC (from EtOH) (Lit.[6] 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=CH), 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, CH_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 – $C_{15}H_{12}BrN$).

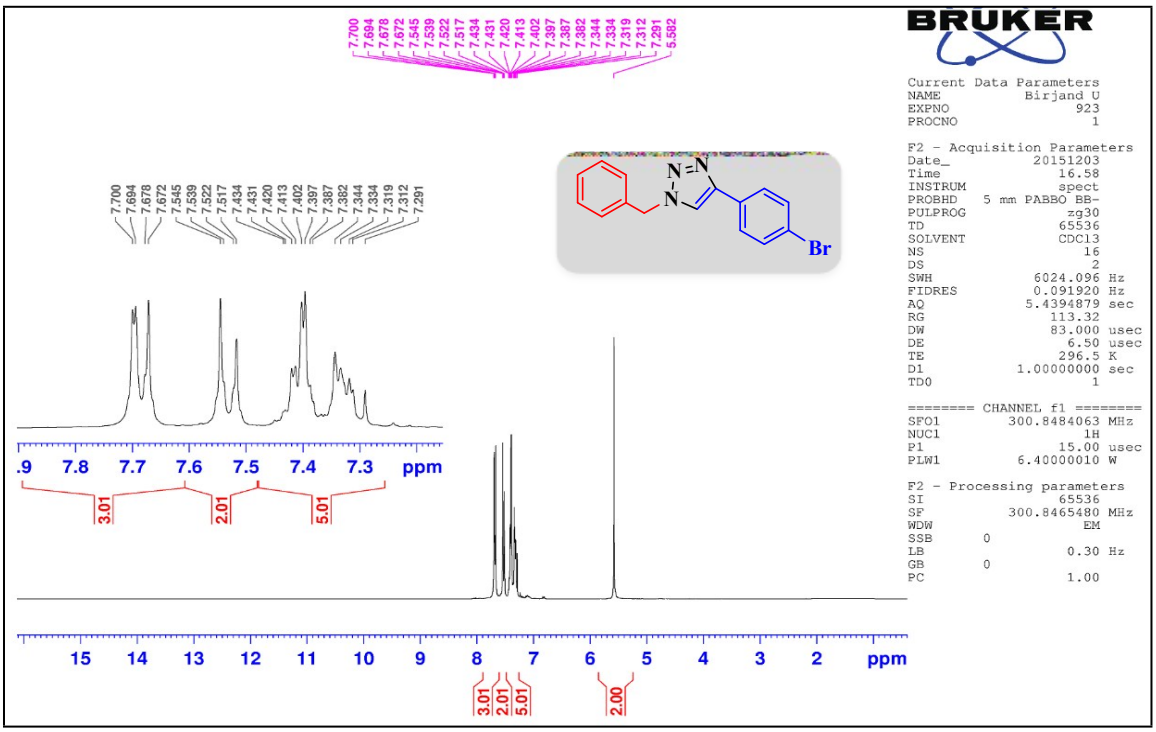


Figure 22: ^{1}H NMR (300 MHz, $CDCl_3$) of 1-benzyl-4-(4-bromophenyl)-1*H*-1,2,3-triazole **(Table 3, Entry 7)**.

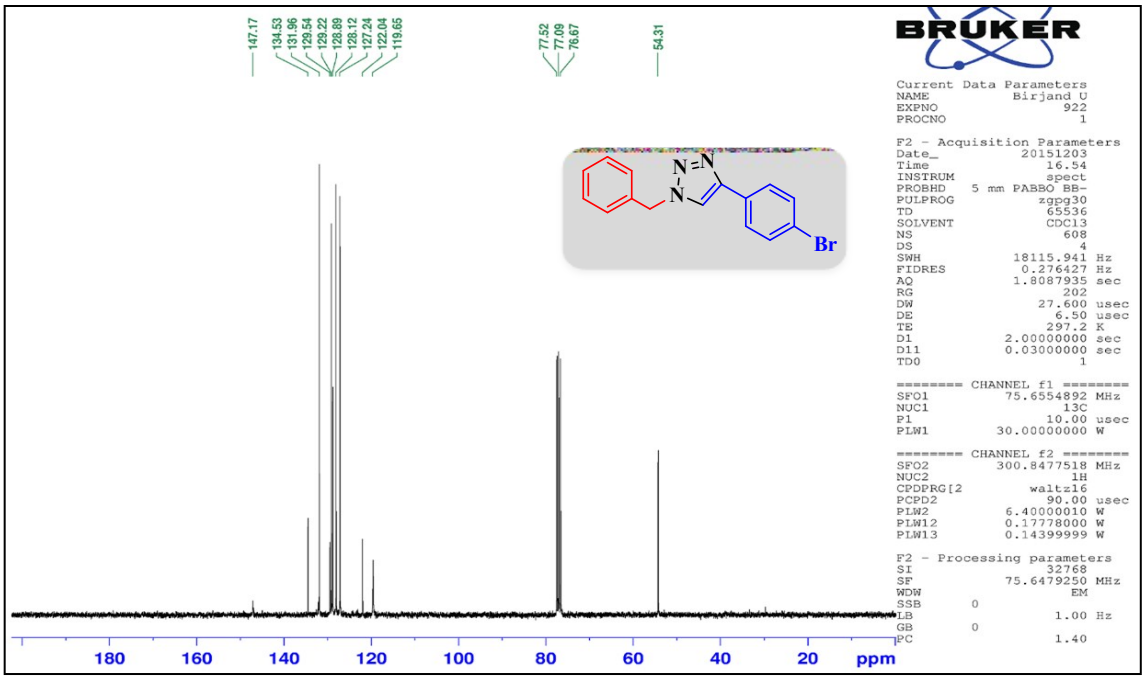


Figure 23: ^{13}C NMR (75MHz, $CDCl_3$) of 1-benzyl-4-(4-bromophenyl)-1*H*-1,2,3-triazole **(Table 3, Entry 7)**.

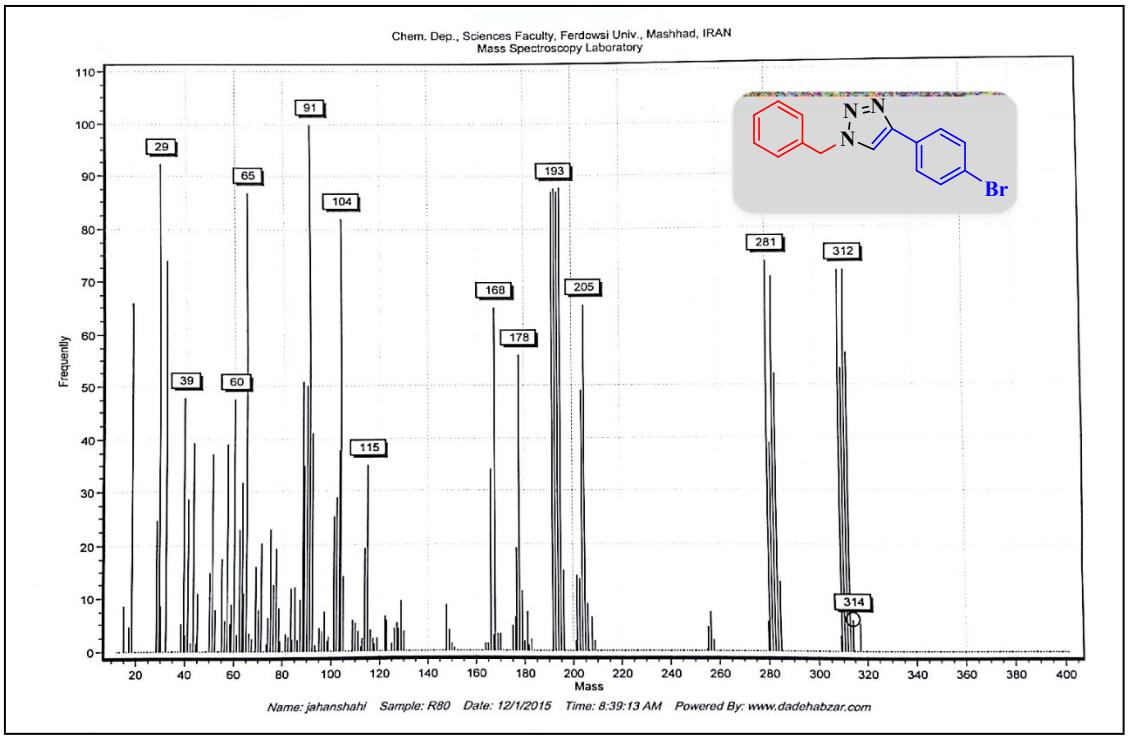


Figure 24: Mass spectrum of 1-benzyl-4-(4-bromophenyl)-1*H*-1,2,3-triazole **(Table 3, Entry 7)**.

1-benzyl-4-(4-nitrophenyl)-1*H*-1,2,3-triazole (Table 3, Entry 8) (0.27 g, 95%); yellow solid (crystals); mp 167–168 ºC (from EtOH) (Lit.[7] 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=CH), 7.29-7.44 (5 H, m, Ar-H), 5.63 (2 H, s, CH_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 – $C_{15}H_{12}N_2O_2$).

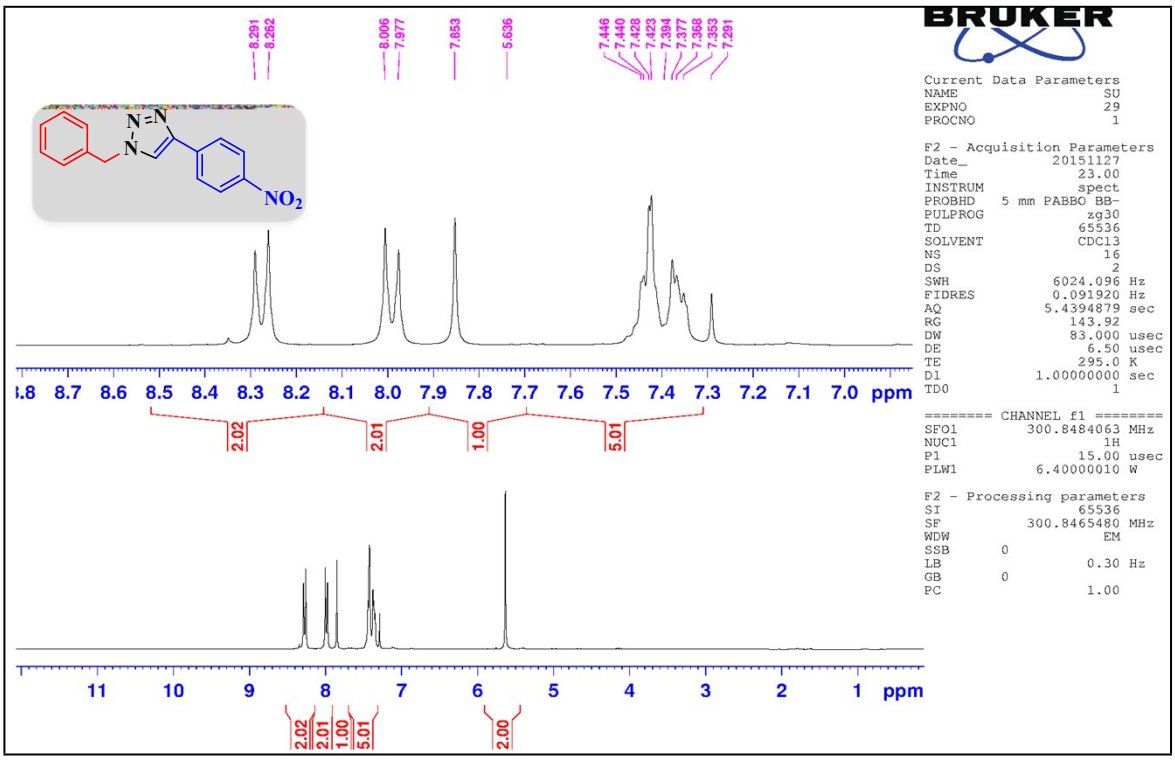


Figure 25: ^{1}H NMR (300 MHz, $CDCl_3$) of 1-benzyl-4-(4-nitrophenyl)-1*H*-1,2,3-triazole **(Table 3, Entry 8)**.

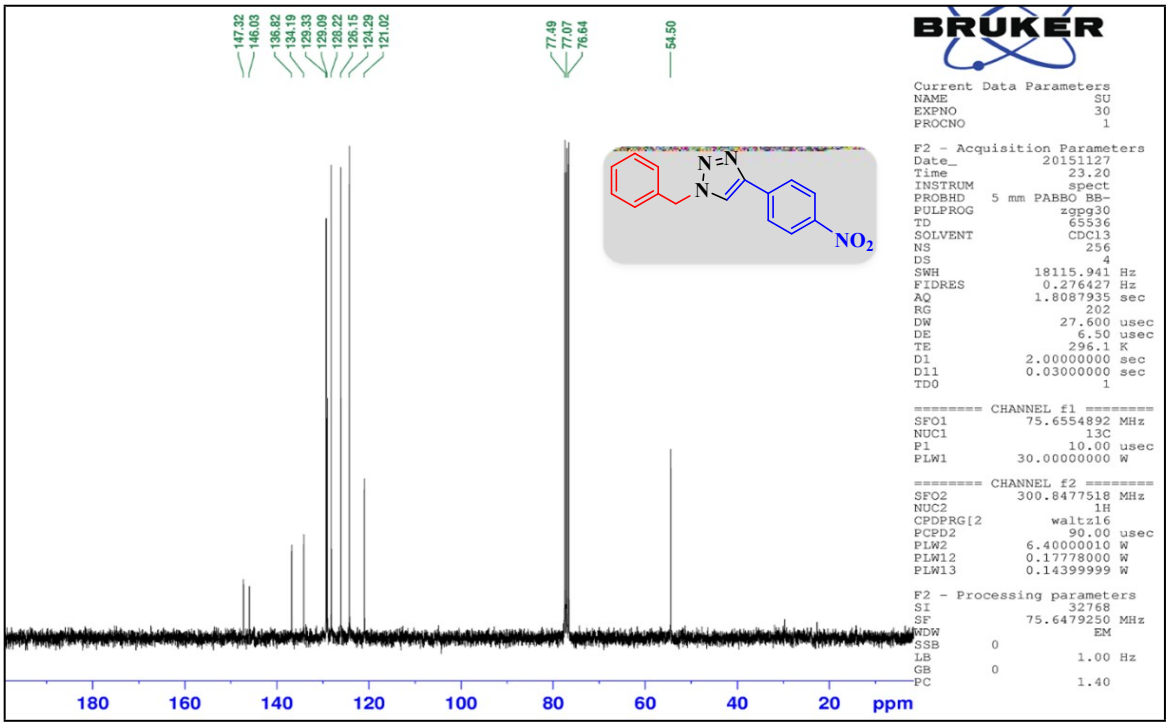


Figure 26: ^{13}C NMR (75MHz, $CDCl_3$) of 1-benzyl-4-(4-nitrophenyl)-1*H*-1,2,3-triazole **(Table 3, Entry 8)**.

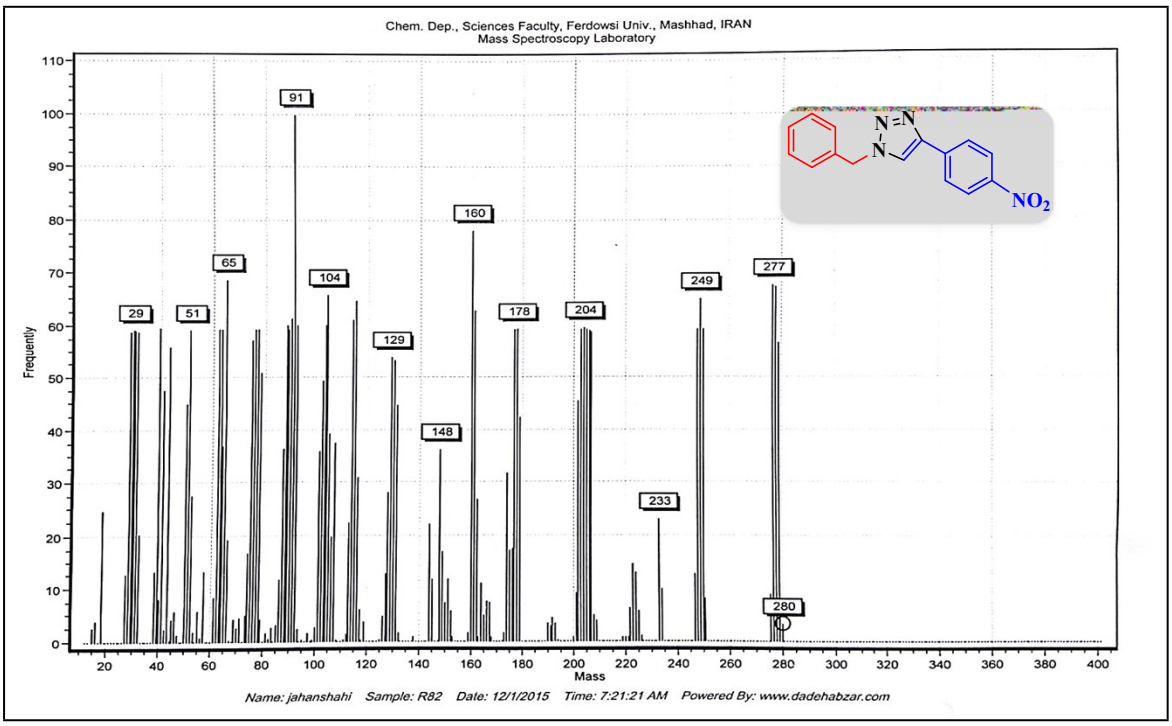


Figure 27: Mass spectrum of 1-benzyl-4-(4-nitrophenyl)-1*H*-1,2,3-triazole **(Table 3, Entry 8)**.

(1-benzyl-1*H*-1,2,3-triazol-4-yl)methanol (Table 3, Entry 9) (0.14 g, 73%); white solid (crystals); mp 77-78 ºC (from EtOH) (Lit.[8] 77 - 79 ºC); ^{1}H NMR: δH (300 MHz; $CDCl_3$; Me_4Si) 7.48 (1 H, s, C=CH), 7.36–7.34 (3 H, m, Ar-H), 7.29–7.24 (2 H, m, Ar-H), 5.48 (2 H, s, CH_2), 4.72 (2 H, s, CH_2OH), 4.19 (1 H, br s, OH); ^{13}C NMR: δC (75 MHz; $CDCl_3$; Me_4Si) 148, 134, 129, 128.7, 128.1, 121, 56, 54; MS, *m/z* 189 (M^+, 9%), 188 (64, M-1H), 187 (64, M – 2H), 159 (63, M – CH_3O), 129 (65), 91 (100, M – $C_3H_4N_3O$), 77 (55, M – $C_4H_6N_3O$), 65 (71), 28 (64, M – $C_{10}H_{11}NO$).

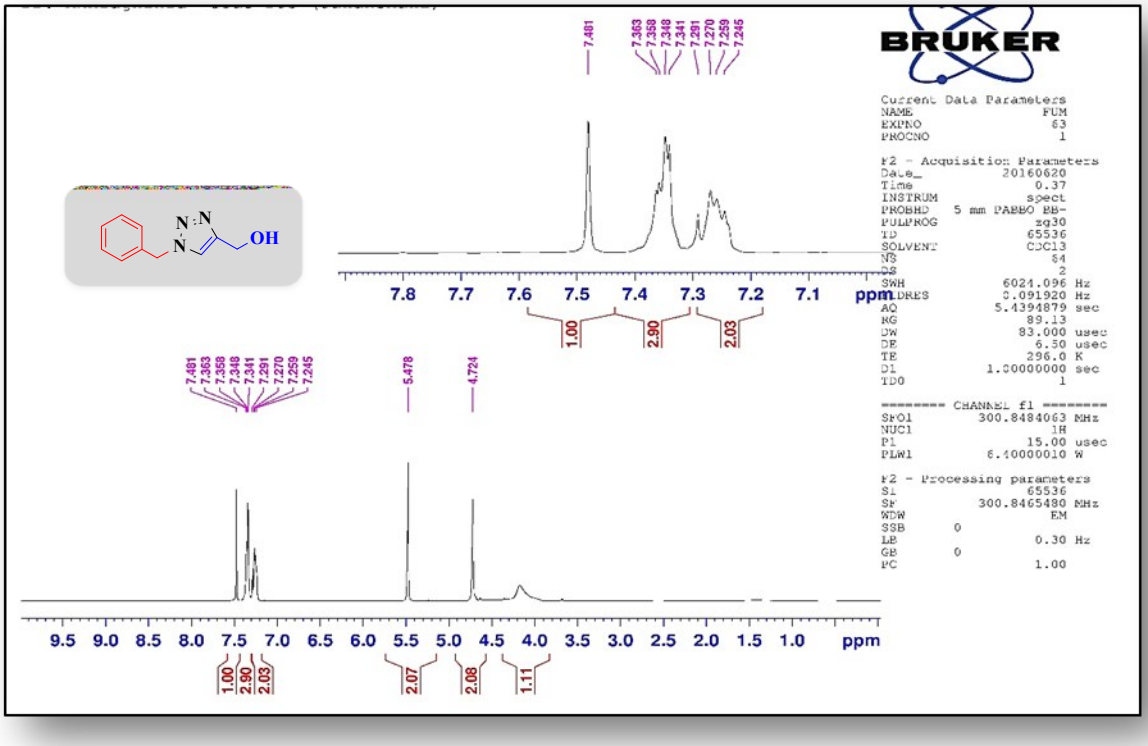


Figure 28: ^{1}H NMR (300 MHz, $CDCl_3$) of (1-benzyl-1*H*-1,2,3-triazol-4-yl)methanol **(Table 3, Entry 9).**

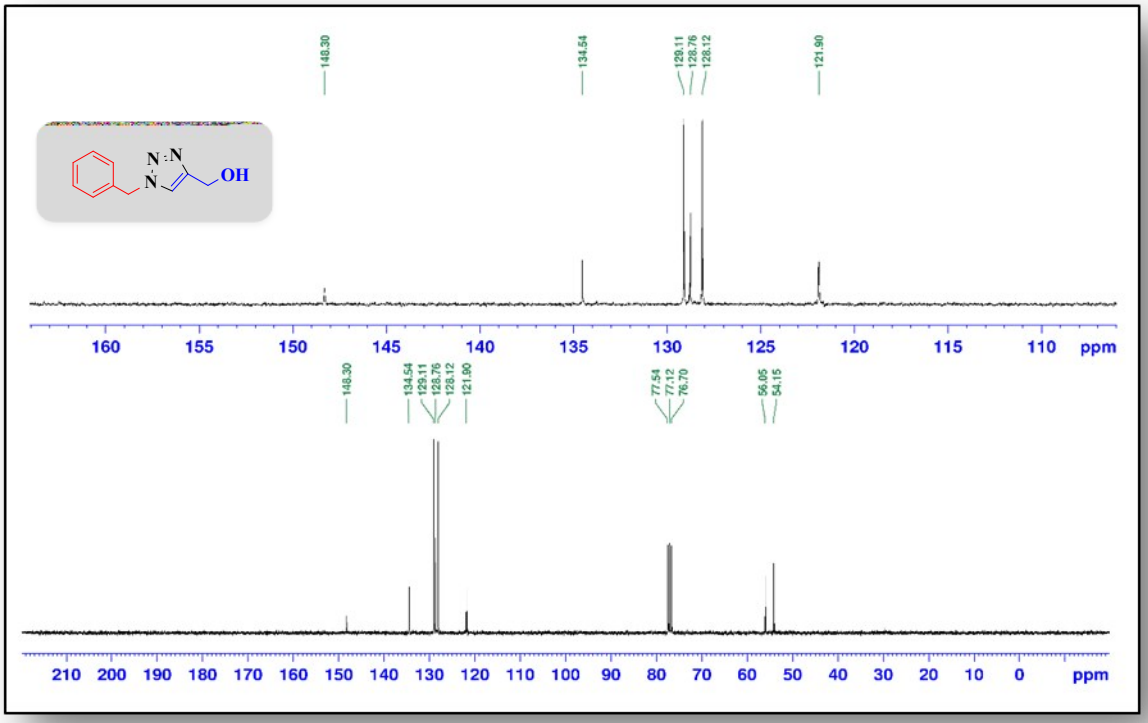


Figure 29: ^{13}C NMR (300 MHz, $CDCl_3$) of (1-benzyl-1*H*-1,2,3-triazol-4-yl)methanol **(Table 3, Entry 9).**

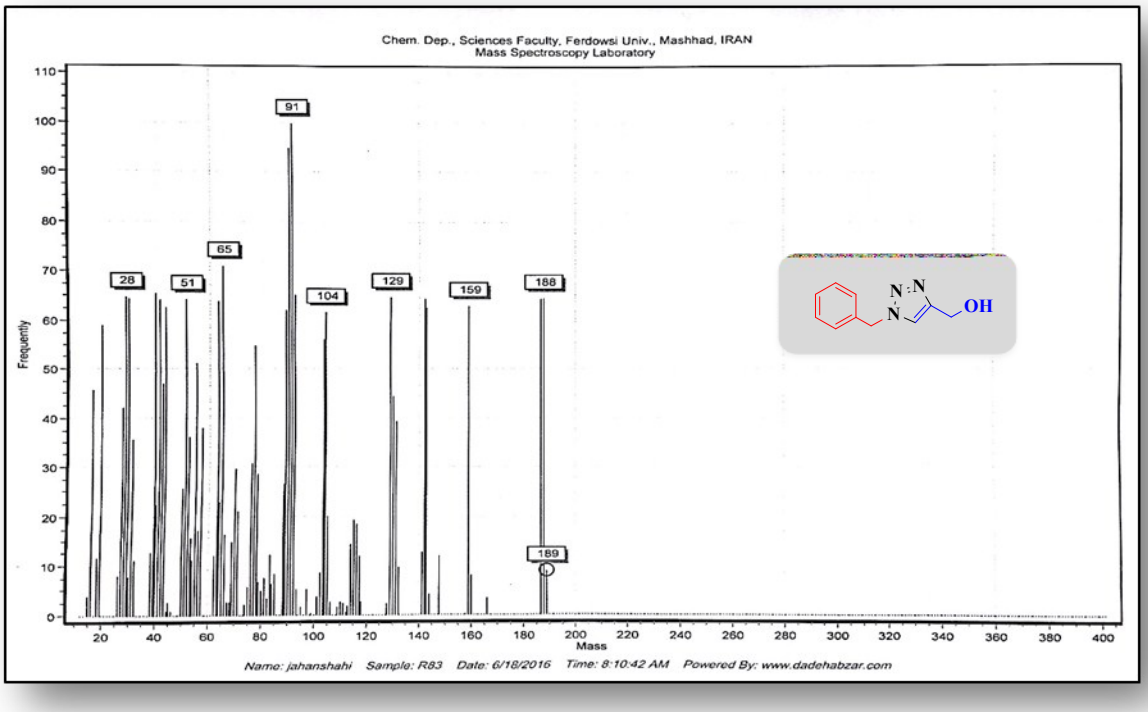


Figure 30: Mass spectrum of 1-benzyl-1*H*-1,2,3-triazol-4-yl)methanol **(Table 3, Entry 9).**

1-benzyl-4-pentyl-1*H*-1,2,3-triazole (Table 3, Entry 10) (0.18 g, 77%); yellow-green solid (crystals); mp 41-42 ºC (from EtOH) (Lit.[9] 42–43 ºC); ^{1}H NMR: δH (300 MHz; $CDCl_3$; Me_4Si) 7.29-7.26 (3 H, m, C=CH , Ar-H), 7.21–7.17 (3 H, m, Ar-H), 5.41 (2 H, s, CH_2), 2.62 (2 H, t, J = 7.8 Hz, CH_2Bt), 1.6 (2 H, qn, J = 7.2 Hz, CH_2CH_2Pr), 1.29-1.22 (4 H, m, Et $CH_2CH_2CH_3$), 0.83 (3 H, t, J = 6.9 Hz, CH_3); ^{13}C NMR: δC (75 MHz; $CDCl_3$; Me_4Si) 148, 135, 129, 128, 127, 120, 54, 31, 29, 25, 22, 14; MS, *m/z* 229 (M^+, 4%), 227 (70, M – 2H), 172 (68, M – C_4H_9), 91 (99, M – $C_7H_{12}N_3$), 83 (70), 57 (70, M – $C_{10}H_{10}N_3$), 43 (67, M – $C_{11}H_{12}N_3$), 29 (47, M – $C_{12}H_{14}N_3$), 28 (75, M – $C_{14}H_{19}N$).

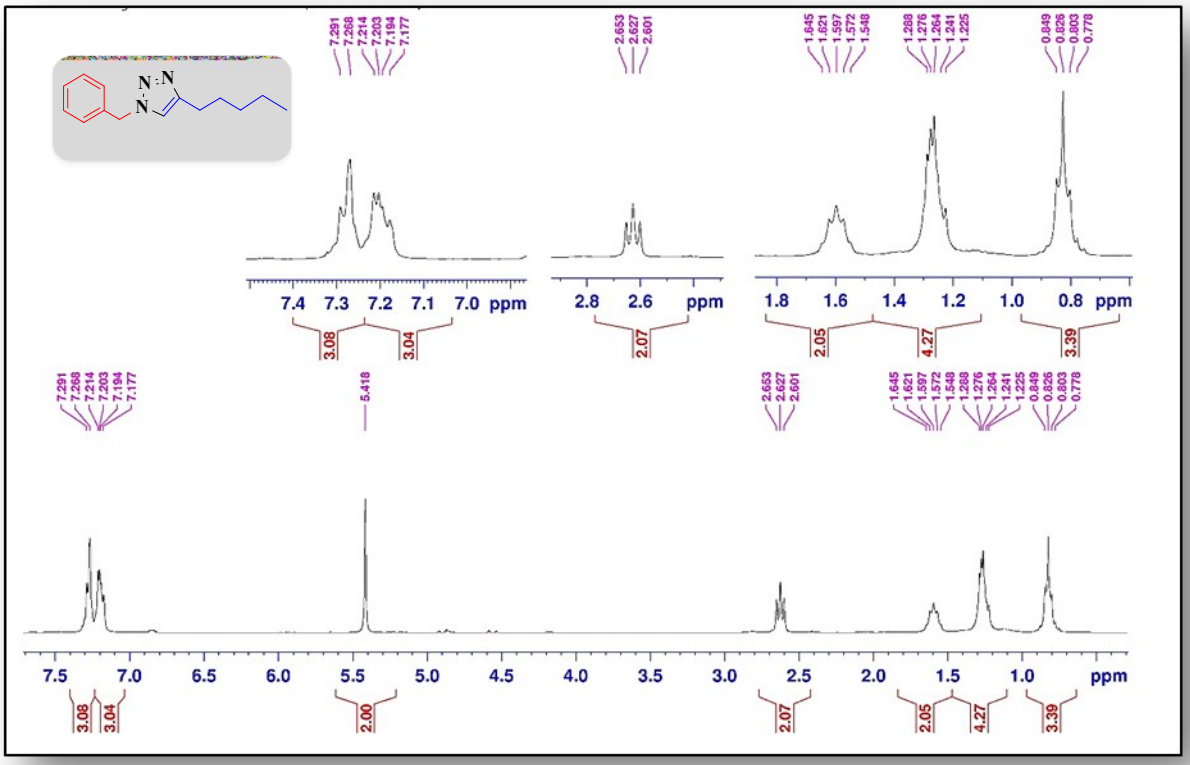


Figure 31: ^{1}H NMR (300 MHz, $CDCl_3$) of 1-benzyl-4-pentyl-1*H*-1,2,3-triazole **(Table 3, Entry 10).**

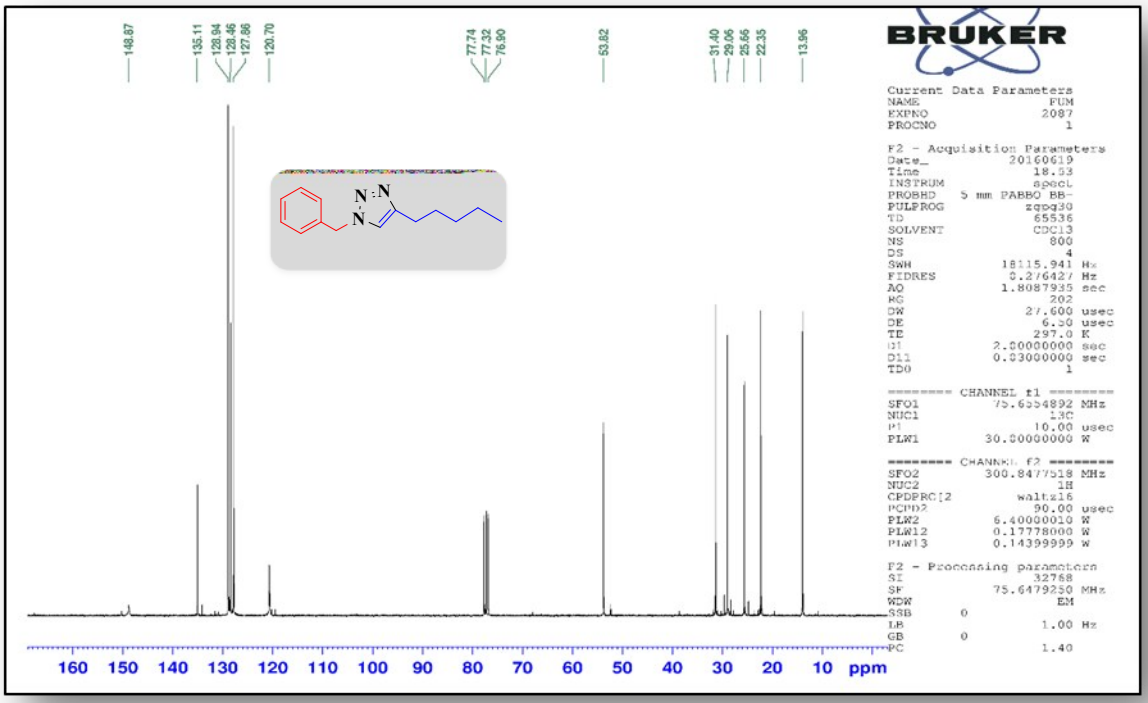


Figure 32: ^{13}C NMR (300 MHz, $CDCl_3$) of 1-benzyl-4-pentyl-1*H*-1,2,3-triazole **(Table 3, Entry 10).**

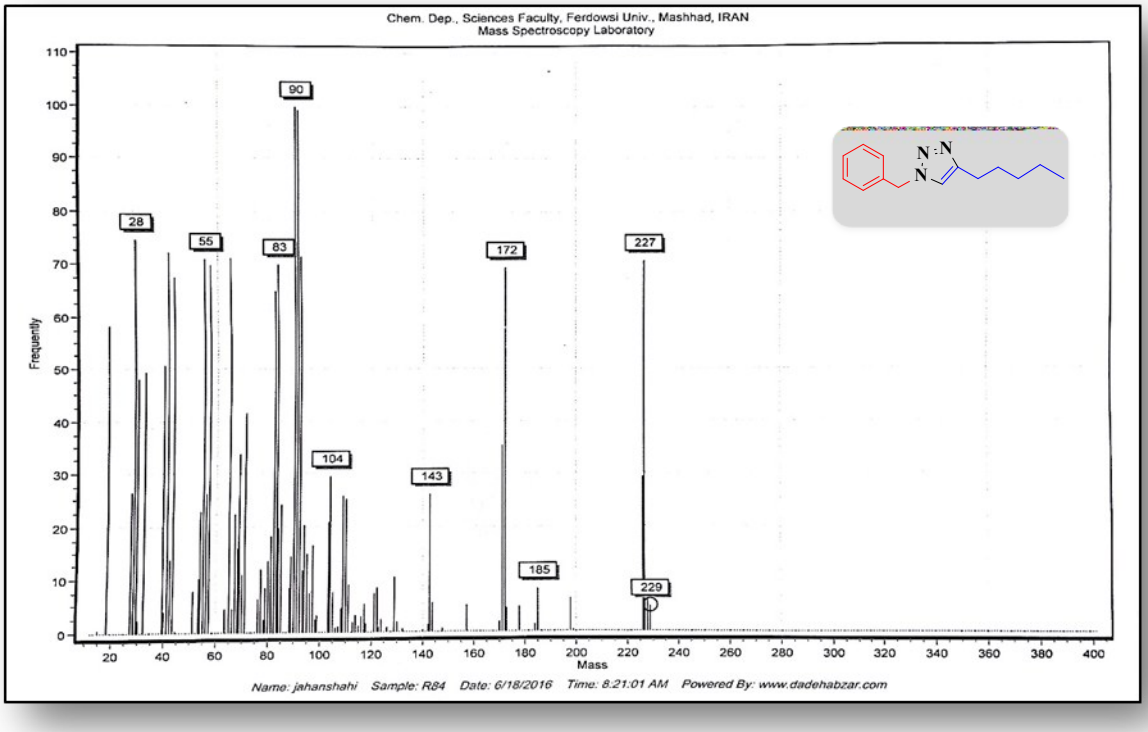


Figure 33: Mass spectrum of 1-benzyl-4-pentyl-1*H*-1,2,3-triazole **(Table 3, Entry 10).**

1-(4-chlorobenzyl)-4-phenyl-1*H*-1,2,3-triazole (Table 3, Entry 11) (0.26 g, 95%); 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=CH), 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, CH_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 – $C_{15}H_{12}ClN$).

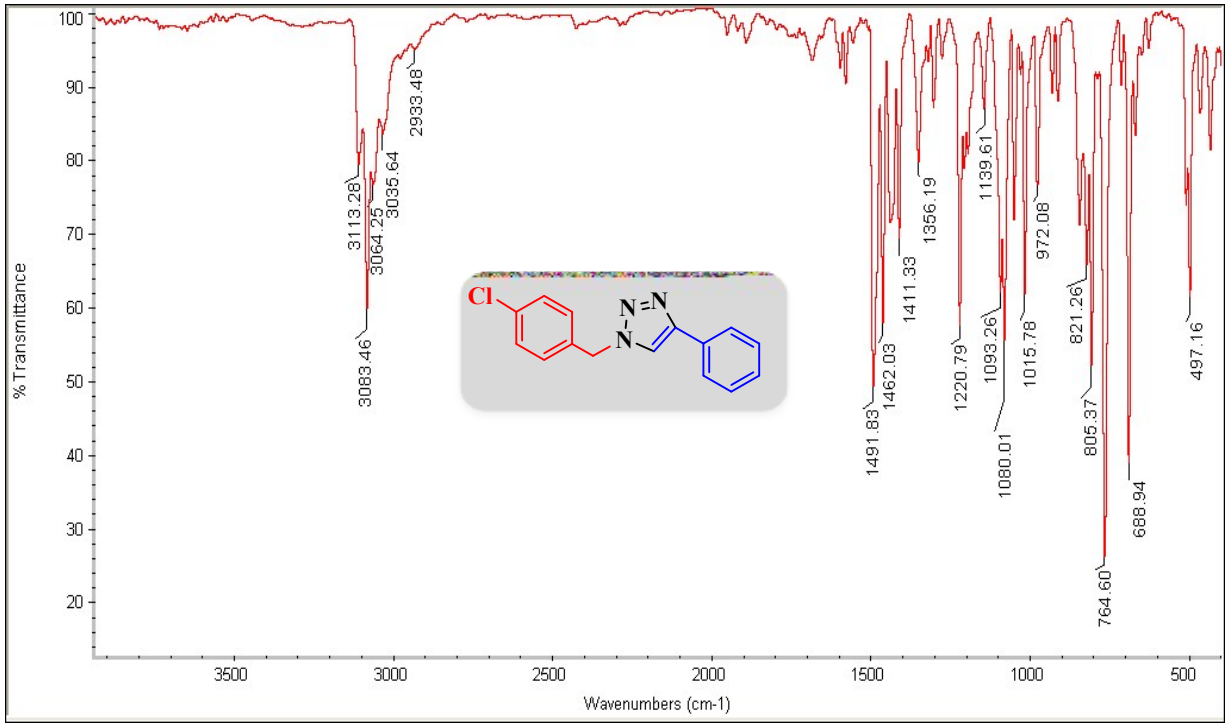


Figure 34: FT-IR (KBr) of 1-(4-chlorobenzyl)-4-phenyl-1*H*-1,2,3-triazole **(Table 3, Entry 11).**

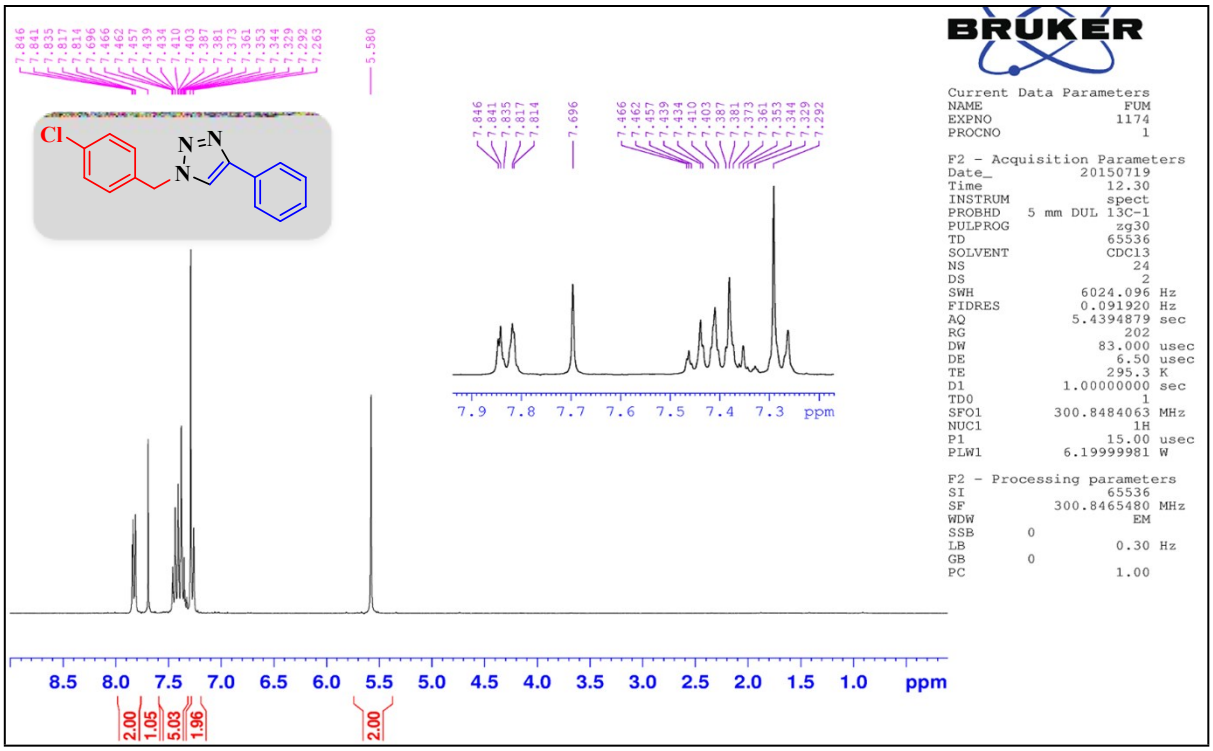


Figure 35: ^{1}H NMR (300 MHz, $CDCl_3$) of 1-(4-chlorobenzyl)-4-phenyl-1*H*-1,2,3-triazole **(Table 3, Entry 11).**

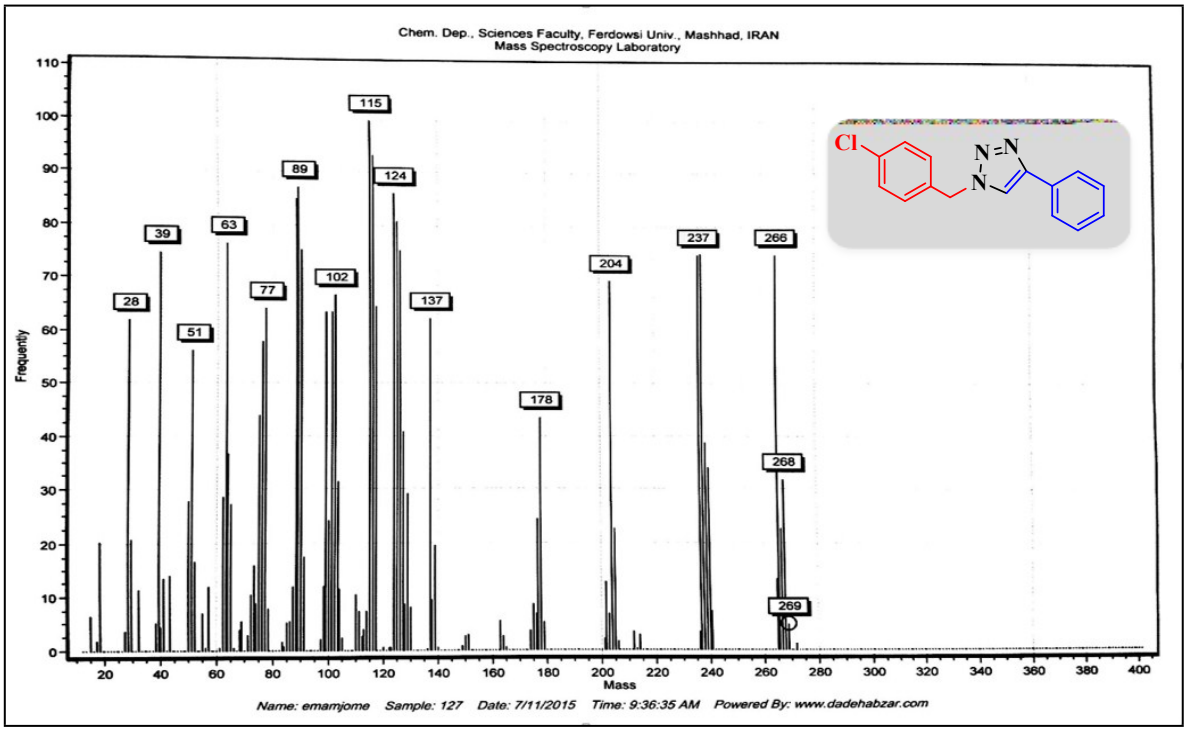


Figure 36: Mass spectrum of 1-(4-chlorobenzyl)-4-phenyl-1*H*-1,2,3-triazole **(Table 3, Entry 11).**

1-(4-chlorobenzyl)-4-(*p*-tolyl)-1*H*-1,2,3-triazole (Table 3, Entry 12) (0.26 g, 91%); 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=CH), 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, CH_2), 2.39 (3 H, s, CH_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 – $C_{15}H_{11}ClN_3$).

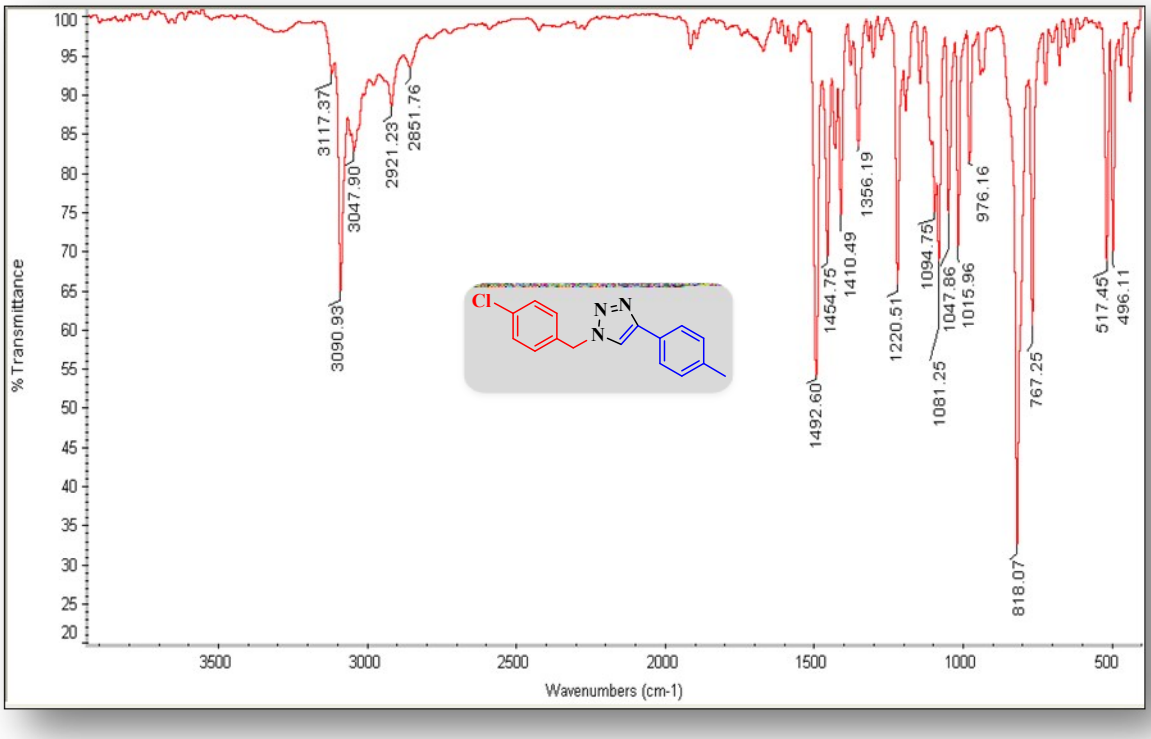


Figure 37: FT-IR (KBr) of 1-(4-chlorobenzyl)-4-(*p*-tolyl)-1*H*-1,2,3-triazole **(Table 3, Entry 12)**.

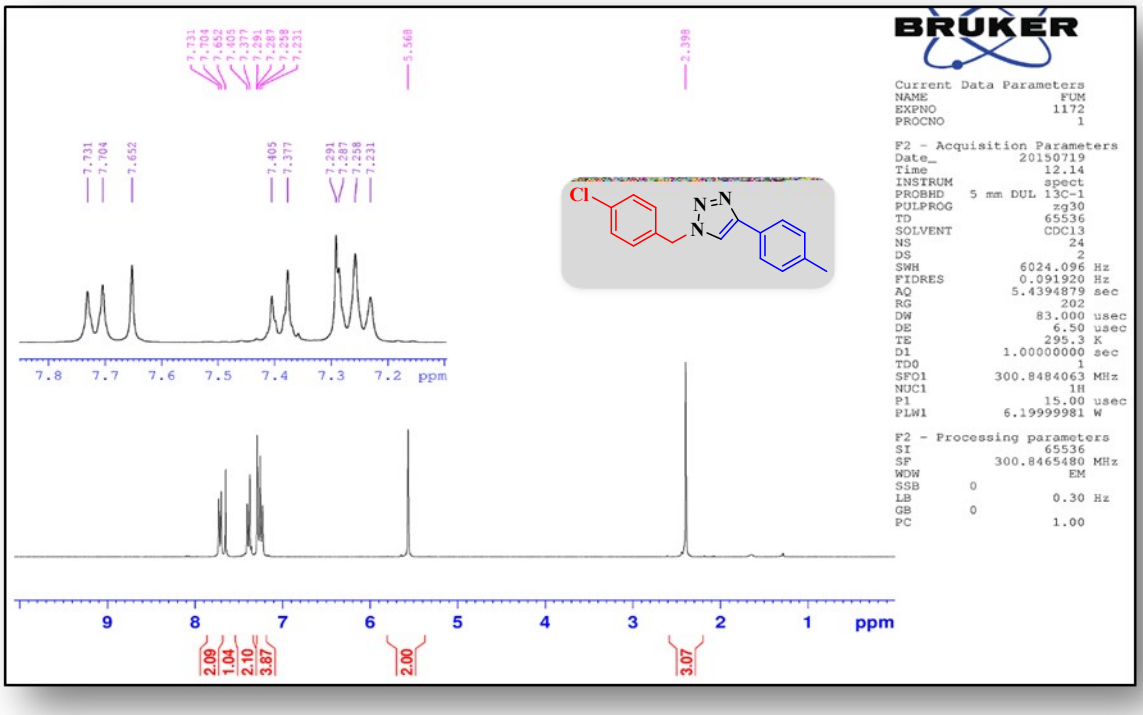


Figure 38: ^{1}H NMR (300 MHz, $CDCl_3$) of 1-(4-chlorobenzyl)-4-(*p*-tolyl)-1*H*-1,2,3-triazole **(Table 3, Entry 12)**.

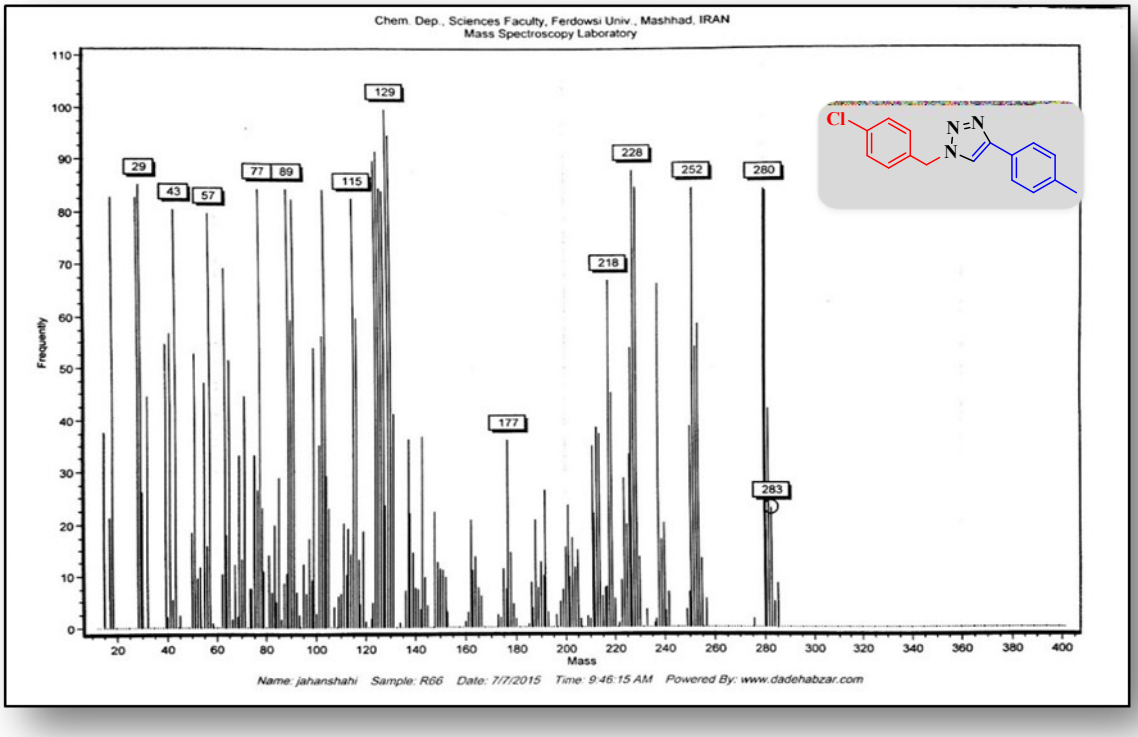
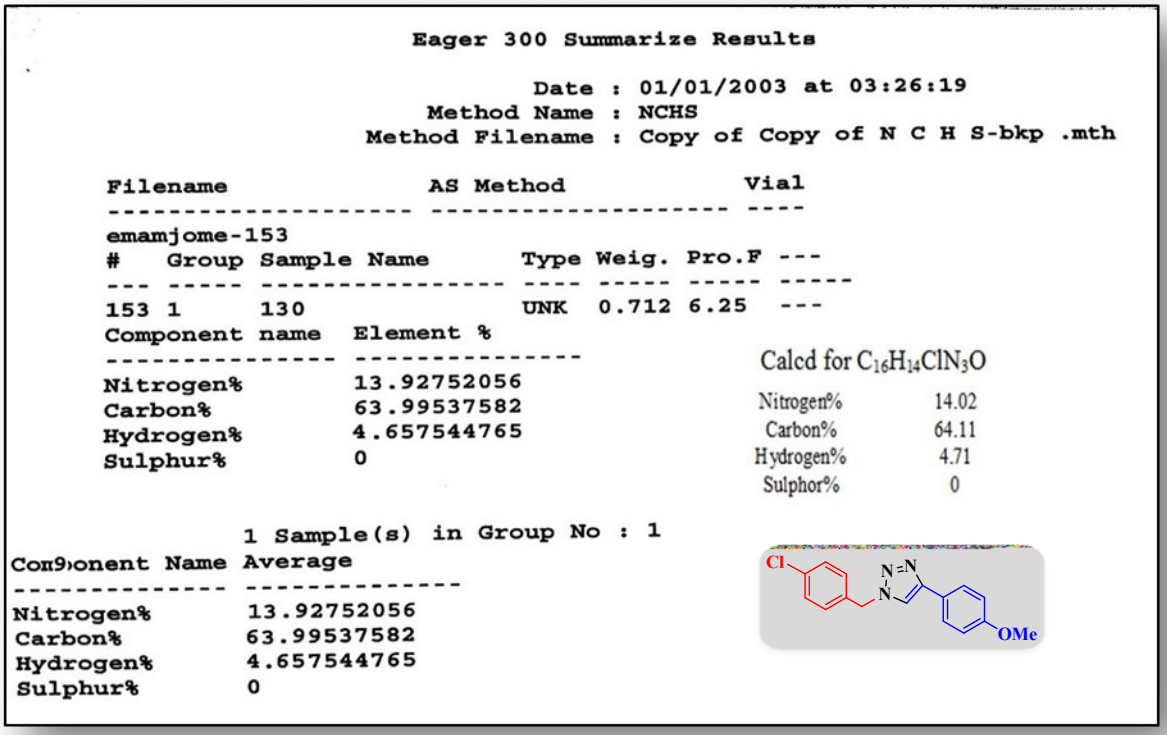


Figure 39: Mass spectrum of 1-(4-chlorobenzyl)-4-(*p*-tolyl)-1*H*-1,2,3-triazole **(Table 3, Entry 12)**.

1-(4-chlorobenzyl)-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (Table 3, Entry 13) (0.26 g, 87%); white solid (crystals); mp 150-151 ºC (from EtOH) (Lit.[10] 150–152 ºC); 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=CH), 6.96 (2 H, d, *J* = 6.3 Hz, Ar-H), 5.55 (2 H, s, CH_2), 2.86 (3 H, s, CH_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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Method Filename : Copy of Copy of N C H S-bkp .mth

Filename	AS Method	Vial
emamjome-153		

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Carbon%	63.99537582
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 40: Elemental analysis of 1-(4-chlorobenzyl)-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole **(Table 3, Entry 13).**

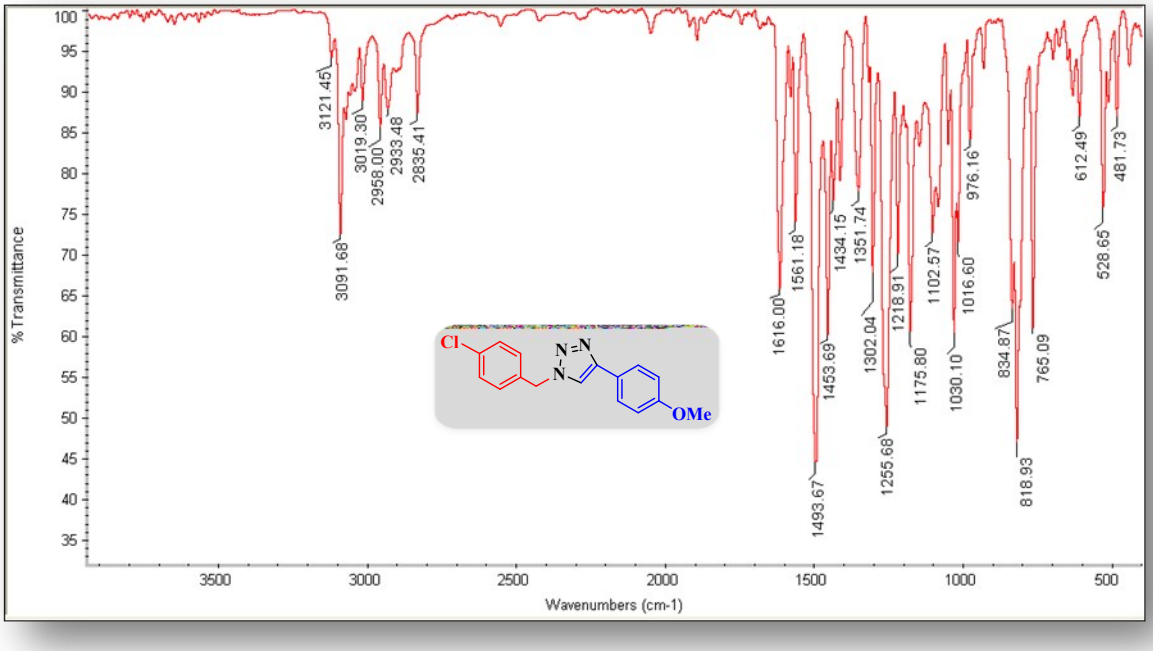

Figure 41: FT-IR (KBr) of 1-(4-chlorobenzyl)-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole **(Table 3, Entry 13).**

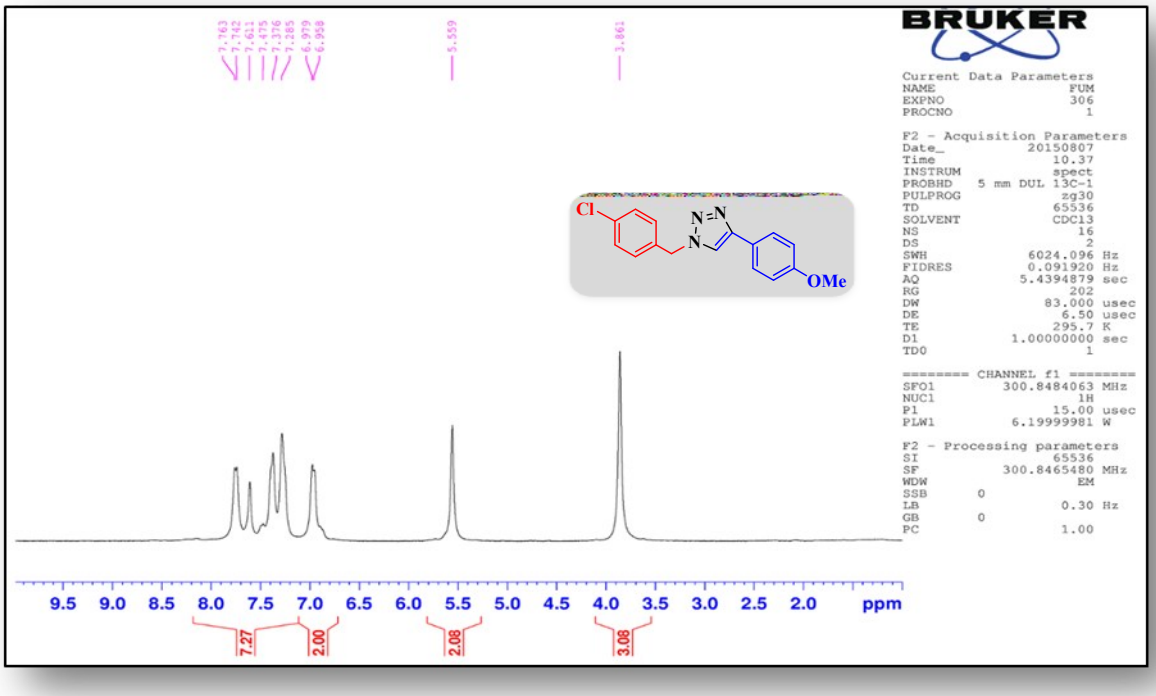

Figure 42: ^{1}H NMR (300 MHz, $CDCl_3$) of 1-(4-chlorobenzyl)-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole **(Table 3, Entry 13).**

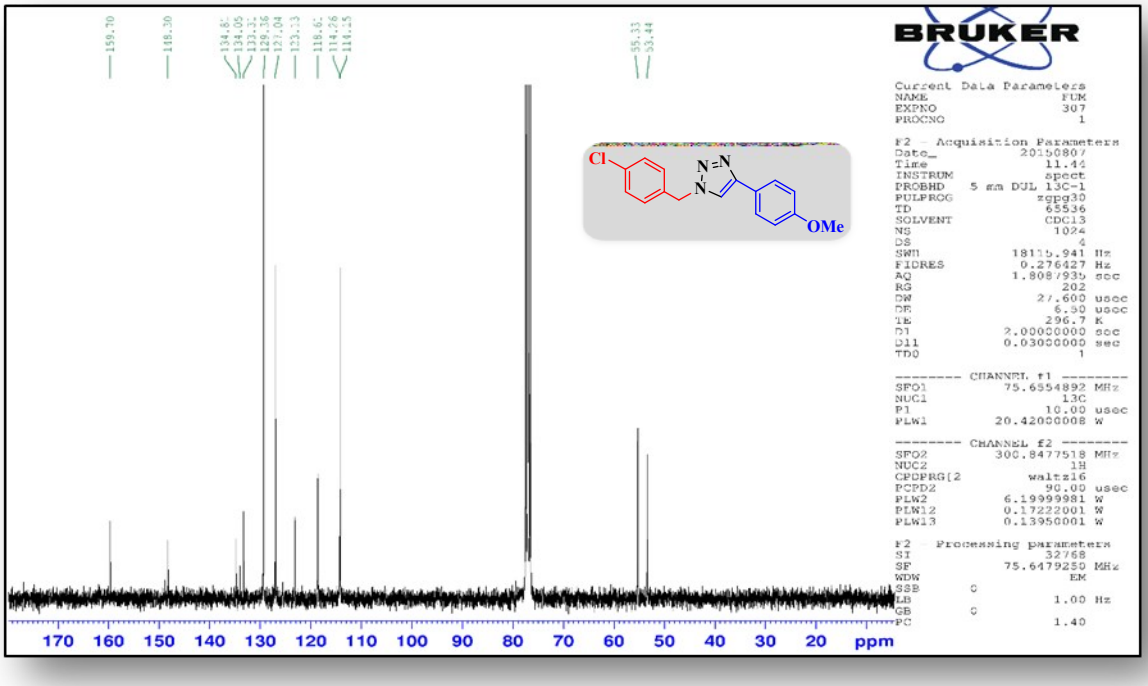

Figure 43: ^{13}C NMR (75MHz, $CDCl_3$) of 1-(4-chlorobenzyl)-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole **(Table 3, Entry 13).**

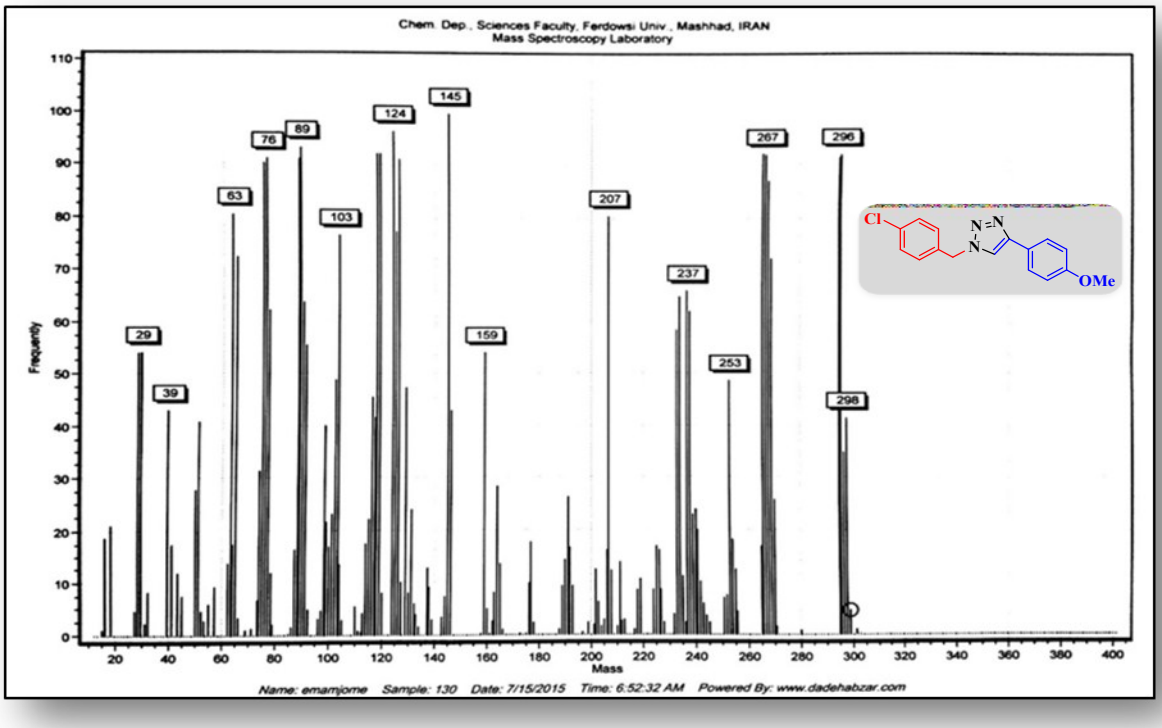

Figure 44: Mass spectrum of 1-(4-chlorobenzyl)-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole **(Table 3, Entry 13).**

4-(4-(*tert*-butyl)phenyl)-1-(4-chlorobenzyl)-1*H*-1,2,3-triazole (Table 3, Entry 14) (0.29 g, 88%); white solid (crystals); mp 153-154ºC (from EtOH) (Lit.[10] 153–154 ºC); 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; ^{1}H 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=CH), 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, CH_2), 1.36 (9 H, s, 3 CH_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).

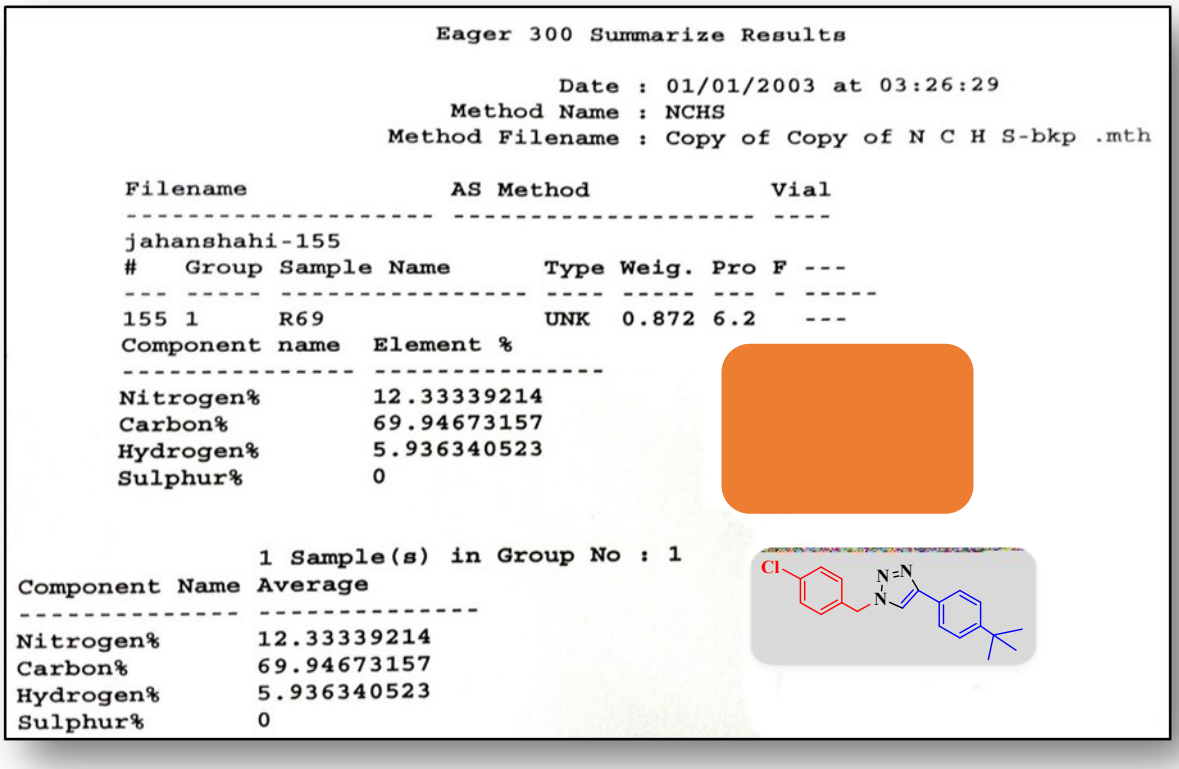

Figure 45: Elemental analysis of 4-(4-(*tert*-butyl)phenyl)-1-(4-chlorobenzyl)-1*H*-1,2,3-triazole **(Table 3, Entry 14).**

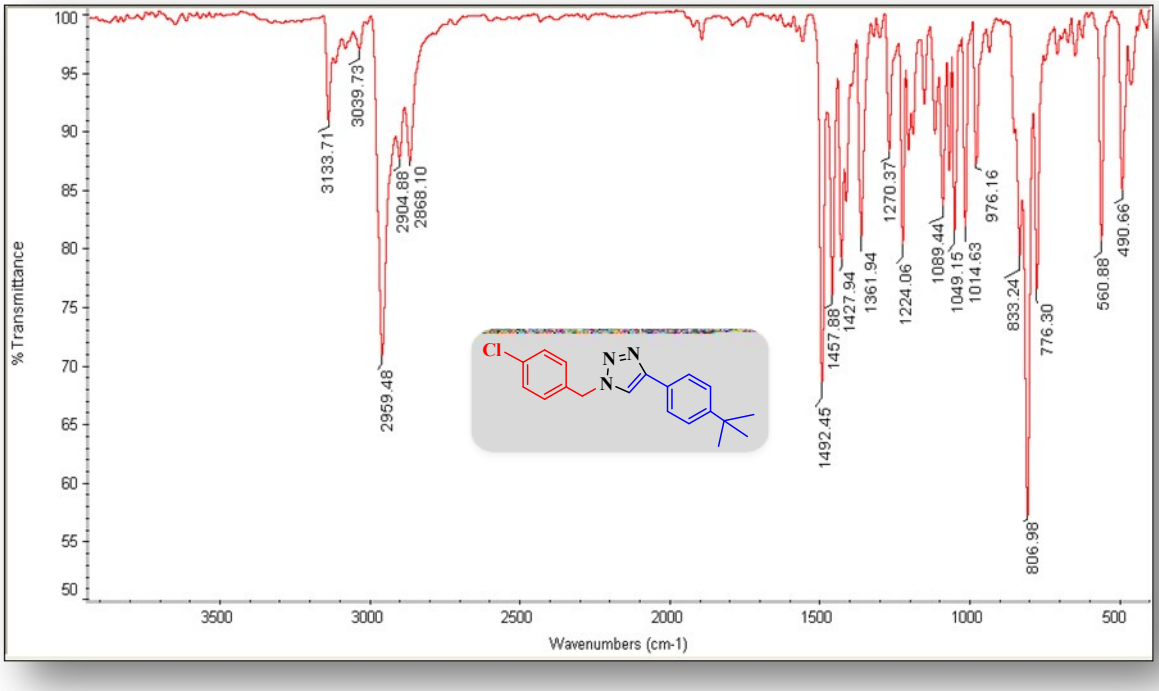

Figure 46: FT-IR (KBr) of 4-(4-(*tert*-butyl)phenyl)-1-(4-chlorobenzyl)-1*H*-1,2,3-triazole **(Table 3, Entry 14)**.

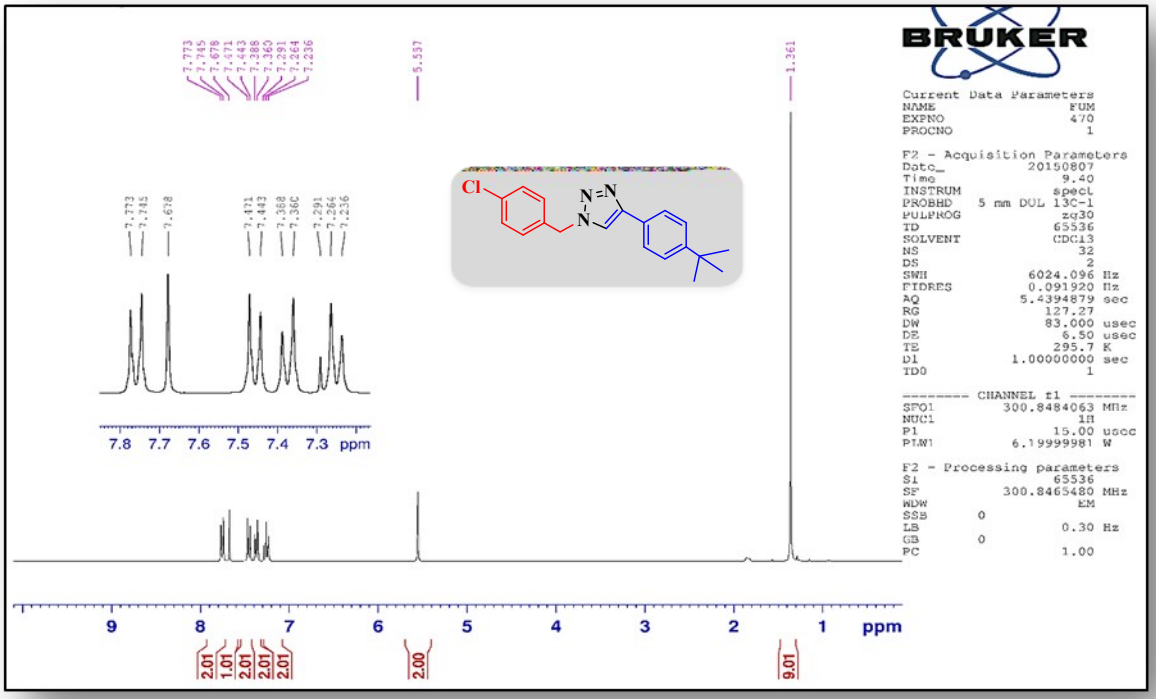

Figure 47: ^{1}H NMR (300 MHz, $CDCl_3$) of 4-(4-(*tert*-butyl)phenyl)-1-(4-chlorobenzyl)-1*H*-1,2,3-triazole **(Table 3, Entry 14)**.

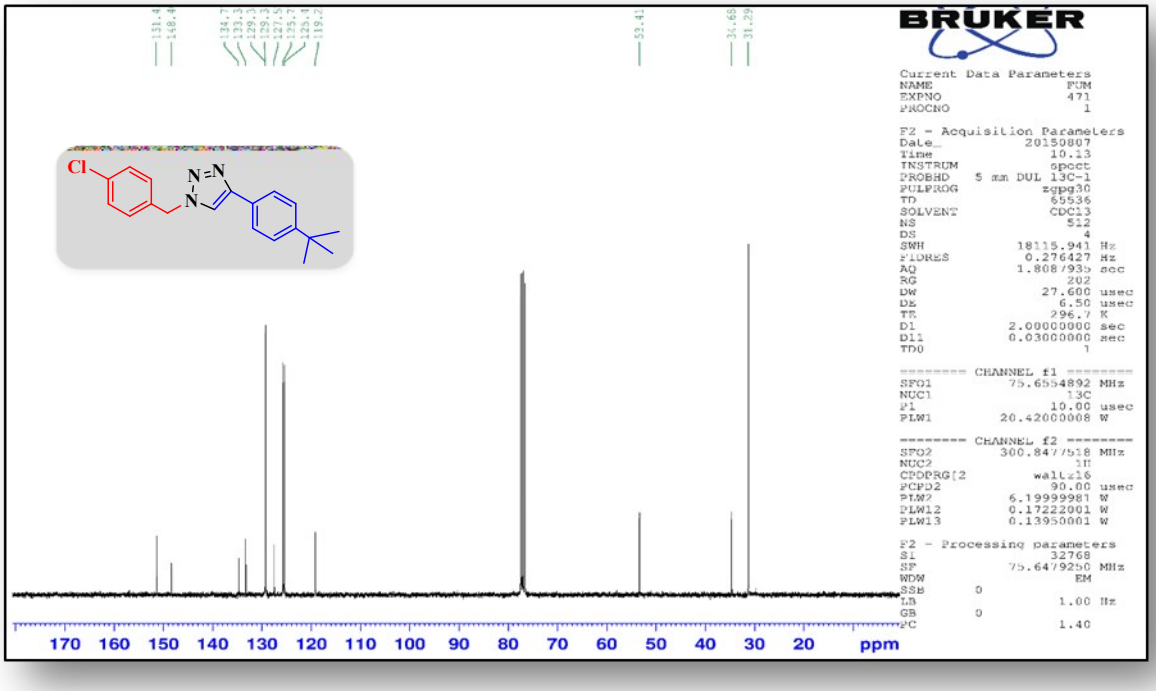

Figure 48: ^{13}C NMR (75MHz, $CDCl_3$) of 4-(4-(*tert*-butyl)phenyl)-1-(4-chlorobenzyl)-1*H*-1,2,3-triazole **(Table 3, Entry 14)**.

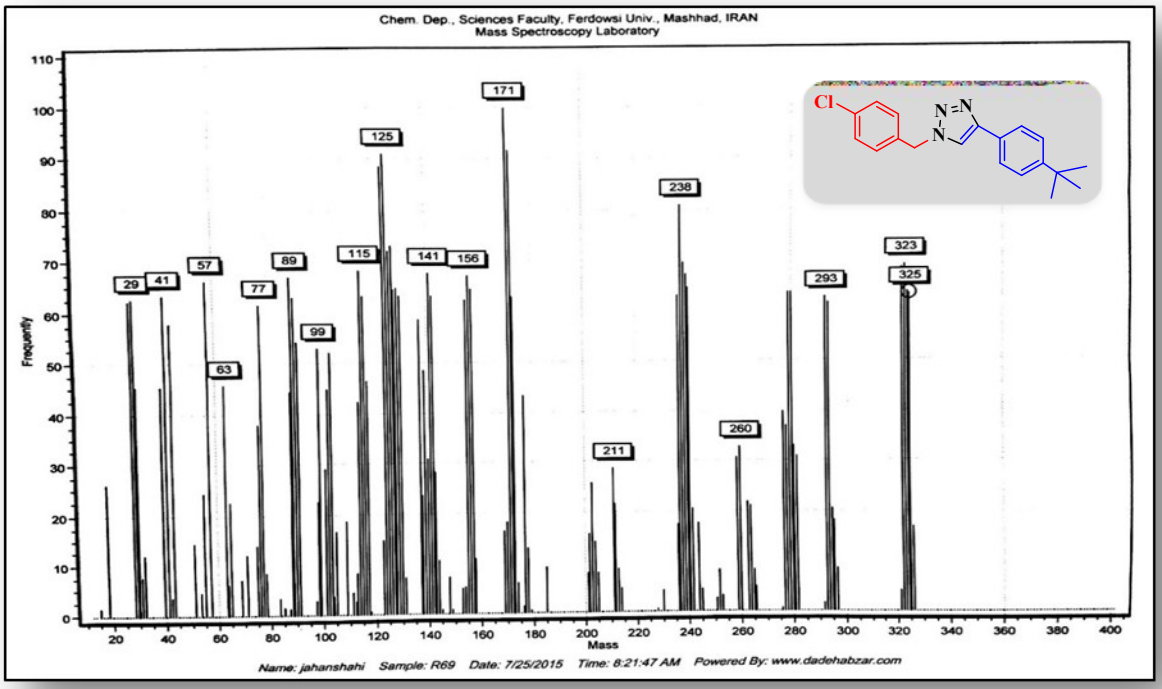

Figure 49: Mass spectrum of 4-(4-(*tert*-butyl)phenyl)-1-(4-chlorobenzyl)-1*H*-1,2,3-triazole **(Table 3, Entry 14)**.

2-(1-(4-chlorobenzyl)-1*H*-1,2,3-triazol-4-yl)pyridine (Table 3, Entry 15) (0.20 g, 74 %); 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=CH), 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, CH_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 – $C_{14}H_{11}ClN_2$).

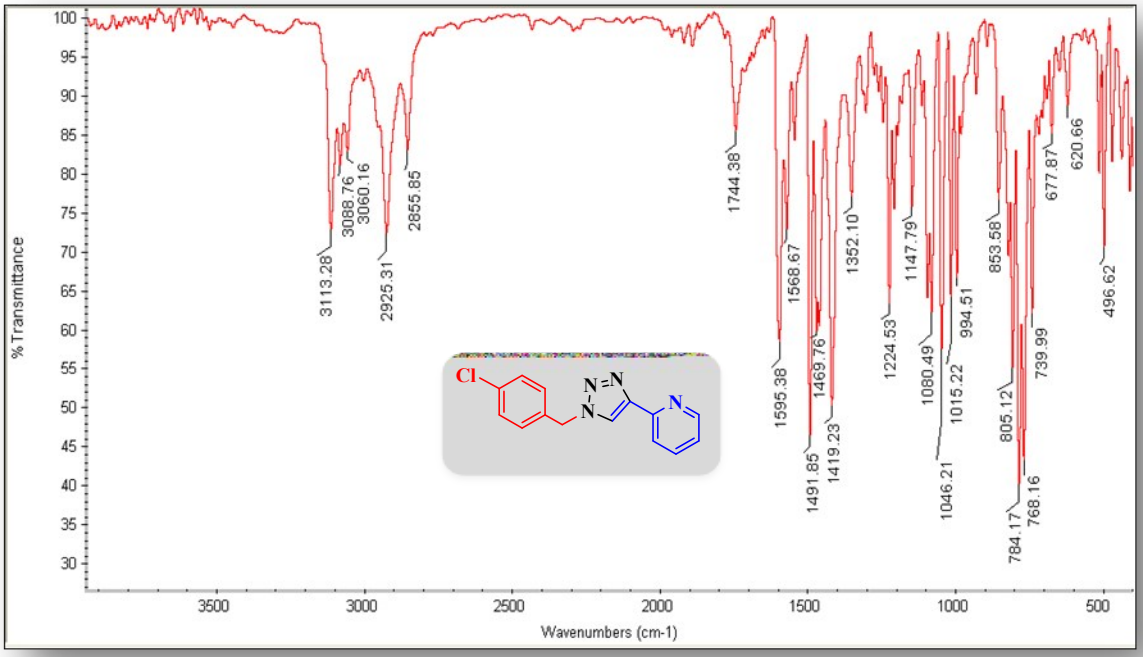

Figure 50: FT-IR (KBr) of 2-(1-(4-chlorobenzyl)-1*H*-1,2,3-triazol-4-yl)pyridine **(Table 3, Entry 15).**

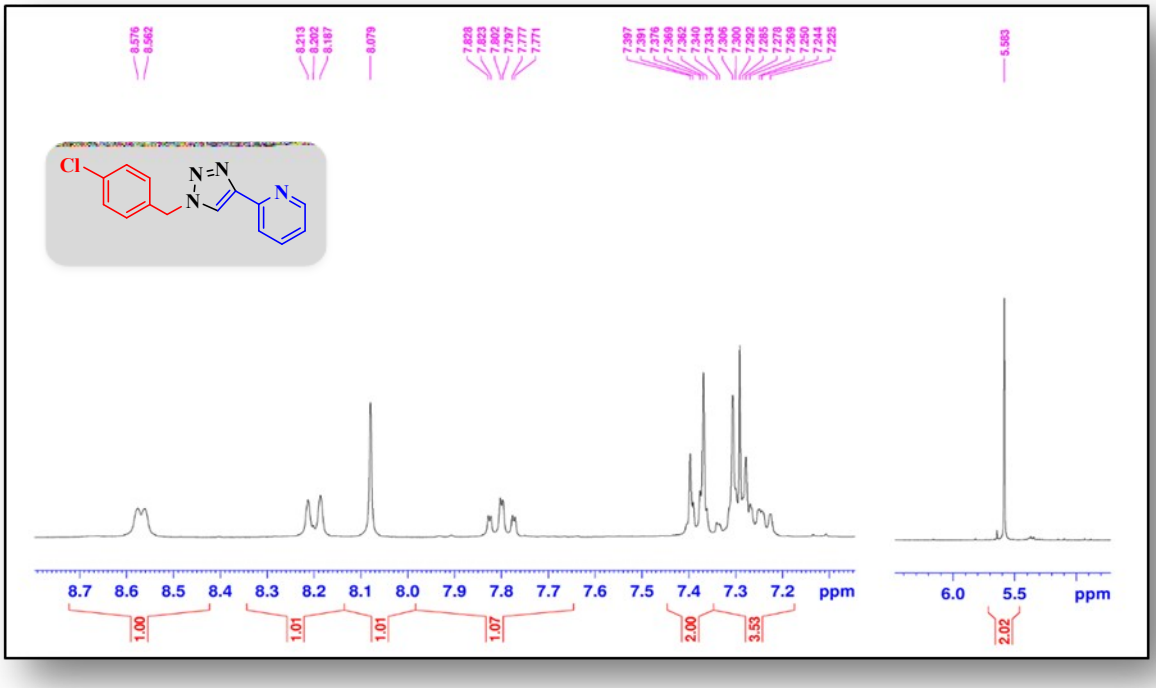

Figure 51: ^{1}H NMR (300 MHz, $CDCl_3$) of 2-(1-(4-chlorobenzyl)-1*H*-1,2,3-triazol-4-yl)pyridine **(Table 3, Entry 15).**

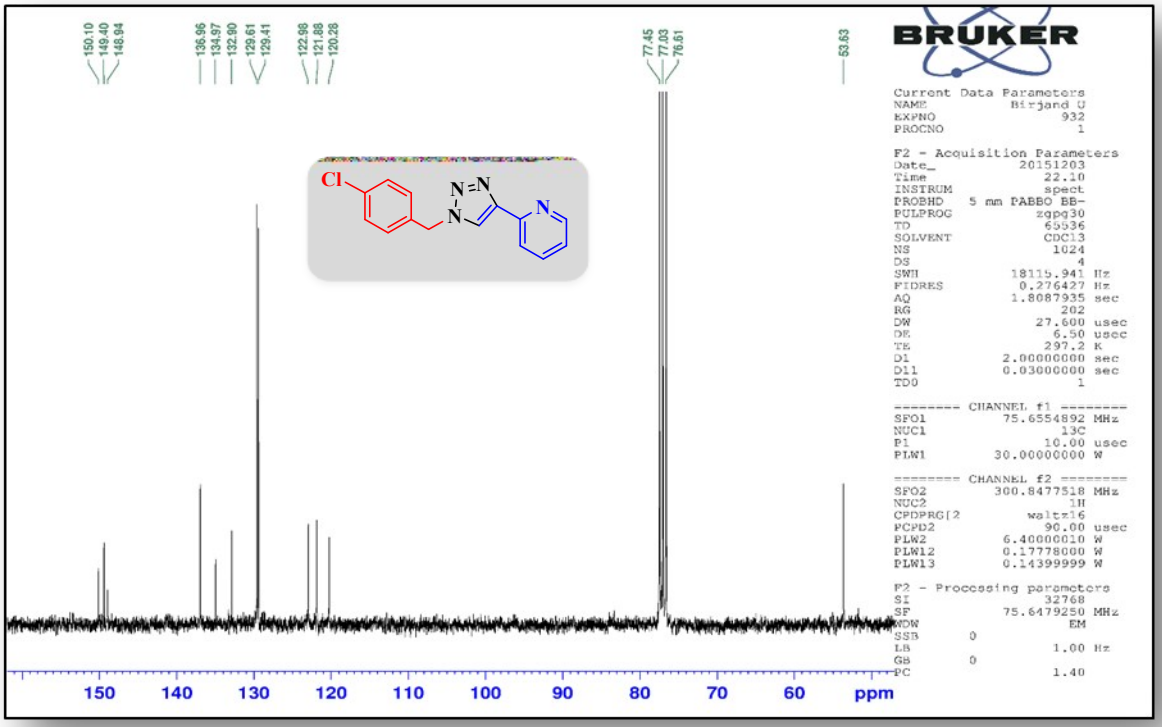

Figure 52: ^{13}C NMR (75MHz, $CDCl_3$) of 2-(1-(4-chlorobenzyl)-1*H*-1,2,3-triazol-4-yl)pyridine **(Table 3, Entry 15).**

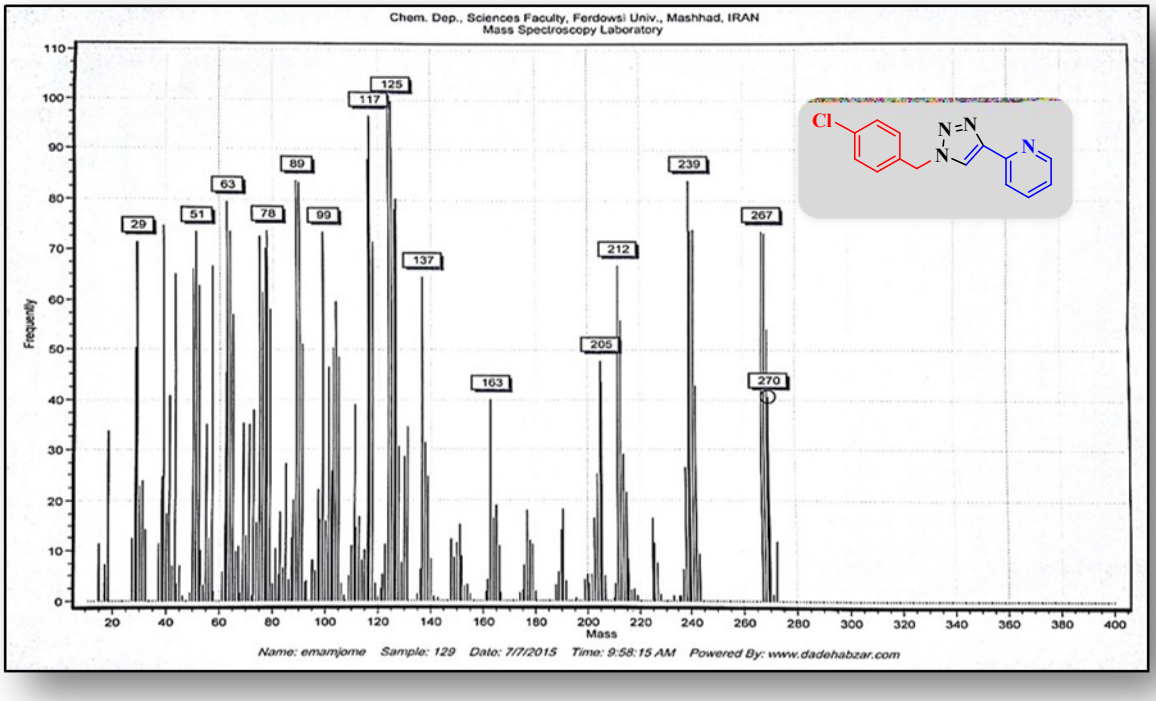

Figure 53: Mass spectrum of 2-(1-(4-chlorobenzyl)-1*H*-1,2,3-triazol-4-yl)pyridine **(Table 3, Entry 15).**

1-(4-nitrobenzyl)-4-phenyl-1*H*-1,2,3-triazole (Table 3, Entry 16) (0.23 g, 85%); white solid (crystals); mp 157–158 ºC (from EtOH) (Lit.[11] 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; ^{1}H 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=CH), 7.48-7.29 (5 H, m, Ar-H), 5.72 (2 H, s, CH_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 – $C_{15}H_{12}N_2O_2$).

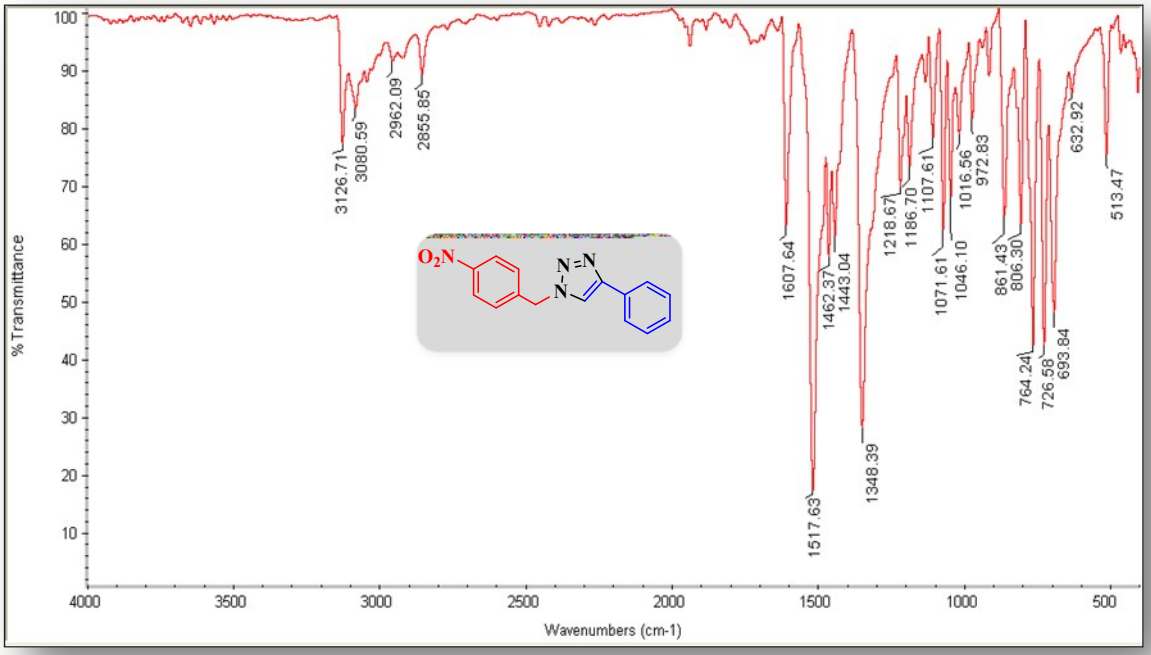

Figure 45: FT-IR (KBr) of 1-(4-nitrobenzyl)-4-phenyl-1*H*-1,2,3-triazole **(Table 3, Entry 16)**.

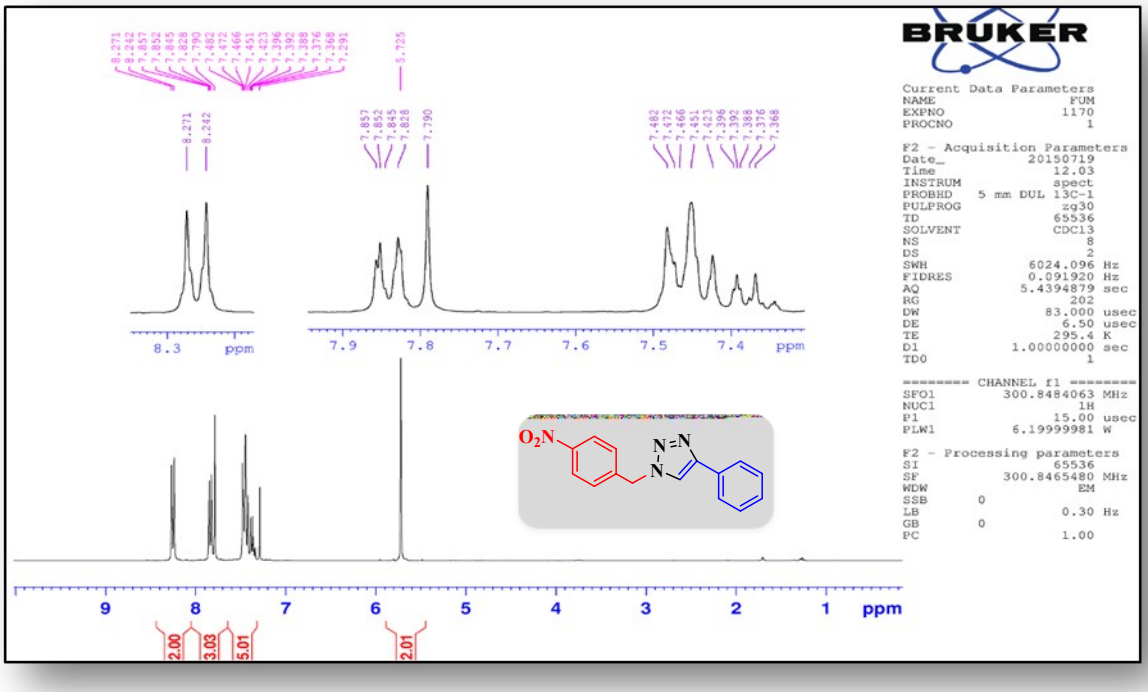

Figure 55: ^{1}H NMR (300 MHz, $CDCl_3$) of 1-(4-nitrobenzyl)-4-phenyl-1*H*-1,2,3-triazole **(Table 3, Entry 16)**.

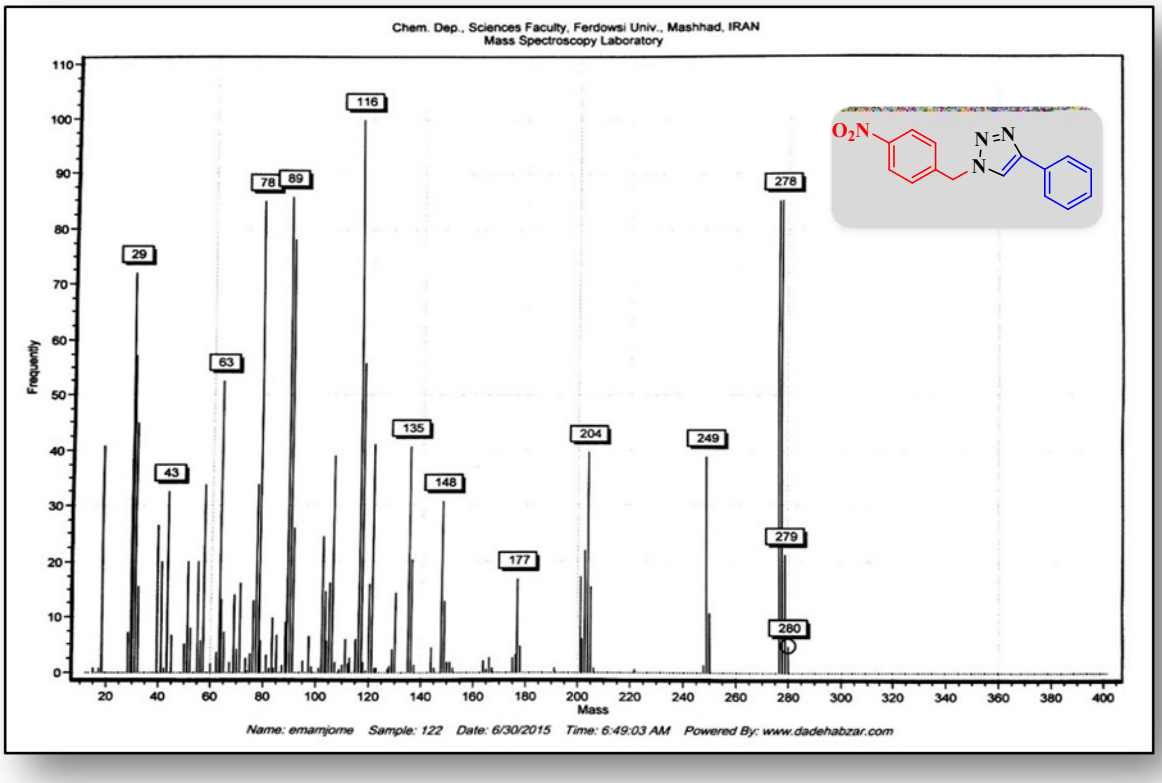

Figure 56: Mass spectrum of 1-(4-nitrobenzyl)-4-phenyl-1*H*-1,2,3-triazole **(Table 3, Entry 16)**.

1-(4-nitrobenzyl)-4-(*p*-tolyl)-1*H*-1,2,3-triazole (Table 3, Entry 17) (0.24 g, 84%); white solid (crystals); mp 145–146 ºC (from EtOH) (Lit.[12] 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 – $C_{16}H_{14}N_2O_2$).

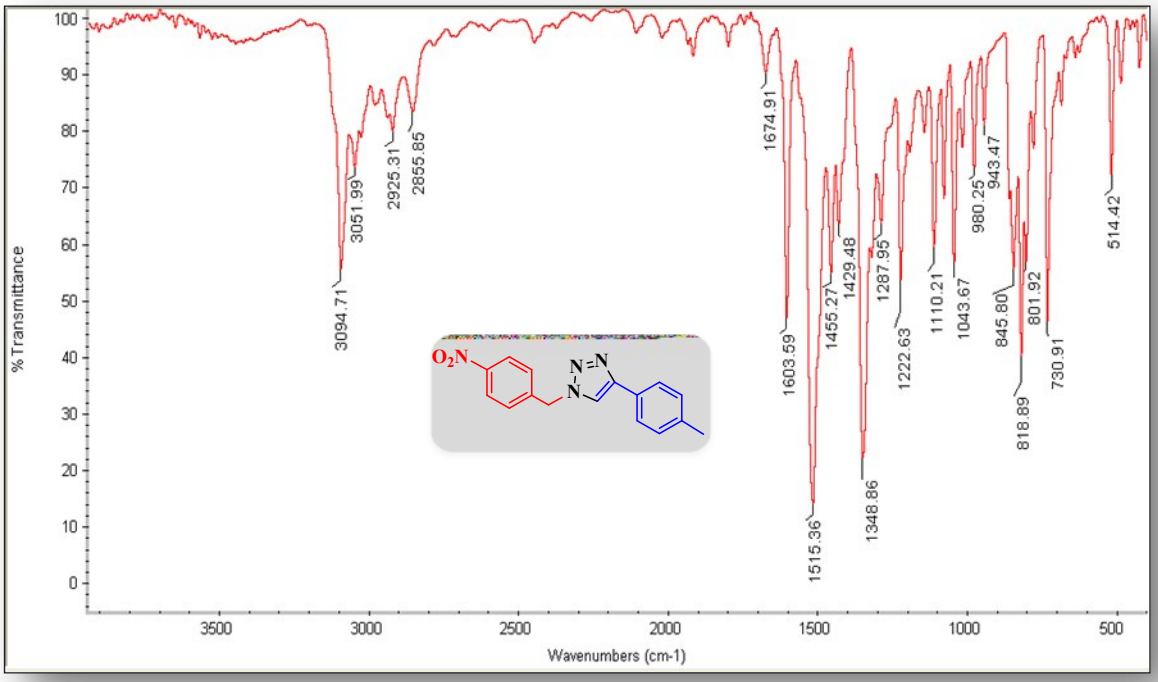

Figure 57: FT-IR (KBr) of 1-(4-nitrobenzyl)-4-(*p*-tolyl)-1*H*-1,2,3-triazole **(Table 3, Entry 17).**

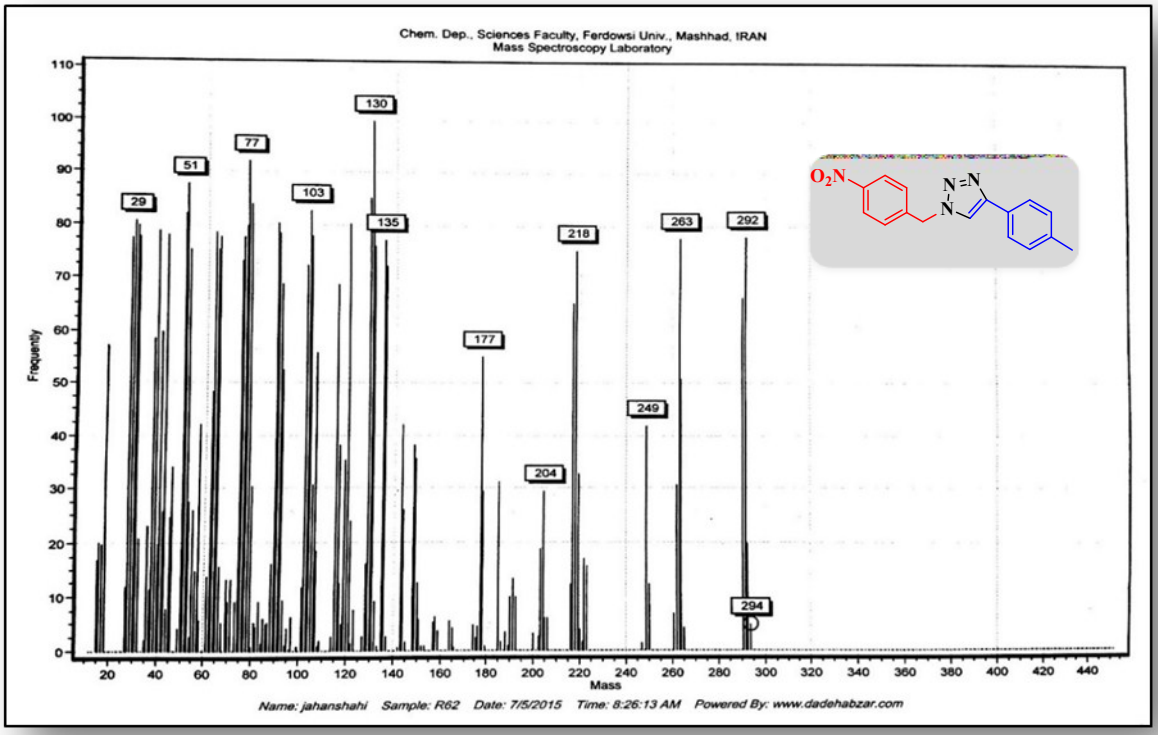

Figure 58: Mass spectrum of 1-(4-nitrobenzyl)-4-(*p*-tolyl)-1*H*-1,2,3-triazole **(Table 3, Entry 17).**

4-(4-methoxyphenyl)-1-(4-nitrobenzyl)-1*H*-1,2,3-triazole (Table 3, Entry 18) (0.27 g, 89%); white solid (crystals); mp 94–96 ºC (from EtOH) (Lit.[13] 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=CH), 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, CH_2), 3.83 (3 H, s, OCH_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 – $C_{16}H_{14}N_2O_3$).

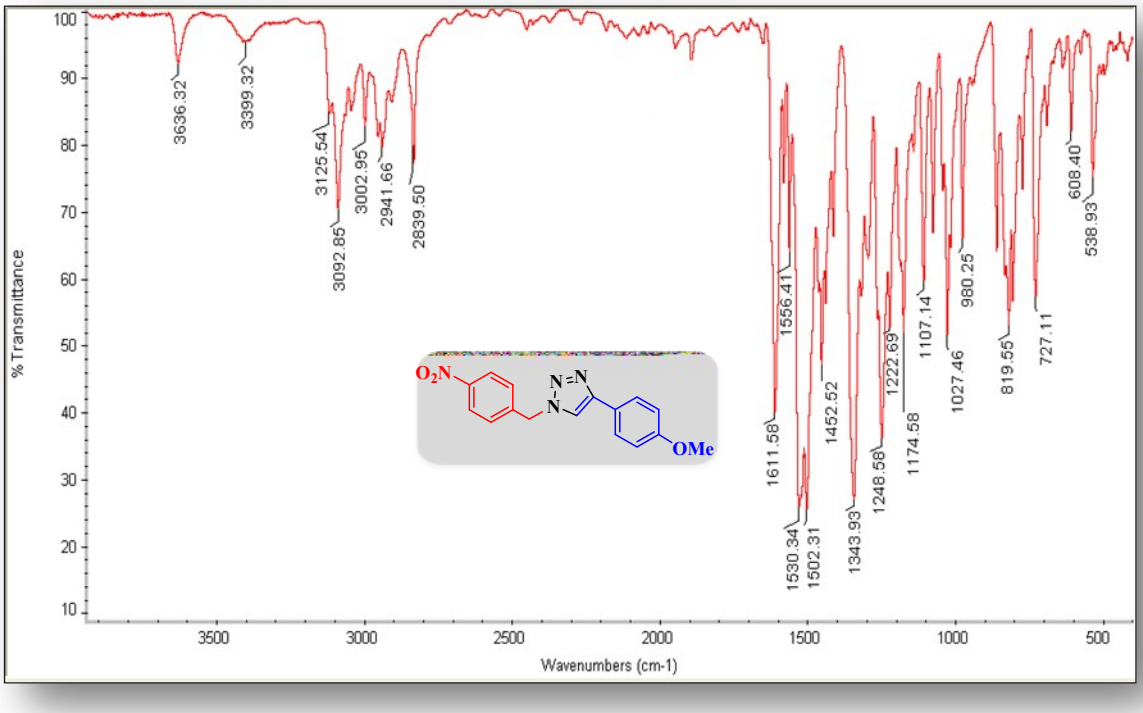

Figure 59: FT-IR (KBr) of 4-(4-methoxyphenyl)-1-(4-nitrobenzyl)-1*H*-1,2,3-triazole **(Table 3, Entry 18).**

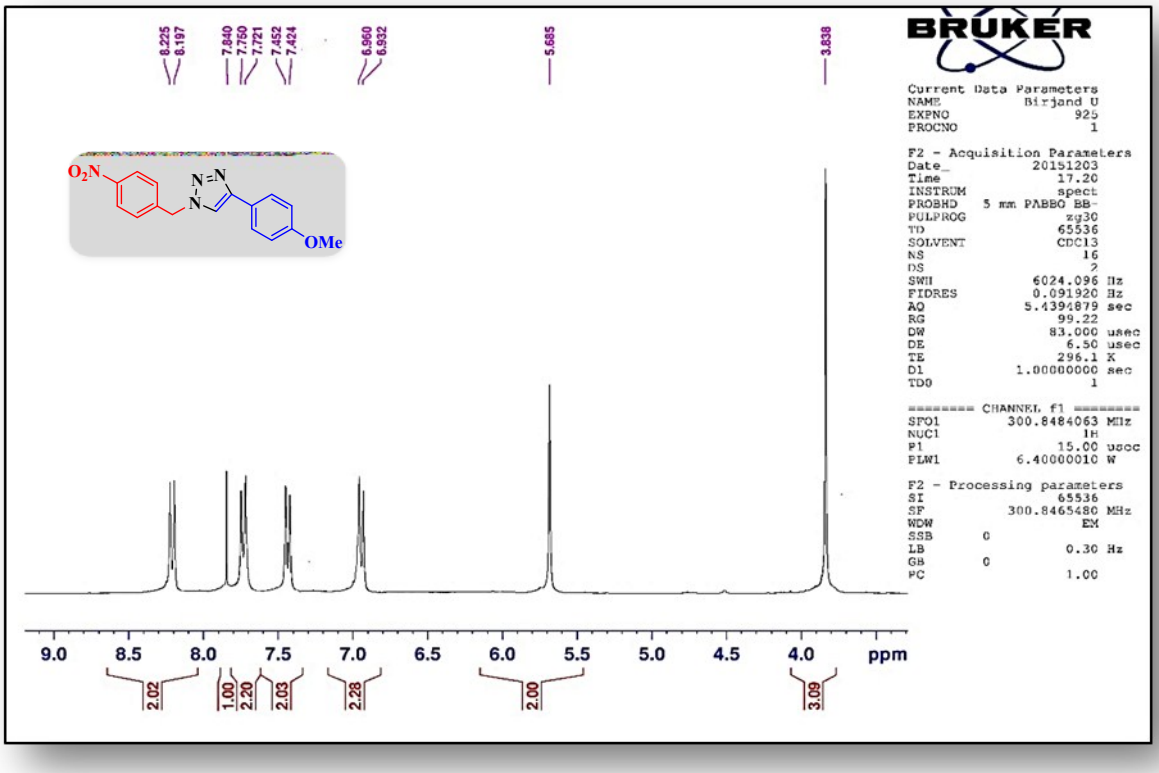

Figure 60: ^{1}H NMR (300 MHz, $CDCl_3$) of 4-(4-methoxyphenyl)-1-(4-nitrobenzyl)-1*H*-1,2,3-triazole **(Table 3, Entry 18).**

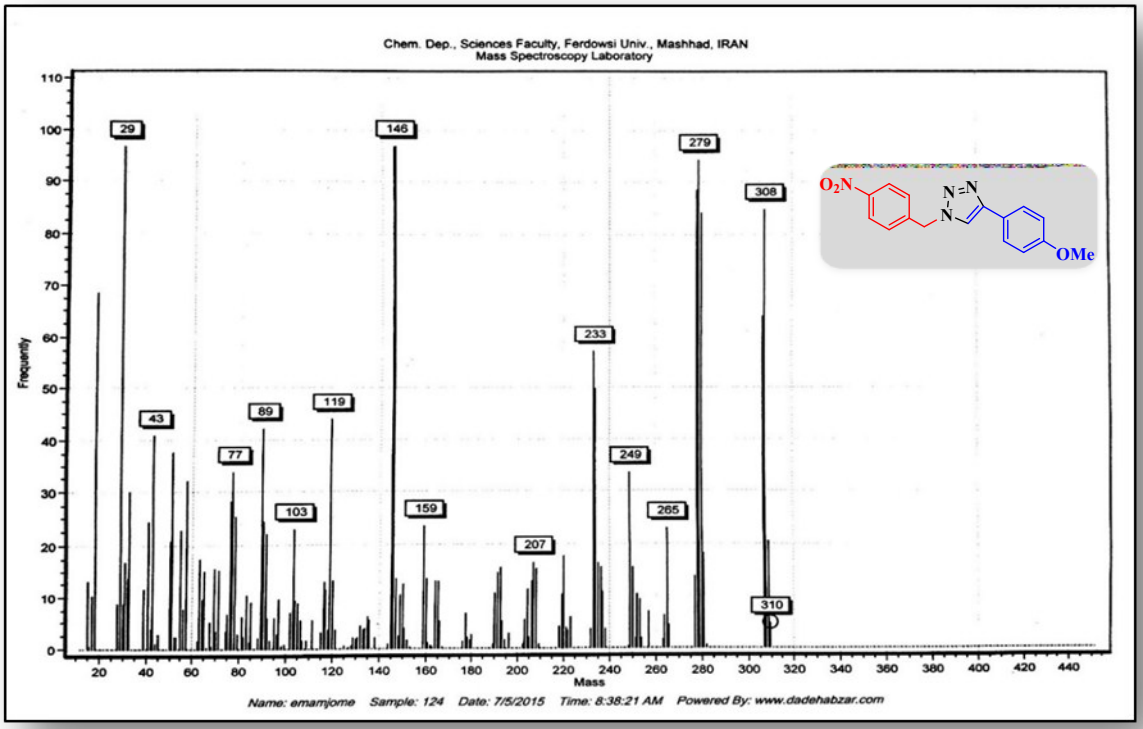

Figure 61: Mass spectrum of 4-(4-methoxyphenyl)-1-(4-nitrobenzyl)-1*H*-1,2,3-triazole **(Table 3, Entry 18).**

4-(4-(*tert*-butyl)phenyl)-1-(4-nitrobenzyl)-1*H*-1,2,3-triazole (Table 3, Entry 19) (0.26 g, 77%); white solid (crystals); mp 146-147 ºC (from EtOH) (Lit.[10] 145–147 ºC); 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=CH), 7.48-7.43 (4 H, m, Ar-H), 5.72 (2 H, s, CH_2), 1.36 (9 H, s, 3 CH_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 – $C_{19}H_{20}N_2O_2$).

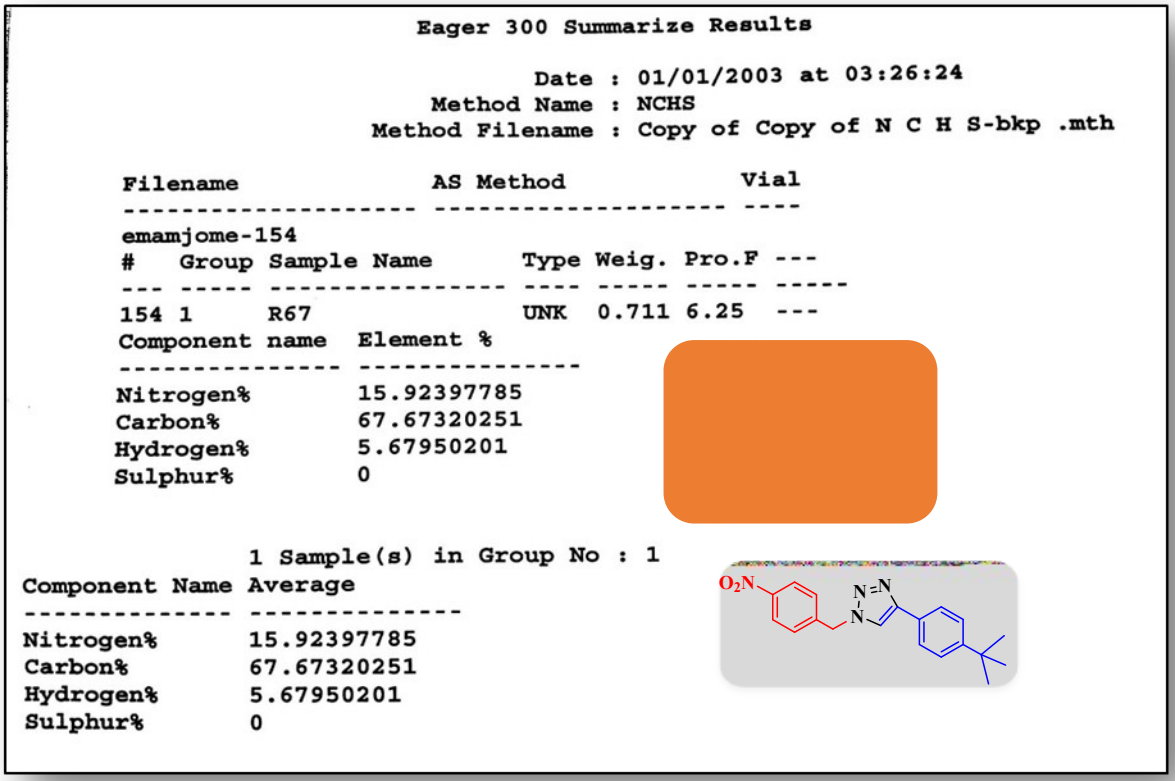

Figure 62: Elemental analysis of 4-(4-(*tert*-butyl)phenyl)-1-(4-nitrobenzyl)-1*H*-1,2,3-triazole **(Table 3, Entry 19).**

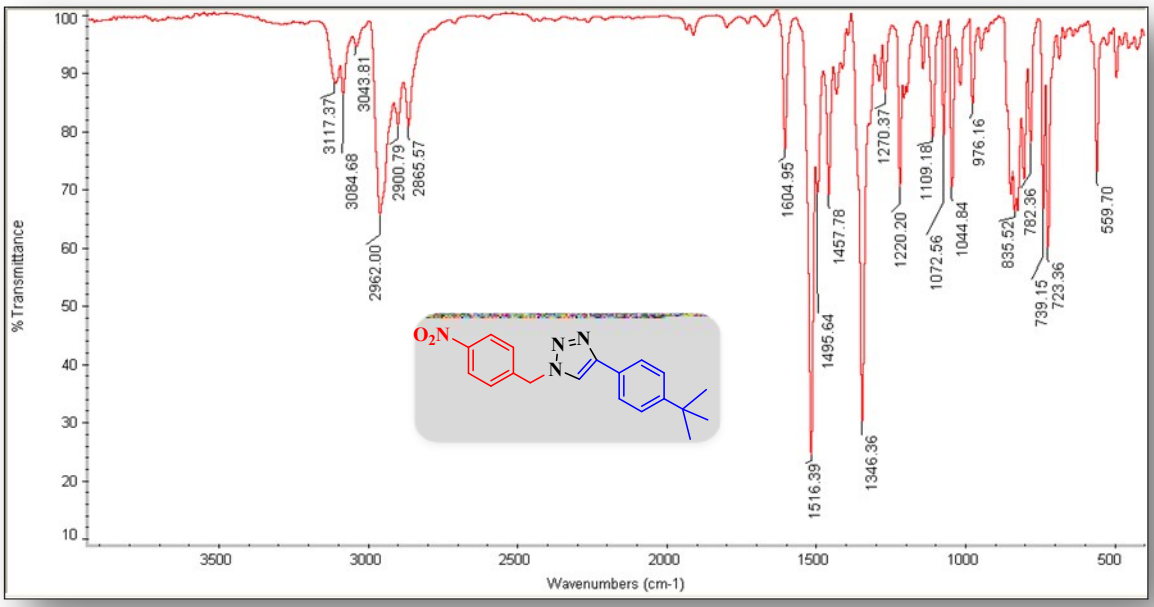

Figure 63: FT-IR (KBr) of 4-(4-(*tert*-butyl)phenyl)-1-(4-nitrobenzyl)-1*H*-1,2,3-triazole **(Table 3, Entry 19).**

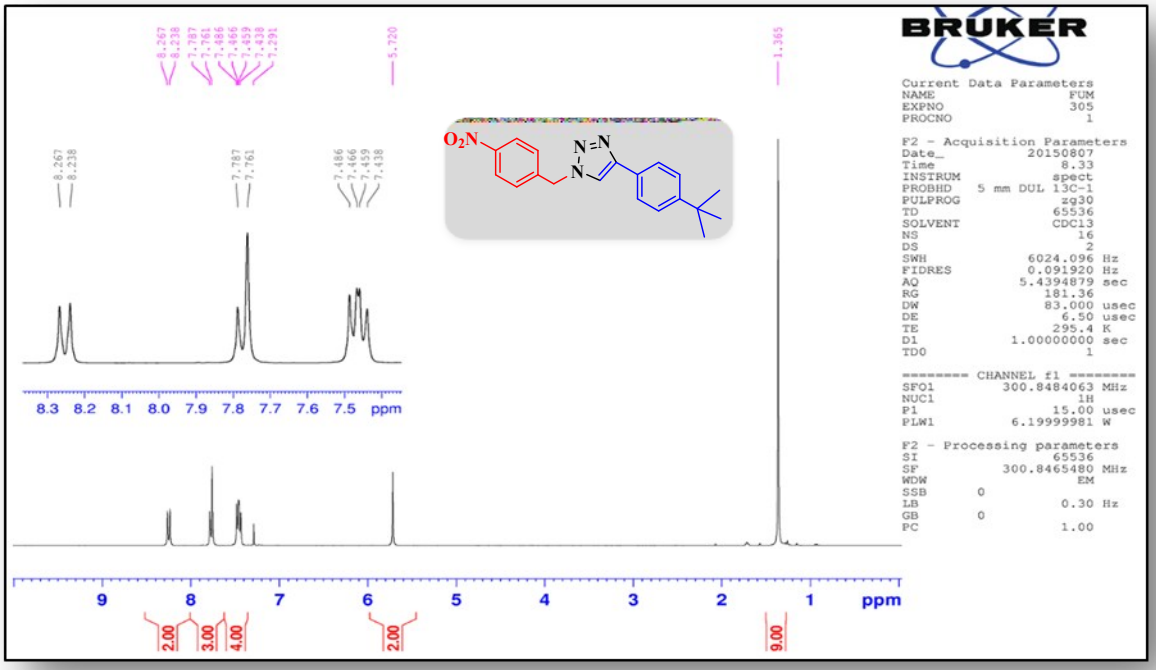

Figure 64: ^{1}H NMR (300 MHz, $CDCl_3$) of 4-(4-(*tert*-butyl)phenyl)-1-(4-nitrobenzyl)-1*H*-1,2,3-triazole **(Table 3, Entry 19).**

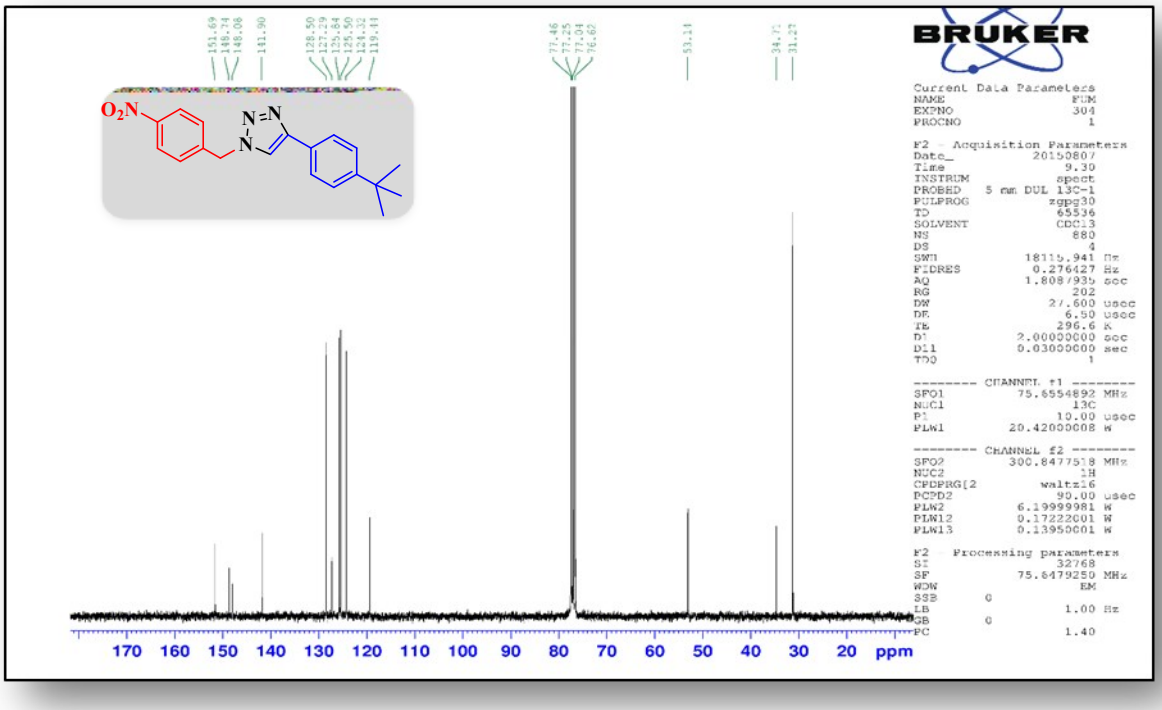

Figure 65: ^{13}C NMR (75 MHz, $CDCl_3$) of 4-(4-(*tert*-butyl)phenyl)-1-(4-nitrobenzyl)-1*H*-1,2,3-triazole **(Table 3, Entry 19).**

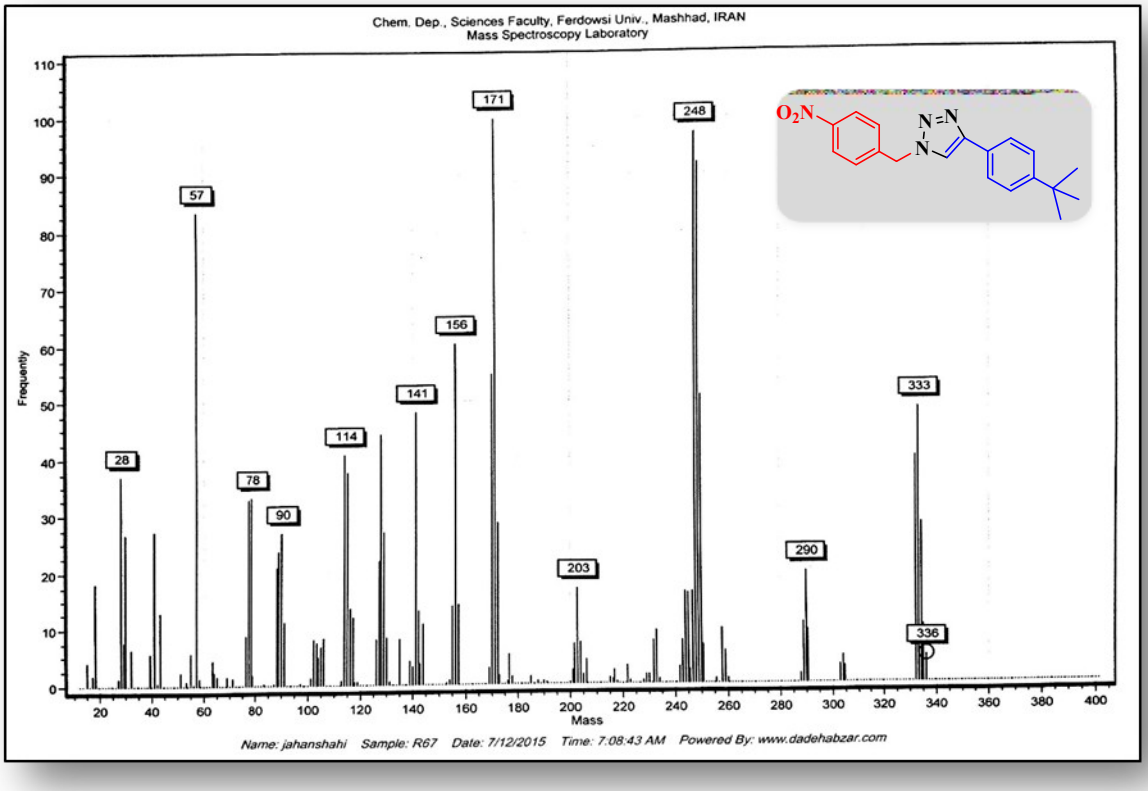

Figure 66: Mass spectrum of 4-(4-(*tert*-butyl)phenyl)-1-(4-nitrobenzyl)-1*H*-1,2,3-triazole **(Table 3, Entry 19).**

2-(1-(4-nitrobenzyl)-1*H*-1,2,3-triazol-4-yl)pyridine (Table 3, Entry 20) (0.20 g, 72%); yellow solid (crystals); mp 175–177 ºC (from EtOH) (Lit.[13] 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 – $C_{14}H_{11}N_3O_2$).

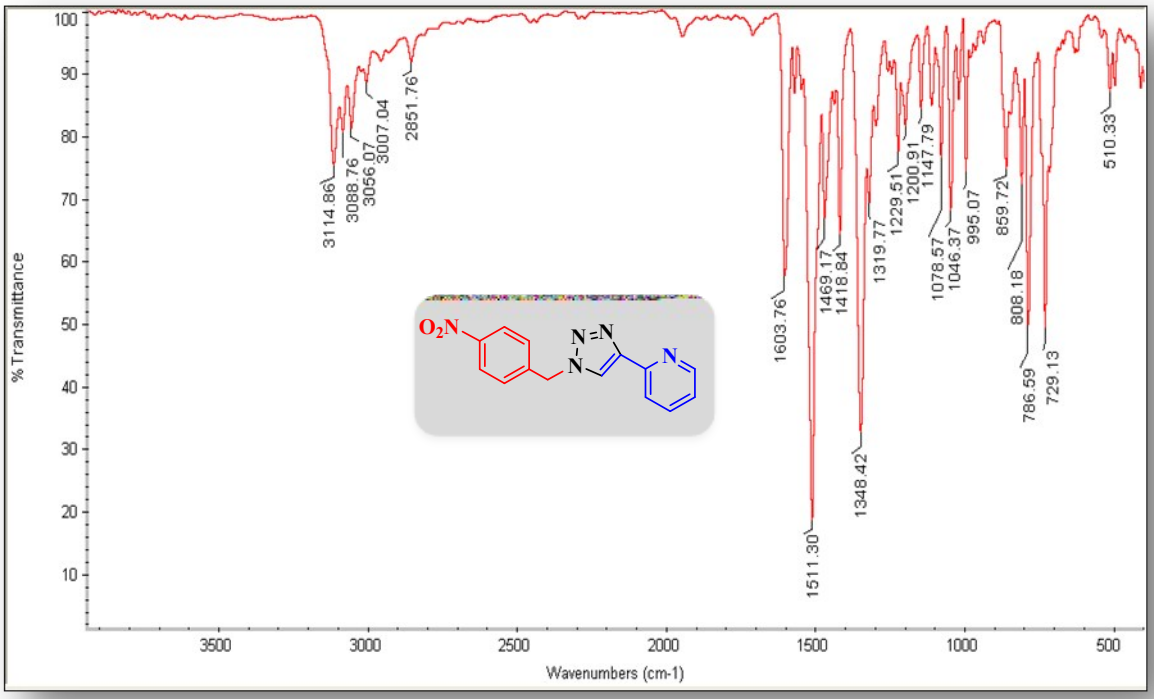

Figure 67: FT-IR (KBr) of 2-(1-(4-nitrobenzyl)-1*H*-1,2,3-triazol-4-yl)pyridine **(Table 3, Entry 20).**

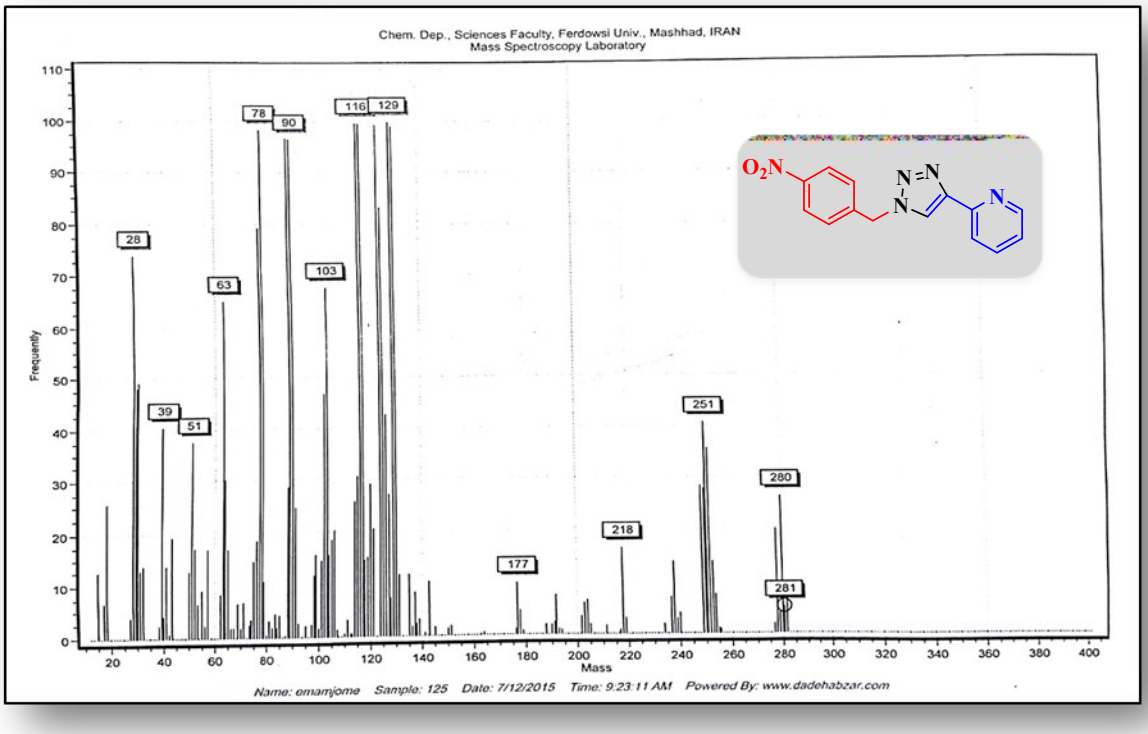

Figure 68: Mass spectrum of 2-(1-(4-nitrobenzyl)-1*H*-1,2,3-triazol-4-yl)pyridine **(Table 3, Entry 20)**.

1-allyl-4-phenyl-1*H*-1,2,3-triazole (Table 3, Entry 21) (0.16 g, 90%); yellow (crystals); mp 40 ºC (from EtOH) (Lit.[14] 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 – $C_{11}H_{11}N$).

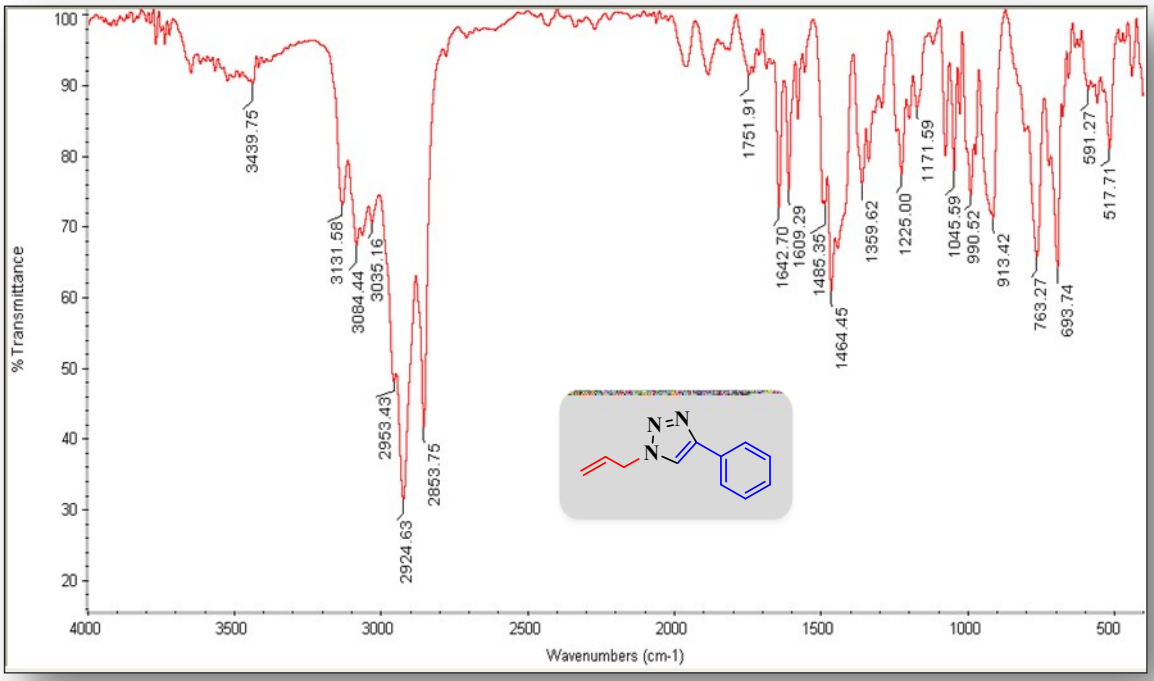

Figure 69: FT-IR (KBr) of 1-allyl-4-phenyl-1H-1,2,3-triazole **(Table 3, Entry 21)**.

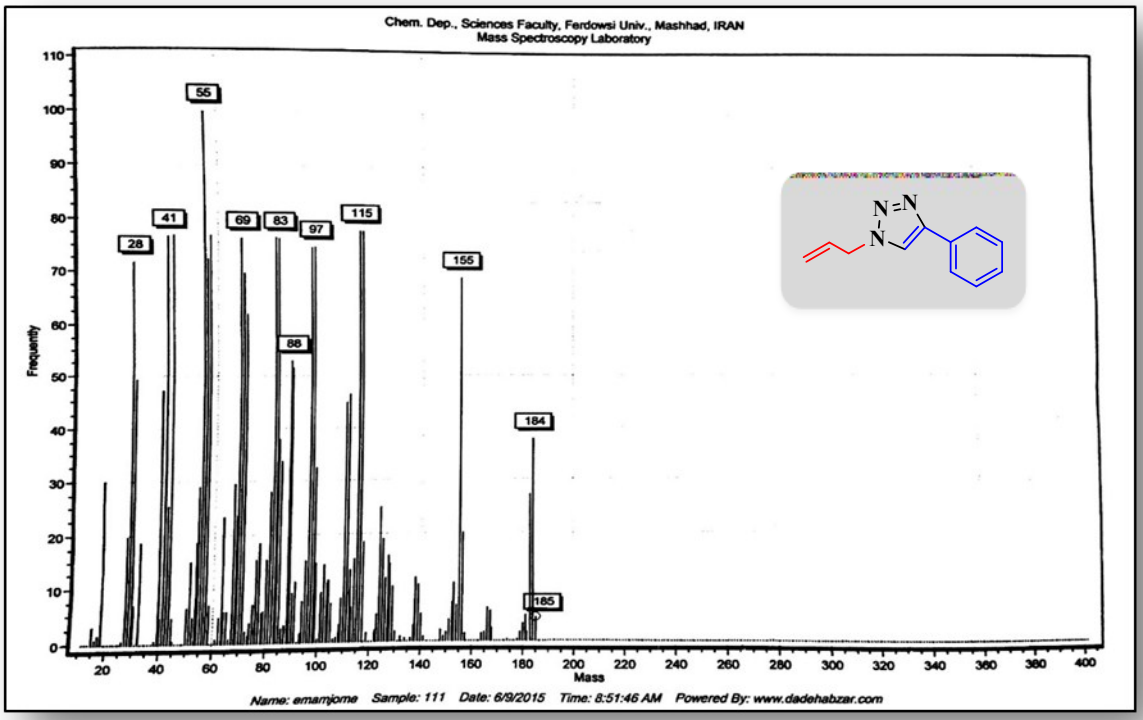

Figure 70: Mass spectrum of 1-allyl-4-phenyl-1H-1,2,3-triazole **(Table 3, Entry 21)**.

1-allyl-4-(*p*-tolyl)-1*H*-1,2,3-triazole[15] **(Table 3, Entry 22)** (0.17 g, 85%); white solid (crystals); mp 82-84 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=CH), 7.26-7.16 (3 H, m, Ar-H), 6.06-6.04 (1 H, m, C=CH), 5.40-5.33 (2 H, m, H_2C=CH), 5.03-4.97 (2 H, m, CH_2), 2.35 (3 H, d, J = 9.6 Hz, CH_3); 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 – $C_{12}H_{13}N$).

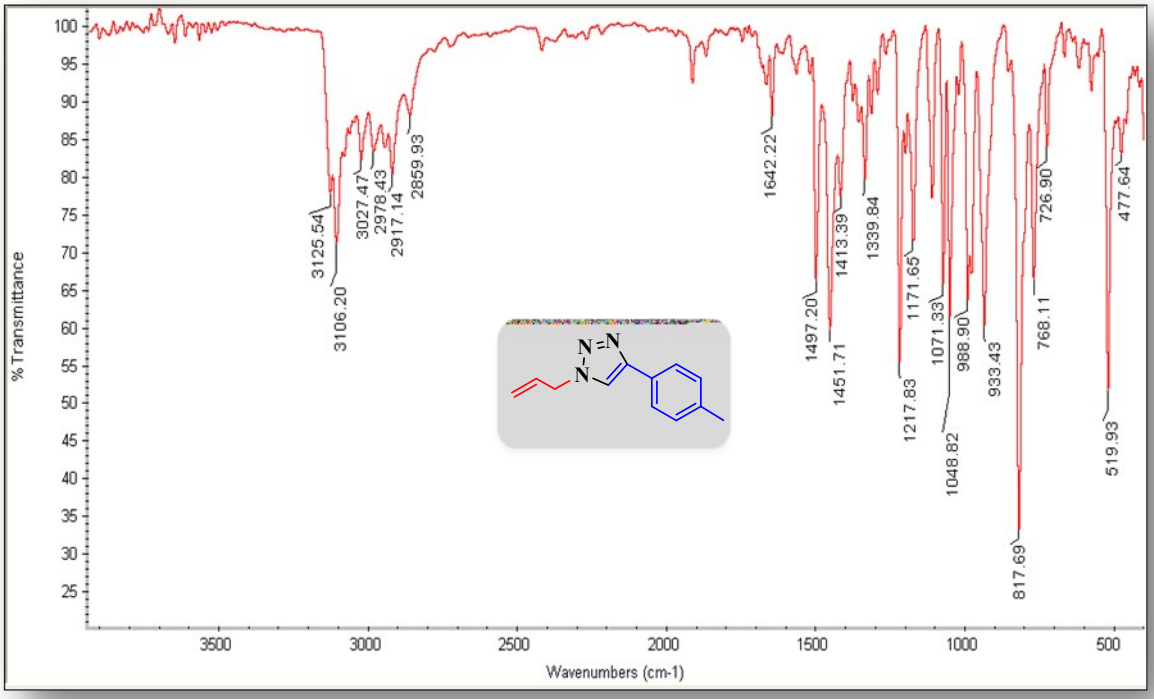

Figure 71: FT-IR (KBr) of 1-allyl-4-(*p*-tolyl)-1*H*-1,2,3-triazole **(Table 3, Entry 22)**.

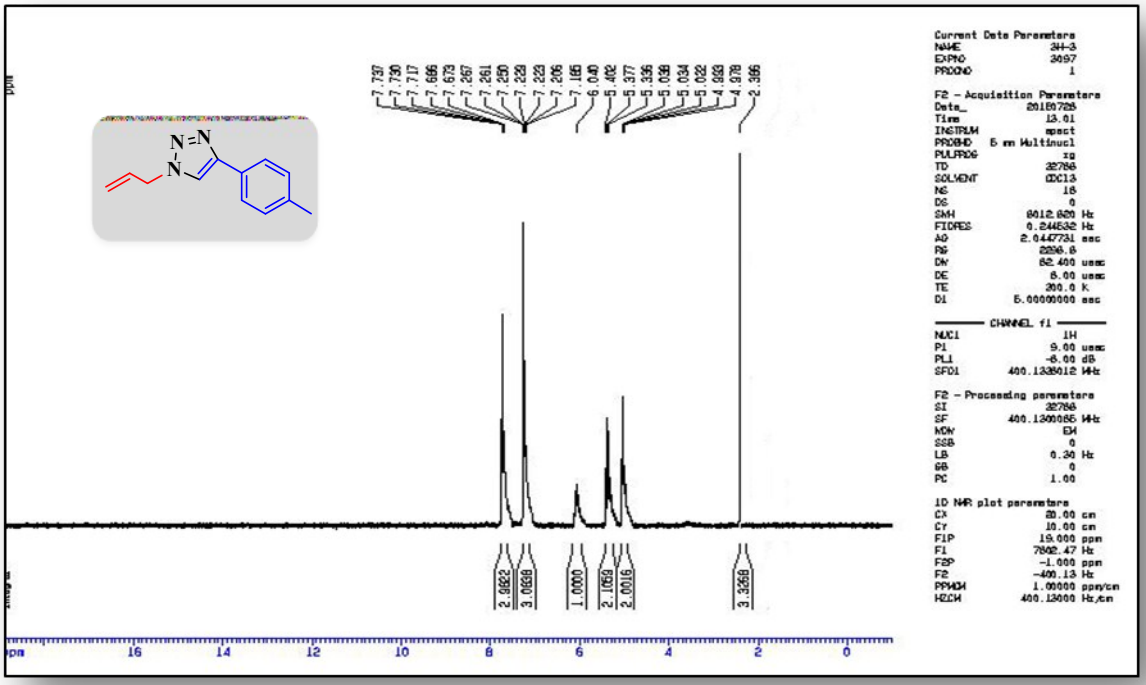

Figure 72: ^{1}H NMR (400 MHz, $CDCl_3$) of 1-allyl-4-(*p*-tolyl)-1*H*-1,2,3-triazole **(Table 3, Entry 22).**

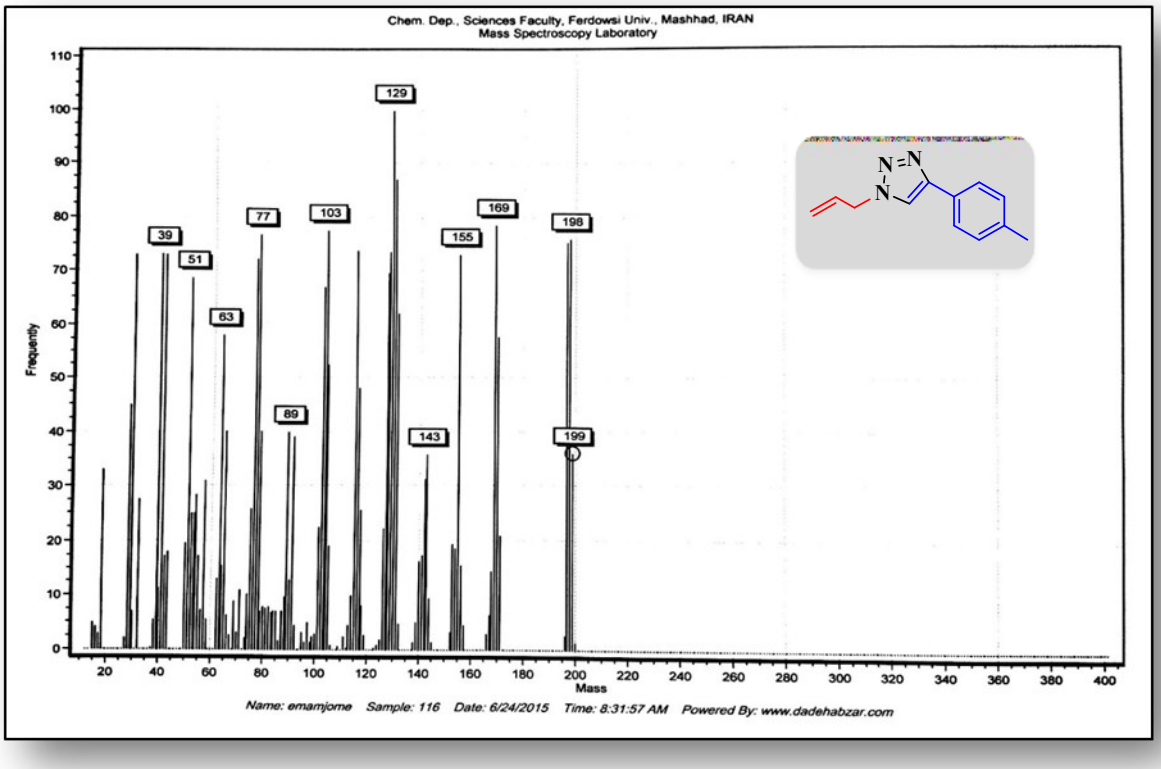

Figure 73: Mass spectrum of 1-allyl-4-(*p*-tolyl)-1*H*-1,2,3-triazole **(Table 3, Entry 22).**

allyl-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (Table 3, Entry 23) (0.18 g, 84%); white solid (crystals); mp 90–91 ºC (from EtOH) (Lit.[16] 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=CH), 6.97 (2 H, d, *J* = 8.7 Hz, Ar-H), 6.14-6.01 (1 H, m, H_2C=CH), 5.40-5.33 (2 H, m, H_2C=CH), 5.02 (2 H, d, *J* = 6 Hz, CH_2), 3.85 (3 H, s, CH_3); ^{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 – $C_{11}H_{11}N$).

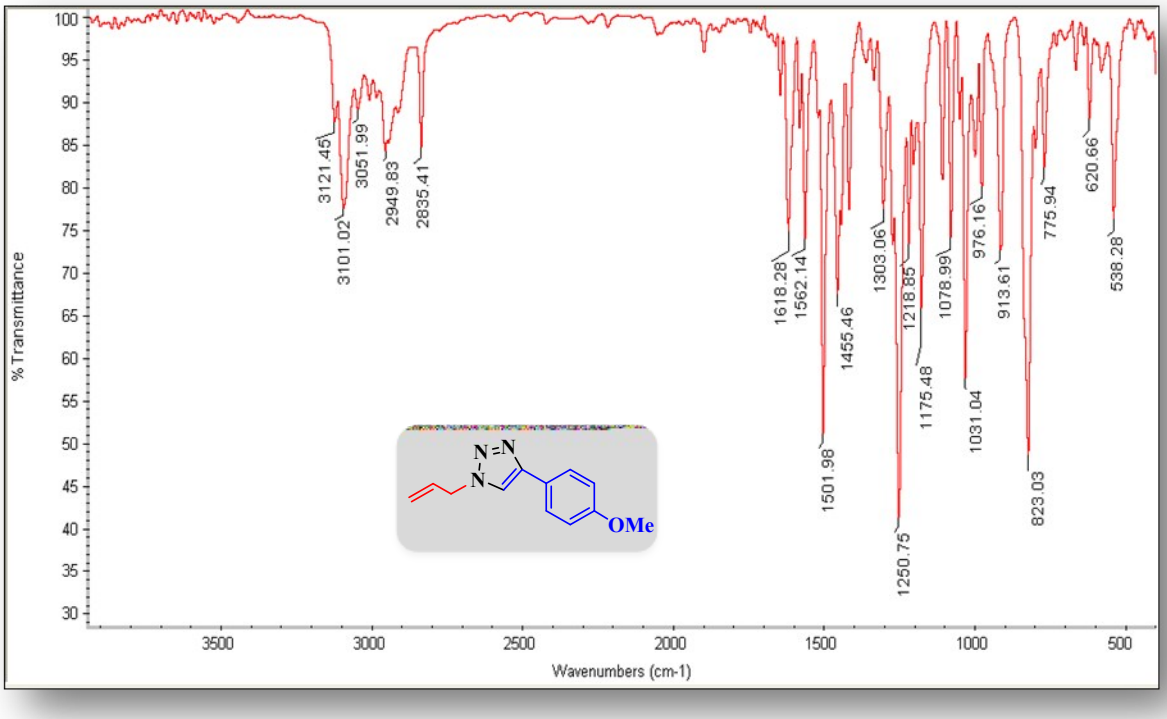

Figure 74: FT-IR (KBr) of 1-allyl-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole **(Table 3, Entry 23)**.

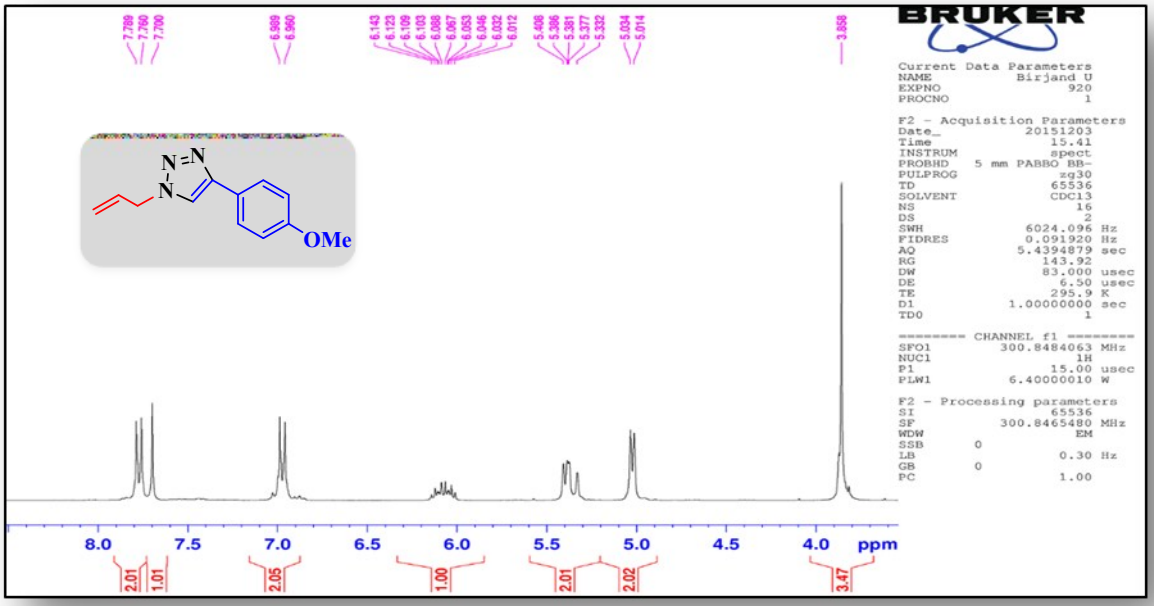

Figure 75: ^{1}H NMR (300 MHz, $CDCl_3$) of 1-allyl-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole **(Table 3, Entry 23)**.

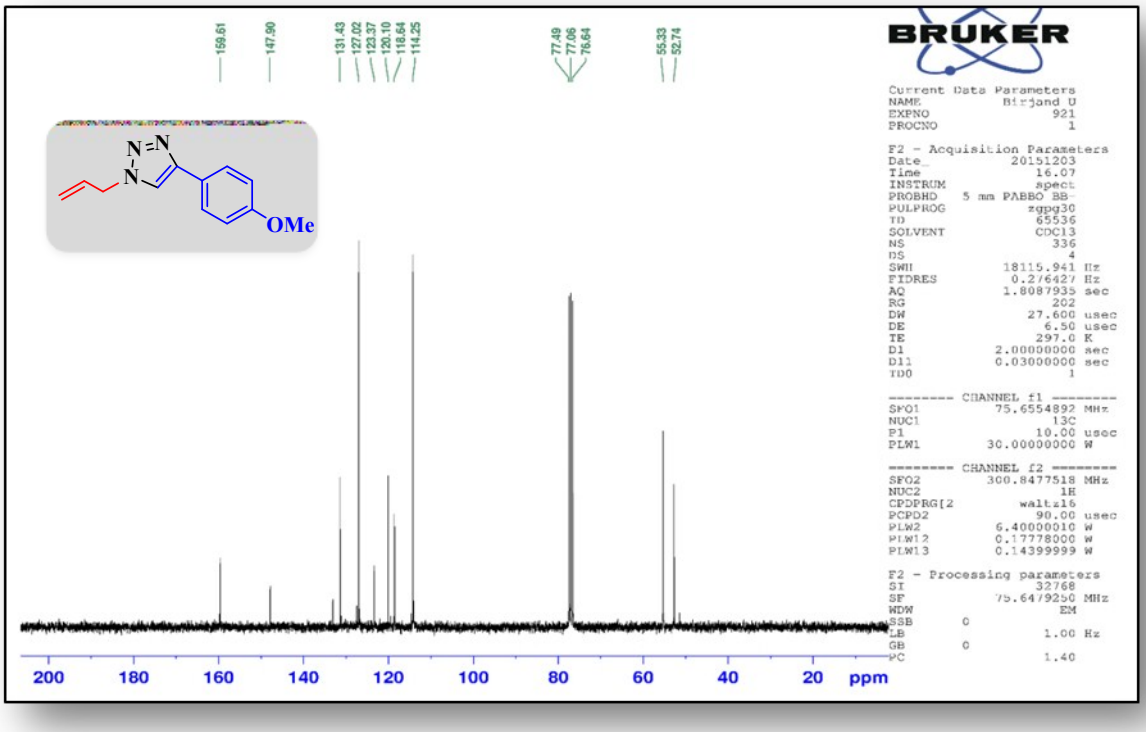

Figure 76: ^{13}C NMR (75 MHz, $CDCl_3$) of 1-allyl-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole **(Table 3, Entry 23)**.

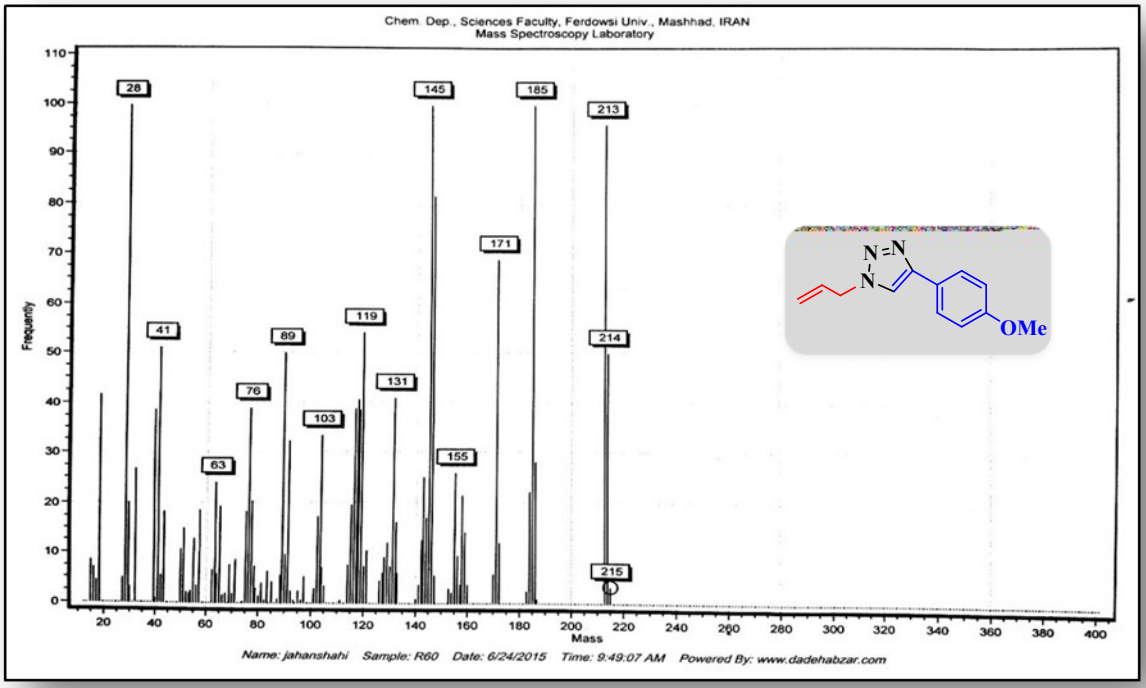

Figure 77: Mass spectrum of 1-allyl-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole **(Table 3, Entry 23)**.

1-allyl-4-(4-(*tert*-butyl)phenyl)-1*H*-1,2,3-triazole[15] **(Table 3, Entry 24)** (0.21 g, 93%); 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 – $C_{15}H_{19}N$).

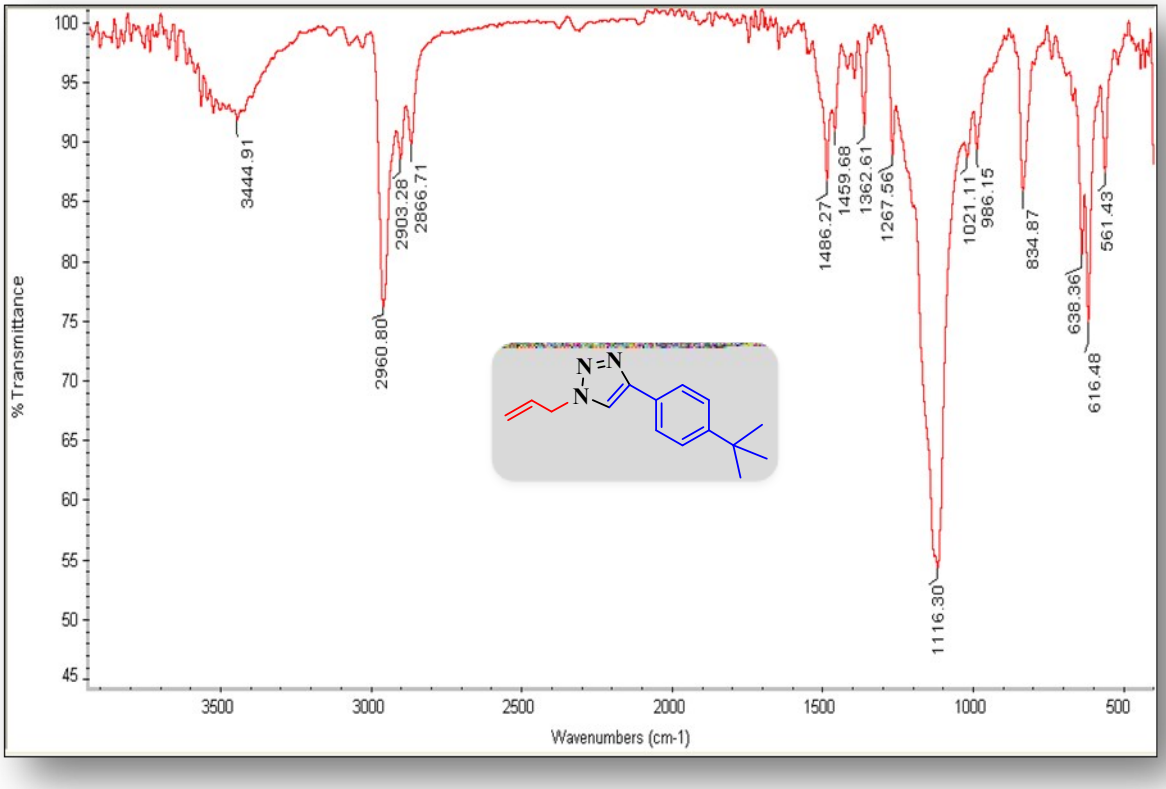

Figure 78: FT-IR (KBr) of 1-allyl-4-(4-(*tert*-butyl)phenyl)-1*H*-1,2,3-triazole **(Table 3, Entry 24).**

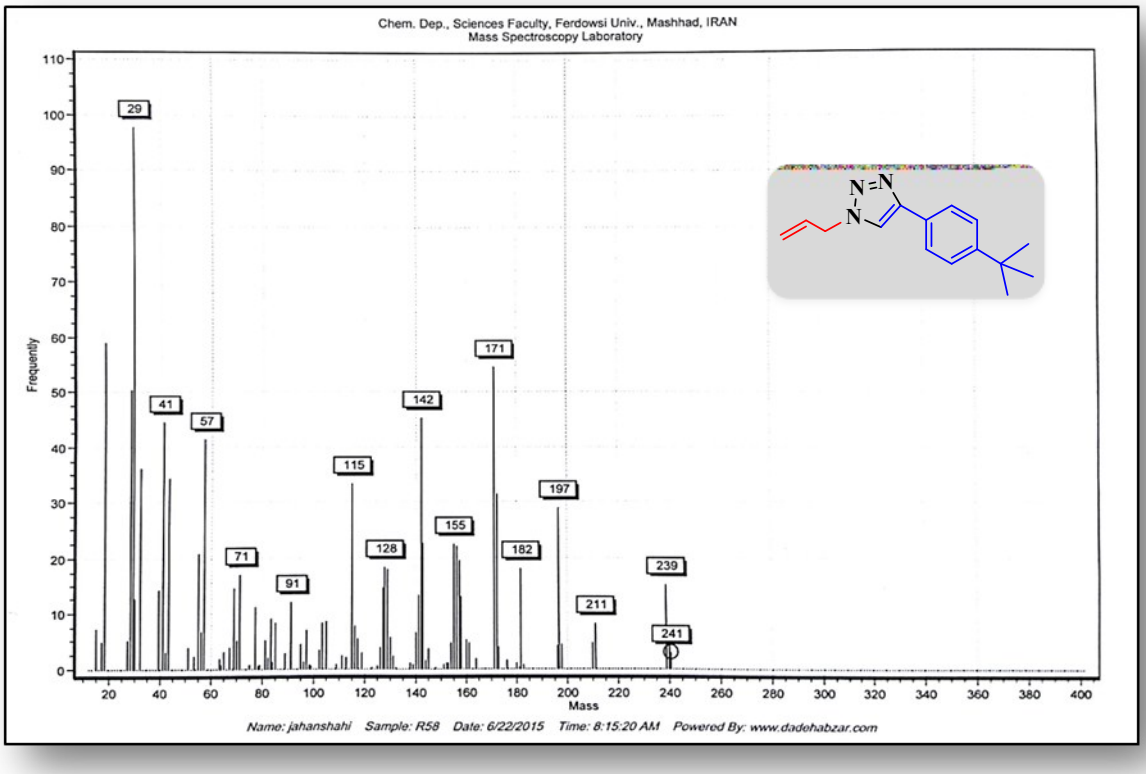

Figure 79: Mass spectrum of 1-allyl-4-(4-(*tert*-butyl)phenyl)-1*H*-1,2,3-triazole **(Table 3, Entry 24)**.

2-(4-phenyl-1H-1,2,3-triazol-1-yl)ethan-1-ol (Table 3, Entry 25) (0.14 g, 76%); green solid (crystals); mp 87-91 ºC (from EtOH) (Lit.[17] 89 - 92ºC); ^{1}H NMR: δH (300 MHz; $CDCl_3$; Me_4Si) 7.74 (1 H, s, C=CH), 7.61 (2 H, d, *J* = 6.6 Hz, Ar-H), 7.46-7.37 (3 H, m, Ar-H), 4.81 (1 H, br s, OH), 4.44 (2 H, t, *J* = 6.0 Hz, H_2C-CH_2OH), 4.06 (2 H, t, *J* = 5.7 Hz, CH_2OH); ^{13}C NMR: δC (75 MHz; $CDCl_3$; Me_4Si) 147, 129, 128.8, 128.2, 125, 121, 61, 52; MS, *m/z* 189 (M^+, 4%), 188 (30, M – H), 172 (12, M – OH), 117 (86, M – C_3H_6NO),116 (33, M – $C_2H_5N_2O$), 102 (33, M – $C_2H_5N_3O$), 77 (48, M – $C_4H_6N_3O$), 45 (17, M – $C_8H_6N_3$), 28 (55, M – $C_{10}H_{11}NO$), 17 (20, M – $C_{10}H_{10}N_3$).

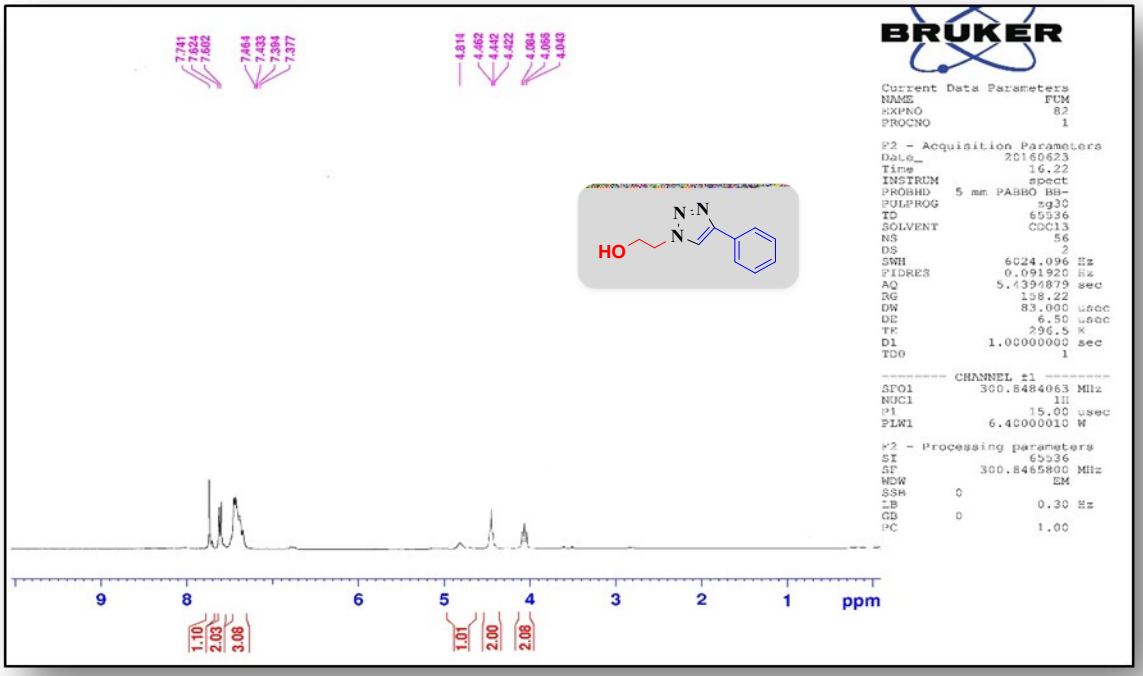

Figure 80: ^{1}H NMR (300 MHz, $CDCl_3$) of 2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)ethan-1-ol **(Table 3, Entry 25).**

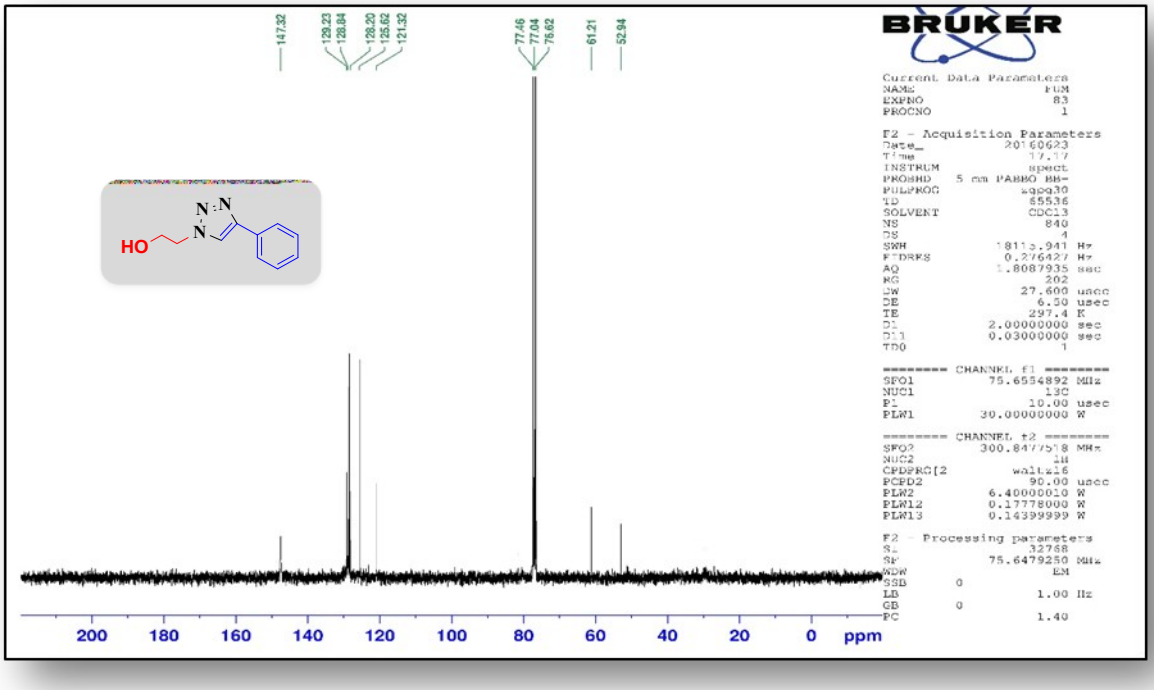

Figure 81: ^{13}C NMR (300 MHz, $CDCl_3$) of 2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)ethan-1-ol

(Table 3, Entry 25).

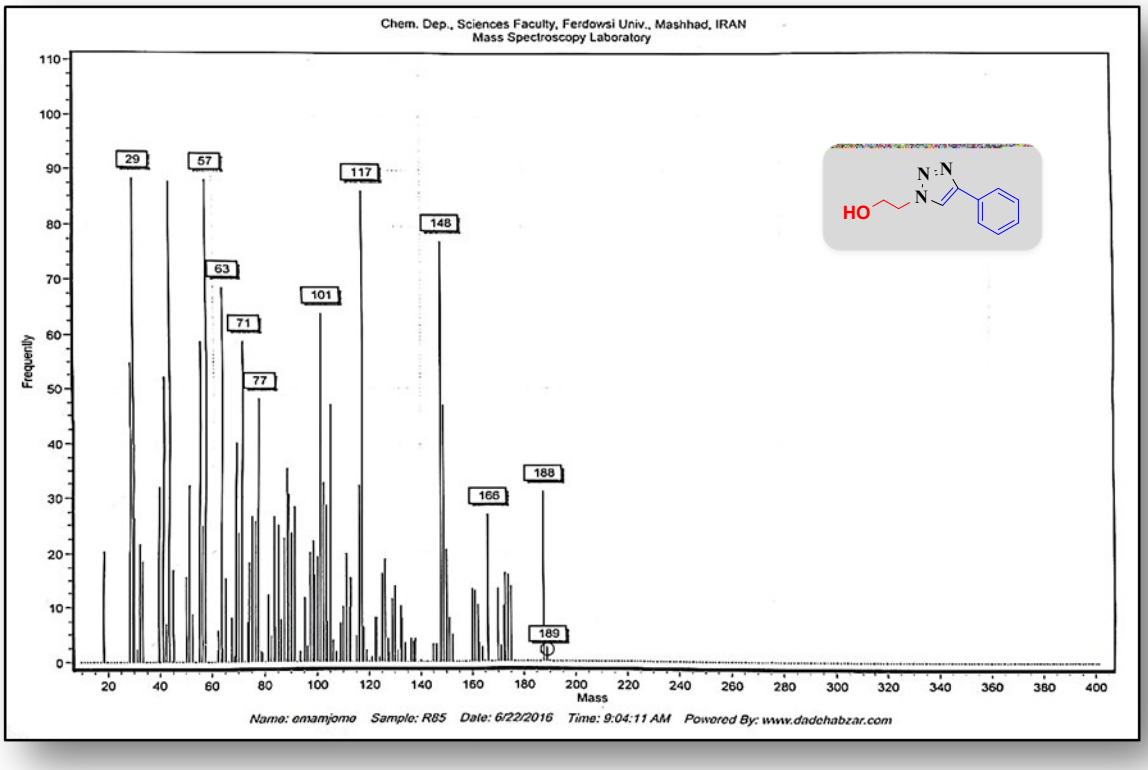

Figure 82: Mass spectrum of 2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)ethan-1-ol **(Table 3, Entry 25).**

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