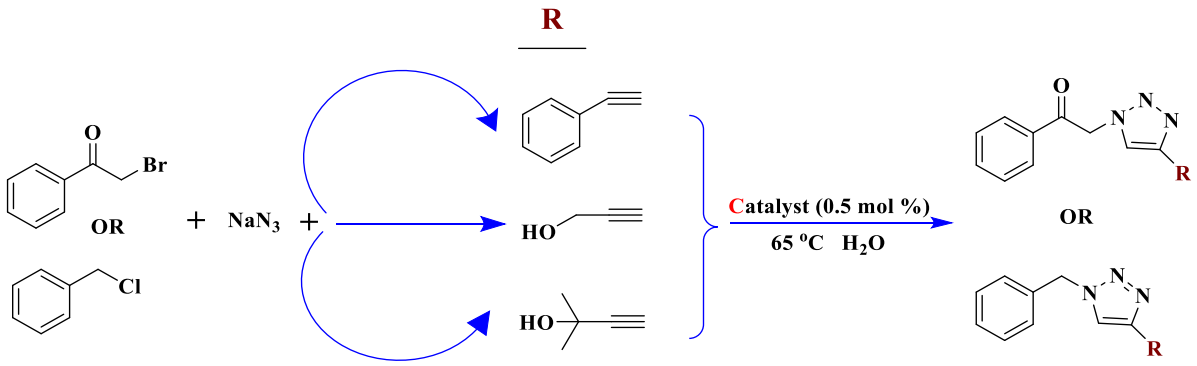
Supporting Information

New Acetamidine Cu (II) Schiff base complex supported on magnetic nanoparticles pectin for the Synthesis of Triazoles Using Click chemistry

Hossein Khashei Siuki, Pouya Ghamari Kargar, & Ghodsieh Bagherzade*

* Corresponding authors: E-mail: gbagherzade@gmail.com; bagherzadeh@birjand.ac.ir. Fax: +98 56 32345192; Tel: +98 56 32345192
[a] Department of Chemistry, Faculty of Sciences, University of Birjand, Birjand, 97175-615, Iran.

Spectra data



Scheme 1: Reaction of synthesis triazole derivatives in the presence of catalyst Fe_3O_4@Pectin@$(CH_2)_3$-Acetamide-Cu(II)

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

^{1}HNMR (DMSO, 300 MHz): δ= 5.66 (s, 2H, CH_2), 7.34-7.45(m, 8H, H-Ar), 7.48 (s, 1H, CH of triazole), 7.85-7.87 (d, 2H, H-Ar) ppm.
^{13}CNMR (DMSO, 75 MHz): δ= 53.51, 122.03, 125.65, 128.37, 129.59, 133.22, 147.14 ppm.
Anal. calcd for $C_{13}H_{15}N_3$: C, 75.57; H, 5.57; N, 17.86; found: C, 75.52; H, 5.58; N, 18.9. Mp (°C): 127-129. [71]

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

^{1}HNMR (DMSO, 300 MHz): δ= 2.308 (s, 3H, CH_3), 5.607 (s, 2H, CH_2), 7.25(q, 3H, H-Ar), 7.36 (t, 2H, H-Ar), 7.45 (t, 2H, h-Ar), 7.69 (s, 1H, CH of triazole), 7.86 (d, 2H, H-Ar) ppm.
^{13}CNMR (DMSO, 75 MHz): δ= 21.18, 53.30, 128.42, 129.36, 129.80, 131.16, 133.48, 137.98, 147.09 ppm.
Anal. calcd for $C_{16}H_{15}N_3$: C, 77.08; H, 6.06; N, 16.85; found: C, 77.11; H, 6.04; N, 16.85. M.p (°C): 103-105. [72]

1-(4-chlorobenzyl)-4-phenyl-1H-1,2,3-triazole (4c):

^{1}HNMR (DMSO, 300 MHz): δ= 5.76 (s, 2H, CH_2), 7.24 (d, 2H, H-Ar), 7.34 (d, 2H, H-Ar), 7.62 (q, 3H, H-Ar), 7.77 (s, 1H, CH of triazole), 7.86 (d, 2H, H-Ar) ppm.
Anal. calcd for $C_{15}H_{12}ClN_3$: C, 66.79; H, 4.48; Cl, 13.14; N, 15.58; found: C, 66.59; H, 4.72; N, 15.54.
M.p (°C): 145-147 [73]

1-(2-chlorobenzyl)-4-phenyl-1H-1,2,3-triazole (4d):

^{1}HNMR (DMSO, 300 MHz): δ= 5.77 (s, 2H, CH_2), 7.34 (3H, H-Ar), 7.45 (3H, H-Ar), 7.57 (d, 1H, H-Ar), 7.67 (s, 1H, CH of triazole), 7.86 (d, 2H, H-Ar) ppm.
^{13}CNMR (DMSO, 75 MHz): δ= 51.27, 125.68, 127.24, 128.28, 129.38, 130.76, 130.99, 133.66, 138.79, 146.94 ppm.
Anal. calcd for $C_{15}H_{12}ClN_3$: C, 66.79; H, 4.48; Cl, 13.14; N, 15.58; found: C, 66.61; H, 4.53; N, 15.561.
Mp (°C): 88-90. [73]

2-(1-benzyl-1H-1,2,3-triazol-4-yl)propan-2-ol (4e):

^{1}HNMR (DMSO, 300 MHz): δ= 1.45 (s, 6H, CH_3), 5.09 (s, 2H, CH_2), 5.55 (s, 1H, OH), 7.40 (5H, H-Ar), 7.91(s, 1H, CH of triazole) ppm.
Anal. calcd for $C_{12}H_{15}N_3O$: C, 66.34; H, 6.96; N, 19.34; O, 7.36; found: C, 66.41; H, 7.01; N, 19.41. Mp (°C): 75-77. [72]

2-(1-(4-methylbenzyl)-1H-1,2,3-triazol-4-yl)propan-2-ol (4f):

^{1}HNMR (DMSO, 300 MHz): δ= 1.44 (s, 6H, CH_3), 2.30 (s, 3H, CH_3), 5.09 (s, 2H, CH_2), 5.49 (s, 1H, OH), 7.23 (5H, H-Ar), 7.87 (s, 1H, CH of triazole) ppm.
^{13}CNMR (DMSO, 75 MHz): δ= 22.90, 31.94, 58.86, 78.40, 122.41, 125.68, 129.38, 131.04, 133.66, 134.80 ppm.
Anal. calcd for $C_{13}H_{17}N_3O$: C, 67.51; H, 7.41; N, 18.17; O, 6.92; found: C, 67.53; H, 7.50; N, 17.98.

2-(1-(4-chlorobenzyl)-1H-1,2,3-triazol-4-yl)propan-2-ol (4g):

^{1}HNMR (DMSO, 300 MHz): δ= 1.46 (s, 6H, CH_3), 5.13 (s, 2H, CH_2), 5.67 (s, 1H, OH), 7.42 (4H, H-Ar), 7.88 (s, 1H, CH of triazole) ppm.
^{13}CNMR (DMSO, 75 MHz): δ= 31.17, 58.64, 78.40, 122.41, 129.38, 130.99, 132.19, 133.66 ppm.
Anal. calcd for $C_{12}H_{14}ClN_3O$: C, 57.26; H, 5.61; Cl, 14.08; N, 16.69; O, 6.36; found: C, 57.31; H, 5.62; N, 16.82.

2-(1-(2-chlorobenzyl)-1H-1,2,3-triazol-4-yl)propan-2-ol (4h):

^{1}HNMR (DMSO, 300 MHz): δ= 1.46 (s, 6H, CH_3), 5.15 (s, 2H, CH_2), 5.66 (s, 1H, OH), 7.27 (d, 1H, H-Ar), 7.51 (d of d, 1H, H-Ar), 7.63 (d of d, 1H, H-Ar), 7.73 (d, 1H, H-Ar), 7.90 (s, 1H, CH of triazole) ppm.
^{13}CNMR (DMSO, 75 MHz): δ= 31.17, 52.89, 78.40, 121.05, 127.24, 127.25, 128.28, 130.76, 131.04, 133.66, 139.41 ppm.
Anal. calcd for $C_{12}H_{14}ClN_3O$: C, 57.26; H, 5.61; Cl, 14.08; N, 16.69; O, 6.36; found: C, 57.34; H, 5.59; N, 16.79.

1-Phenyl-2-(4-phenyl-1H-1,2,3-triazol-1-yl)ethanone (4i):

^{1}HNMR (DMSO, 300 MHz): δ= 6.29 (s, 2H, CH_2), 7.35–7.40 (t, 1H, H-Ar), 7.46–7.68 (m, 4H, H-Ar), 7.75–7.81 (t, 1H, H-Ar), 7.88–7.92 (d, 2H, H-Ar), 8.11–8.15 (d, 2H, H-Ar), 8.55 (s, 1H, CH of triazole) ppm.
^{13}CNMR (DMSO, 75 MHz): δ= 56.49, 123.53, 125.64, 128.36, 128.72, 129.45, 129.51, 131.24, 134.61, 134.79, 146.78, 192.70 ppm. Mp (℃): 170-172 [71].
Anal. calcd for $C_{16}H_{13}N_3O$: C, 72.99; H, 4.98; N, 15.96; found: C, 72.67; H, 5.01; N, 15.94. Mp (℃): 170-172 [71].

1-(4-Bromophenyl)-2-(4-phenyl-1H-1,2,3-triazol-1-yl) ethanone (4j).

^{1}HNMR (DMSO, 300 MHz): δ= 6.27 (s, 2H, CH_2), 7.35–7.52 (t,t, 3H, H -Ar), 7.85–7.91 (m, 4H, H-Ar), 8.03– 8.07 (d, 2H, H-Ar), 8.33–8.37 (d, 2H, H-Ar), 8.54 (s, 1H, CH of triazole) ppm.
^{13}CNMR (DMSO, 75 MHz): δ= 56.47, 121.53, 127.54, 128.06, 128.86, 129.82, 129.85, 130.51, 131.54, 133.61, 148.78, 192.70 ppm. Mp (℃): 116-120 [71].
Anal. calcd for $C_{16}H_{12}BrN_3O$: C, 56.16; H, 3.53; N, 12.28; found: C, 56.24; H, 3.55; N, 12.14. Mp (℃): 116-120 [71].

1-(4-Nitro phenyl)-2-(4-phenyl-1H-1,2,3-triazol-1-yl)ethanone (4k):

^{1}HNMR (DMSO, 300 MHz): δ= 6.37 (s, 2H, CH_2), 7.35– 7.41 (t, 1H, H-Ar), 7.47–7.52 (t, 2H, H-Ar), 7.89–7.92 (t, 2H, H-Ar), 8.33–8.37 (d, 2H, H-Ar), 8.44–8.48 (d, 2H, H-Ar), 8.55 (s, 1H, CH of triazole) ppm.
^{13}CNMR (DMSO, 75 MHz): δ= 56.47, 121.23, 123.54, 128.06, 128.76, 129.72, 129.80, 130.41, 140.58, 148.88, 150.51, 192.71 ppm.
Anal. calcd for $C_{16}H_{12}N_4O_3$: C, 62.33; H, 3.92; N, 18.17; found: C, 61.94; H, 3.62; N, 18.21. Mp (℃): 184-185. [74]

2-(4-(2-Hydroxypropan-2-yl)-1H-1,2,3-triazol-1-yl)-1- phenylethanone (4l).

^{1}HNMR (DMSO, 300 MHz): δ= 1.51 (s, 2×3H, CH_3), 5.16 (s, 1H, OH), 6.15 (s, 2H, CH_2), 7.61–7.66 (t, 2H, H-Ar), 7.73–7.79 (t, 2H, CH-Ar), 7.86 (s, 1H, CH of triazole), 8.08–8.11 (d,d, 2H, H-Ar) ppm.
^{13}CNMR (DMSO, 75 MHz): δ= 31.30, 56.46, 78.32, 122.92, 128.75, 130.78, 133.14, 133.53, 134.53, 190.90 ppm.
Anal. calcd for $C_{11}H_{11}N_3O_2$: C, 60.82; H, 5.10; N, 19.34; found: C, 60.79; H, 5.13; N, 19.37. Mp (℃): 96–98. [74]

1-(4-Bromophenyl)-2-(4-(2-hydroxypropan-2-yl)-1H-1,2,3- triazol-1-yl)ethanone (4m).

^{1}HNMR (DMSO, 300 MHz): δ= 1.51 (s, 6H, CH_3), 5.16 (s, 1H, OH), 6.13 (s, 1H, CH_2), 7.84–7.87 (d, 3H, CH of triazole and H-Ar), 8.00–8.03 (d, 2H, H-Ar) ppm.
^{13}CNMR (DMSO, 75 MHz): δ= 31.29, 56.50, 78.29, 122.52, 127.32, 128.75, 129.88, 131.54, 133.53, 152.58, 190.91 ppm. Mp (℃): 167–169 [75].
Anal. calcd for $C_{13}H_{14}N_4O_4$: C, 53.79, H, 4.86; N, 19.30; found: C, 53.63; H, 4.80; N, 19.39.

2-(4-(2-Hydroxypropan-2-yl)-1H-1,2,3-triazol-1-yl)-1-(4- nitrophenyl)ethanone (4n).

^{1}HNMR (DMSO, 300 MHz): δ= 1.38 (s, 6H, CH_3), 4.90 (s, 2H, CH_2), 5.53 (s, 1H, OH), 7.75 (s, 1H, CH of triazole), 8.31–8.33 (d,d, 2H, H-Ar), 8.41–8.44 (d, 2H, j ¼ 8.7, H-Ar) ppm.
^{13}CNMR (DMSO, 75 MHz): δ= 31.18, 56.49, 78.29, 122.82, 123.83, 129.75, 131.24, 140.58, 152.58, 190.90 ppm.
Anal. calcd for $C_{13}H_{14}N_4O_4$: C, 53.79, H, 4.86; N, 19.30; found: C, 53.63; H, 4.80; N, 19.39. Mp (°C): 126-128 [74].

2-(4-(Hydroxymethyl)-1H-1,2,3-triazol-1-yl)-1- phenylethanone (4o).

^{1}HNMR (DMSO, 300 MHz): δ= 4.58–4.59 (d, 2H, CH_2–OH), 5.23–5.27 (t, 1H, OH), 6.18 (s, 2H, CH_2), 7.60– 7.66 (t, 2H, H-Ar), 7.73–7.79 (t, 1H, H-Ar), 7.95 (s, 1H, CH of triazole), 8.08–8.11 (d, 2H, H-Ar) ppm.
^{13}CNMR (DMSO, 75 MHz): δ= 55.57, 56.20, 124.87, 128.64, 129.47, 134.67, 148.41, 192.76 ppm.
Anal. calcd for $C_{11}H_{11}N_3O_2$: C, 60.82; H, 5.10; N, 19.34; found: C, 60.79; H, 5.13; N, 19.37. Mp (°C): 111-113 [75].

1-(4-Bromophenyl)-2-(4-(hydroxymethyl)-1H-1,2,3-triazol-1- yl)ethanone (4p).

^{1}HNMR (DMSO, 300 MHz): δ= 4.38 (s, 2H, CH_2), 5.00 (s, 2H, CH_2–OH), 5.75 (s, 1H, OH), 7.98 (s, 1H, CH of triazole), 8.33–8.37 (d, 2H, H-Ar), 8.44–8.48 (d, 2H, H-Ar) ppm.
^{13}CNMR (DMSO, 75 MHz): δ= 55.57, 56.20, 122.77, 127.72, 129.47, 131.41, 134.67, 147.41, 192.76 ppm.
Anal. calcd for C11H10BrN3O2: C, 44.62; H, 3.40; Br, 26.98; N, 14.19; found: C, 44.48; H, 3.44; N, 14.21. Mp (°C): 156–158 [74].

Green chemistry metrics analysis

The following formulae were used for calculating atom economy (AE), atom efficiency (AEf), carbon efficiency (CE), reaction mass efficiency (RME), optimum efficiency (OE), process mass intensity (PMI), E factor, solvent and water intensity (SI and WI).

$$AE = \frac{Molecular\ weight\ of\ the\ product}{Total\ molecular\ weight\ of\ reactants}$$

$$AE_f = AE \cdot Yield\ (\%)$$

$$CE = \frac{Amount\ of\ carbon\ in\ the\ product}{Total\ carbon\ present\ in\ reactants}$$

$$RME = \frac{Mass\ of\ isolated\ product}{Total\ mass\ of\ reactants} \times 100$$

$$OE = \frac{RME}{AE} \times 100$$

$$PMI = \frac{Total\ mass\ of\ input\ material\ in\ the\ whole\ process}{Mass\ of\ product}$$

$$E\ factor = PMI - 1$$

$$SI = \frac{Total\ mass\ of\ solvents\ excluding\ water\ in\ the\ whole\ process}{Mass\ of\ product}$$

$$WI = \frac{Total\ mass\ of\ water\ used\ in\ the\ whole\ process}{Mass\ of\ product}$$

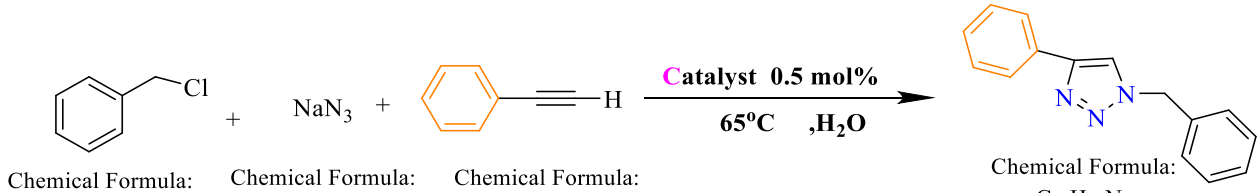
Synthesis of 1-benzyl-4-phenyl-1H-1,2,3-triazole catalyzed by Fe_3O_4@Pectin@$(CH_2)_3$-Acetamide-Cu(II) (Table 2, entry 1)

Experimental procedure:

Benzyl chloride (1.0 mmol), Sodium azide (1.2 mmol), phenylacetylene (1.0mmol), catalyst (0.5 mol %) in the presence of water solvent (2ml). The reaction mixture was heated at 65 °C and stirred until TLC monitoring indicated no further progress in the reaction. Then, the reaction mixture was cooled to room temperature. After completion of the reaction, the catalyst was removed by a magnet. A pure product was obtained by recrystallization from EtOAC-water.

Materials used for metrics calculations:

Benzyl chloride (0.126 g, 1.0 mmol), Sodium azide (0.078 g, 1.2 mmol), phenylacetylene (0.102 g, 1.0mmol), H_2O (1.994 g, 2ml), product (0.228 g, 0.97 mmol).



Chemical Formula: C_7H_7Cl Molecular Weight: 126/58

Chemical Formula: N_3Na Molecular Weight: 65/01

Chemical Formula: C_8H_6 Molecular Weight: 102/14

Chemical Formula: $C_{15}H_{13}N_3$ Molecular Weight: 235/29

$$AE = \frac{235.29}{126.58+78.012+102.14} \times 100 = 76.70$$

$$AE_f = 76.70 \times 97\% = 74.39$$

$$CE = \frac{15 \times 0.00097}{7 \times 0.001 + 8 \times 0.001} \times 100 = 97$$

$$RME = \frac{0.228}{0.126+0.078+0.102} \times 100 = 76$$

$$OE = \frac{76}{76.70} \times 100 = 99.08$$

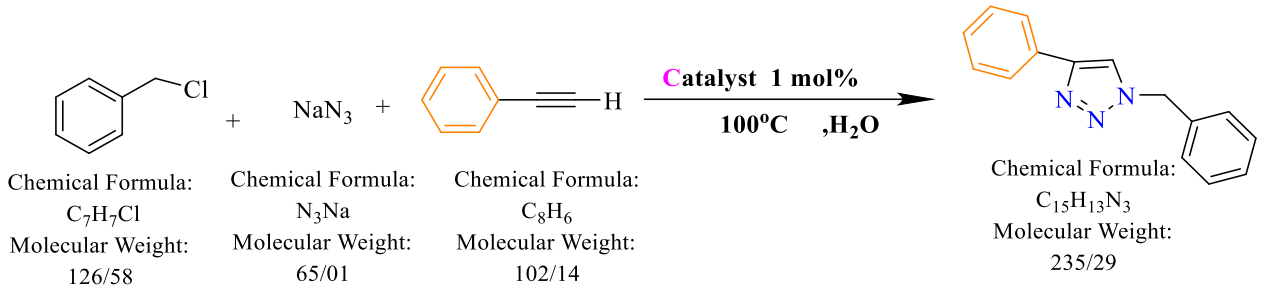
$$PMI = \frac{0.126+0.078+0.102+1.994}{0.228} = 10.08$$

$$E\ factor = 10.08 - 1 = 9.08$$

$$SI = 0$$

$$WI = \frac{2 \times 0.997}{0.228} = 8.74$$

Synthesis of 1-benzyl-4-phenyl-1H-1,2,3-triazole catalyzed by Cu/C (Table 3, entry 1)



Chemical Formula: C_7H_7Cl Molecular Weight: 126/58

Chemical Formula: N_3Na Molecular Weight: 65/01

Chemical Formula: C_8H_6 Molecular Weight: 102/14

Chemical Formula: $C_{15}H_{13}N_3$ Molecular Weight: 235/29

Materials used for metrics calculations:

Benzyl chloride (0.126 g, 1.0 mmol), Sodium azide (0.071 g, 1.1 mmol), phenylacetylene (0.102 g, 1.0mmol), H_2O (0.997 g, 1 ml), product (0.214 g, 0.91 mmol).

$$AE = \frac{235.29}{126.58+71.511+102.14} \times 100 = 78.37$$

$$AE_f = 78.37 \times 91\% = 71.31$$

$$CE = \frac{15 \times 0.00091}{7 \times 0.001 + 8 \times 0.001} \times 100 = 91$$

$$RME = \frac{0.214}{0.126+0.071+0.102} \times 100 = 71.57$$

$$OE = \frac{71.57}{78.37} \times 100 = 91.32$$

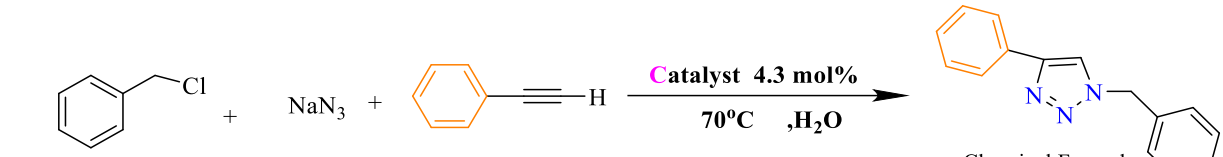
$$PMI = \frac{0.126+0.071+0.102+0.997}{0.214} = 6.05$$

$$E\ factor = 6.05 - 1 = 5.05$$

$$SI = 0$$

$$WI = \frac{1 \times 0.997}{0.214} = 4.66$$

Synthesis of 1-benzyl-4-phenyl-1H-1,2,3-triazole catalyzed by CuNPs/MagSilica (Table 3, entry 4)



Chemical Formula: C_7H_7Cl Molecular Weight: 126/58

Chemical Formula: N_3Na Molecular Weight: 65/01

Chemical Formula: C_8H_6 Molecular Weight: 102/14

Chemical Formula: $C_{15}H_{13}N_3$ Molecular Weight: 235/29

Materials used for metrics calculations:

Benzyl chloride (0.126 g, 1.0 mmol), Sodium azide (0.071 g, 1.1 mmol), phenylacetylene (0.102 g, 1.0mmol), H_2O (1.99 g, 2 ml), product (0.195 g, 0.83 mmol).

$$AE = \frac{235.29}{126.58+71.511+102.14} \times 100 = 78.37$$

$$AE_f = 78.37 \times 83\% = 65.04$$

$$CE = \frac{15 \times 0.00083}{7 \times 0.001 + 8 \times 0.001} \times 100 = 83$$

$$RME = \frac{0.195}{0.126+0.071+0.102} \times 100 = 65.21$$

$$OE = \frac{65.21}{78.37} \times 100 = 83.20$$

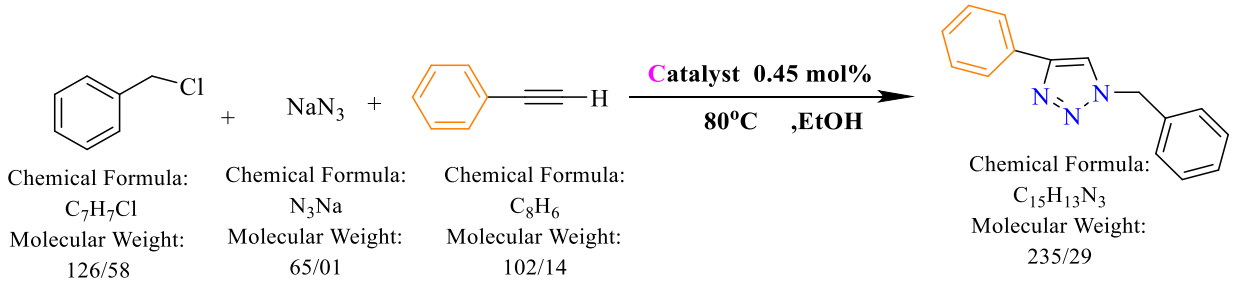
$$PMI = \frac{0.126+0.071+0.102+1.99}{0.195} = 11.73$$

$$E\ factor = 11.73 - 1 = 10.73$$

$$SI = 0$$

$$WI = \frac{2 \times 0.997}{0.195} = 10.20$$

Synthesis of 1-benzyl-4-phenyl-1H-1,2,3-triazole catalyzed by HCP-NHC–Cu (Table 3, entry 7)



Chemical Formula: C_7H_7Cl
Molecular Weight: 126/58

Chemical Formula: N_3Na
Molecular Weight: 65/01

Chemical Formula: C_8H_6
Molecular Weight: 102/14

Chemical Formula: $C_{15}H_{13}N_3$
Molecular Weight: 235/29

Materials used for metrics calculations:

Benzyl chloride (0.126 g, 1.0 mmol), Sodium azide (0.071 g, 1.1 mmol), phenylacetylene (0.102 g, 1.0mmol), EtOH (1.58 g, 2 ml), product (0.214 g, 0.91 mmol).

$$AE = \frac{235.29}{126.58+71.511+102.14} \times 100 = 78.37$$

$$AE_f = 78.37 \times 91\% = 71.31$$

$$CE = \frac{15 \times 0.00091}{7 \times 0.001+8 \times 0.001} \times 100 = 91$$

$$RME = \frac{0.214}{0.126+0.071+0.102} \times 100 = 71.57$$

$$OE = \frac{71.57}{78.37} \times 100 = 91.32$$

$$PMI = \frac{0.126+0.071+0.102+1.58}{0.214} = 8.78$$

$$E\ factor = 8.78 - 1 = 7.78$$

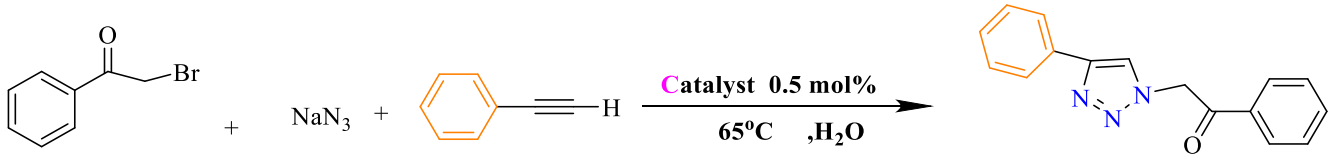
$$SI = \frac{2 \times 0.789}{0.214} = 7.37$$

$$WI = 0$$

Synthesis of 1-Phenyl-2-(4-phenyl-1H-1,2,3-triazol-1-yl)ethanone catalyzed by Fe_3O_4@Pectin@$(CH_2)_3$-Acetamide-Cu(II) (Table 2, entry 9)

Experimental procedure:

Phenacyl bromide (1.0 mmol), Sodium azide (1.2 mmol), phenylacetylene (1.0mmol), catalyst (0.5 mol %) in the presence of water solvent (2ml). The reaction mixture was heated at 65 °C and stirred until TLC monitoring indicated no further progress in the reaction. Then, the reaction mixture was cooled to room temperature. After completion of the reaction, the catalyst was removed by a magnet. A pure product was obtained by recrystallization from EtOAC-water.



Chemical Formula: C_8H_7BrO Molecular Weight: 199/05

Chemical Formula: N_3Na Molecular Weight: 65/01

Chemical Formula: C_8H_6 Molecular Weight: 102/14

Chemical Formula: $C_{16}H_{13}N_3O$ Molecular Weight: 263/30

Materials used for metrics calculations:

Phenacyl bromide (0.199 g, 1.0 mmol), Sodium azide (0.078 g, 1.2 mmol), phenylacetylene (0.102 g, 1.0mmol), H_2O (1.994 g, 2ml), product (0.258 g, 0.98 mmol).

$$AE = \frac{263.30}{199.05+78.012+102.14} \times 100 = 69.43$$

$$AE_f = 69.43 \times 98\% = 68.04$$

$$CE = \frac{16 \times 0.00098}{8 \times 0.001 + 8 \times 0.001} \times 100 = 98$$

$$RME = \frac{0.258}{0.199+0.078+0.102} \times 100 = 68.07$$

$$OE = \frac{68.07}{69.43} \times 100 = 98.04$$

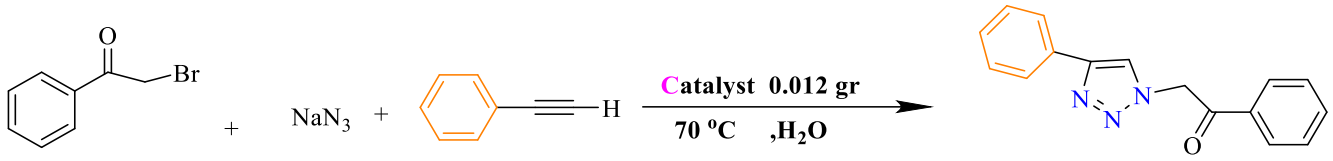
$$PMI = \frac{0.199+0.078+0.102+1.994}{0.258} = 9.19$$

$$E\ factor = 9.19 - 1 = 8.19$$

$$SI = 0$$

$$WI = \frac{2 \times 0.997}{0.258} = 7.72$$

Synthesis of 1-Phenyl-2-(4-phenyl-1H-1,2,3-triazol-1-yl)ethanone by $CuFe_2O_4$ (Table 4, entry 2)



Chemical Formula: C_8H_7BrO Molecular Weight: 199/05

Chemical Formula: N_3Na Molecular Weight: 65/01

Chemical Formula: C_8H_6 Molecular Weight: 102/14

Chemical Formula: $C_{16}H_{13}N_3O$ Molecular Weight: 263/30

Materials used for metrics calculations:

Phenacyl bromide (0.199 g, 1.0 mmol), Sodium azide (0.071 g, 1.1 mmol), phenylacetylene (0.102 g, 1.0mmol), H_2O (1.99 g, 2 ml), product (0.205 g, 0.78 mmol).

$$AE = \frac{263.30}{199.05+71+102.14} \times 100 = 70.74$$

$$AE_f = 70.74 \times 78\% = 55.17$$

$$CE = \frac{16 \times 0.00078}{8 \times 0.001 + 8 \times 0.001} \times 100 = 78$$

$$RME = \frac{0.205}{0.199+0.071+0.102} \times 100 = 55.10$$

$$OE = \frac{55.10}{70.74} \times 100 = 77.89$$

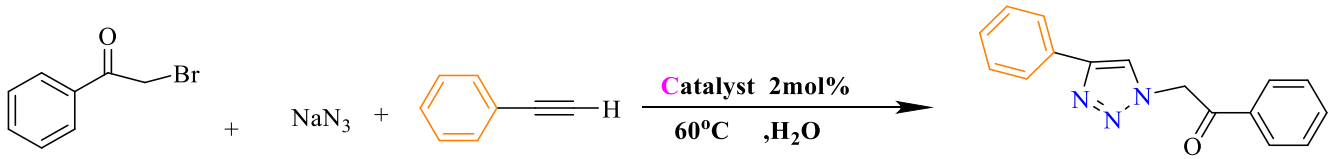
$$PMI = \frac{0.199+0.071+0.102+1.99}{0.205} = 11.52$$

$$E\ factor = 11.52 - 1 = 10.52$$

$$SI = 0$$

$$WI = \frac{2 \times 0.997}{0.205} = 9.70$$

Synthesis of 1-Phenyl-2-(4-phenyl-1H-1,2,3-triazol-1-yl)ethanone by PANS2FCu (Table 4, entry 3)



Chemical Formula: C_8H_7BrO Molecular Weight: 199/05

Chemical Formula: N_3Na Molecular Weight: 65/01

Chemical Formula: C_8H_6 Molecular Weight: 102/14

Chemical Formula: $C_{16}H_{13}N_3O$ Molecular Weight: 263/30

Materials used for metrics calculations:

Phenacyl bromide (0.199 g, 1.0 mmol), Sodium azide (0.078 g, 1.2 mmol), phenylacetylene (0.102 g, 1.0mmol), H_2O (4.98 g, 5ml), product (0.239 g, 0.91 mmol).

$$AE = \frac{263.30}{199.05+78.012+102.14} \times 100 = 69.43$$

$$AE_f = 69.43 \times 91\% = 63.18$$

$$CE = \frac{16 \times 0.00091}{8 \times 0.001 + 8 \times 0.001} \times 100 = 91$$

$$RME = \frac{0.239}{0.199+0.078+0.102} \times 100 = 63.06$$

$$OE = \frac{63.06}{69.43} \times 100 = 90.82$$

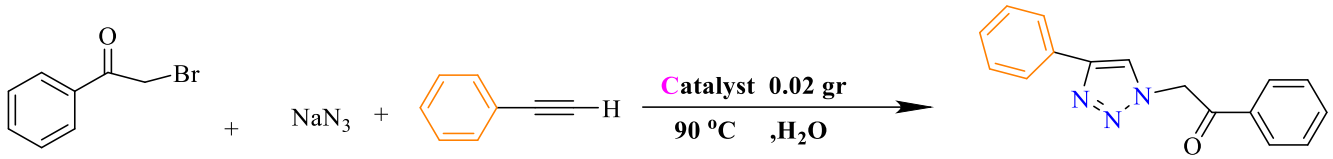
$$PMI = \frac{0.199+0.078+0.102+4.98}{0.239} = 22.42$$

$$E\ factor = 22.42 - 1 = 21.42$$

$$SI = 0$$

$$WI = \frac{5 \times 0.997}{0.239} = 20.85$$

Synthesis of 1-Phenyl-2-(4-phenyl-1H-1,2,3-triazol-1-yl)ethanone by CuI-USY (Table 4, entry 7)



Chemical Formula: C_8H_7BrO Molecular Weight: 199/05

Chemical Formula: N_3Na Molecular Weight: 65/01

Chemical Formula: C_8H_6 Molecular Weight: 102/14

Chemical Formula: $C_{16}H_{13}N_3O$ Molecular Weight: 263/30

Materials used for metrics calculations:

Phenacyl bromide (0.199 g, 1.0 mmol), Sodium azide (0.071 g, 1.1 mmol), phenylacetylene (0.102 g, 1.0mmol), H_2O (1.99 g, 2 ml), product (0.163 g, 0.62 mmol).

$$AE = \frac{263.30}{199.05+71+102.14} \times 100 = 70.74$$

$$AE_f = 70.74 \times 62\% = 43.85$$

$$CE = \frac{16 \times 0.00062}{8 \times 0.001 + 8 \times 0.001} \times 100 = 62$$

$$RME = \frac{0.163}{0.199+0.071+0.102} \times 100 = 43.81$$

$$OE = \frac{43.81}{70.74} \times 100 = 61.93$$

$$PMI = \frac{0.199+0.071+0.102+1.99}{0.163} = 14.49$$

$$E\ factor = 14.49 - 1 = 13.49$$

$$SI = 0$$

$$WI = \frac{2 \times 0.997}{0.163} = 12.20$$

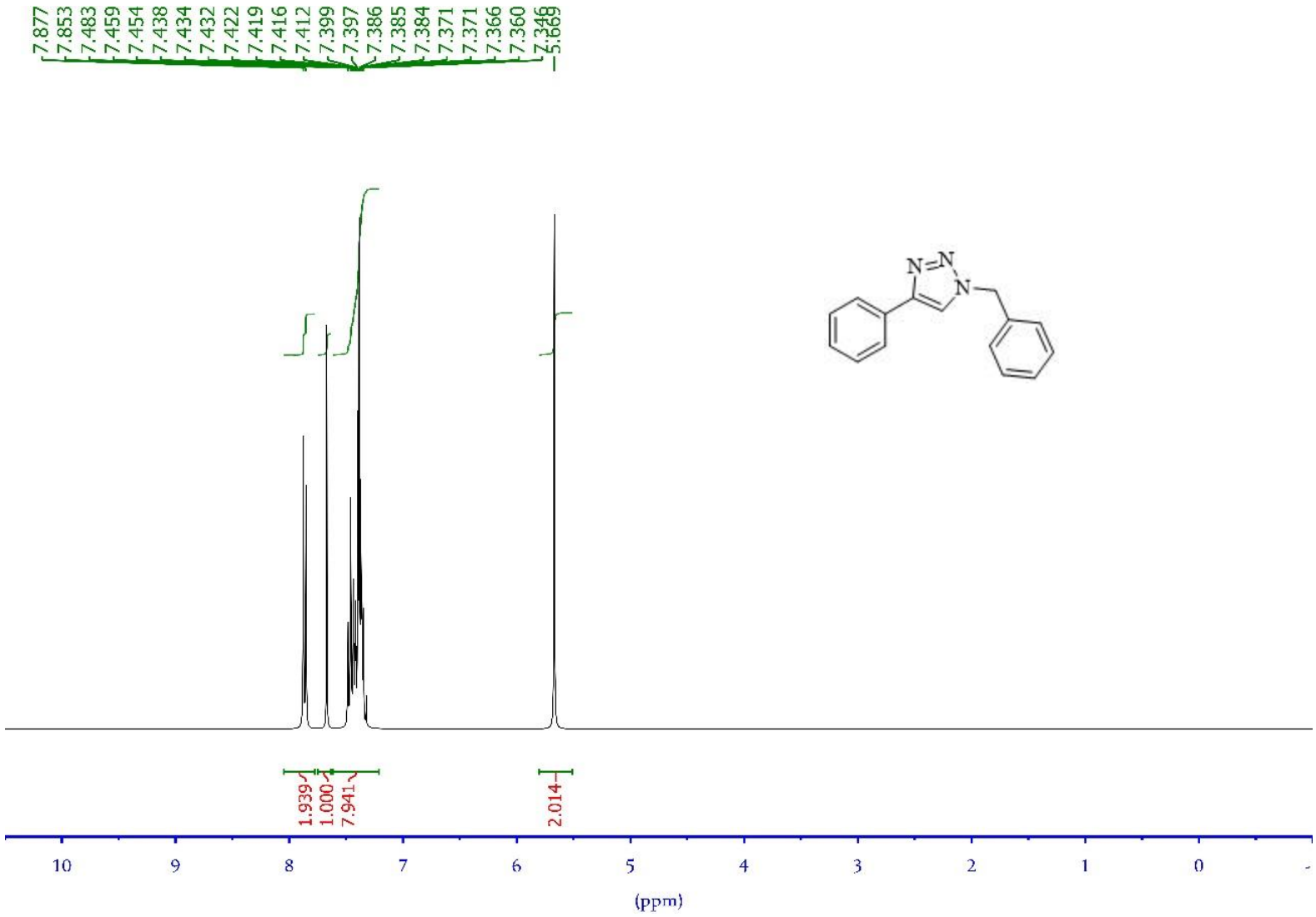


Figure S1: ^{1}H-NMR of 1-benzyl-4-phenyl-1H-1,2,3-triazole

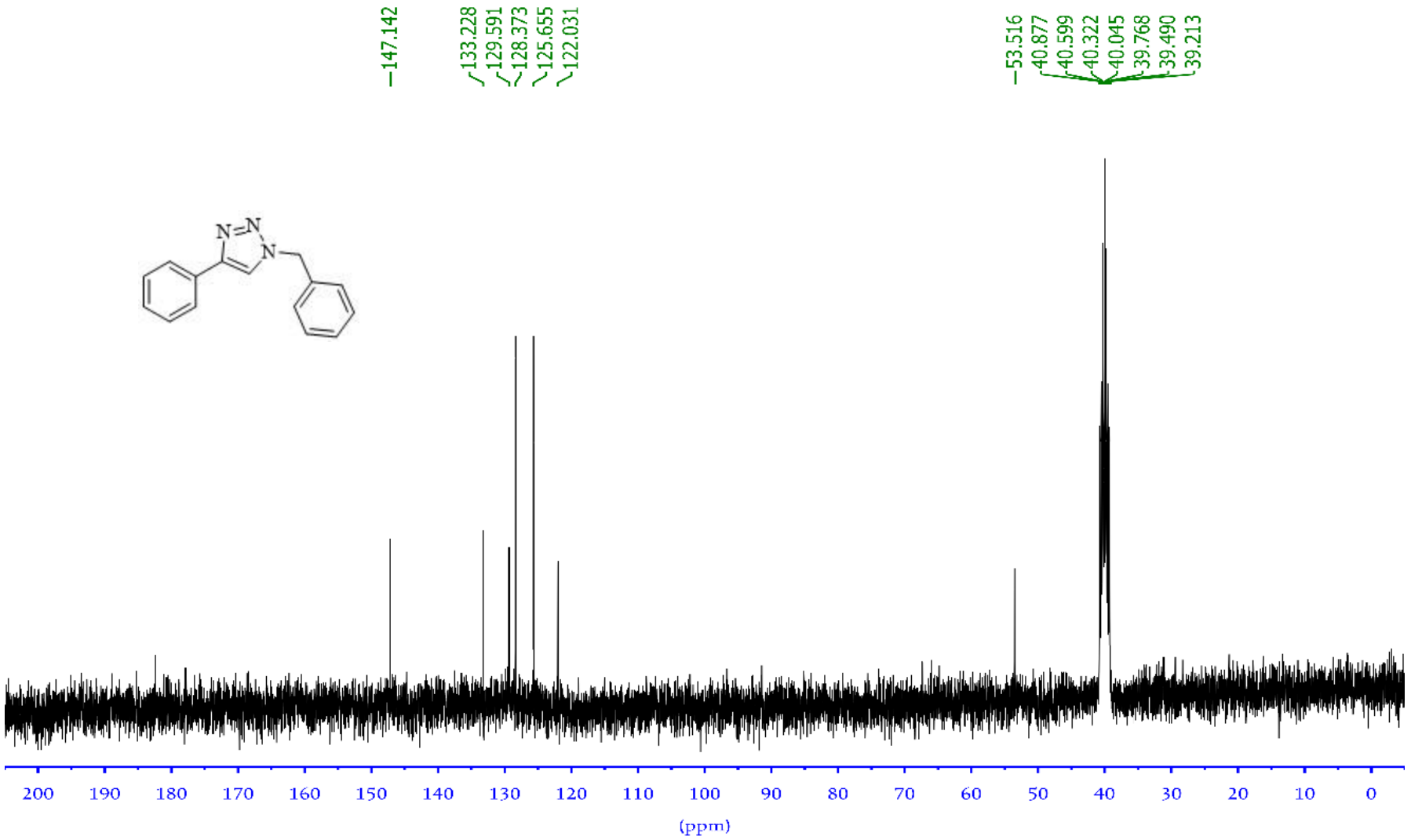


Figure S2: ^{13}C-NMR of 1-benzyl-4-phenyl-1H-1,2,3-triazole

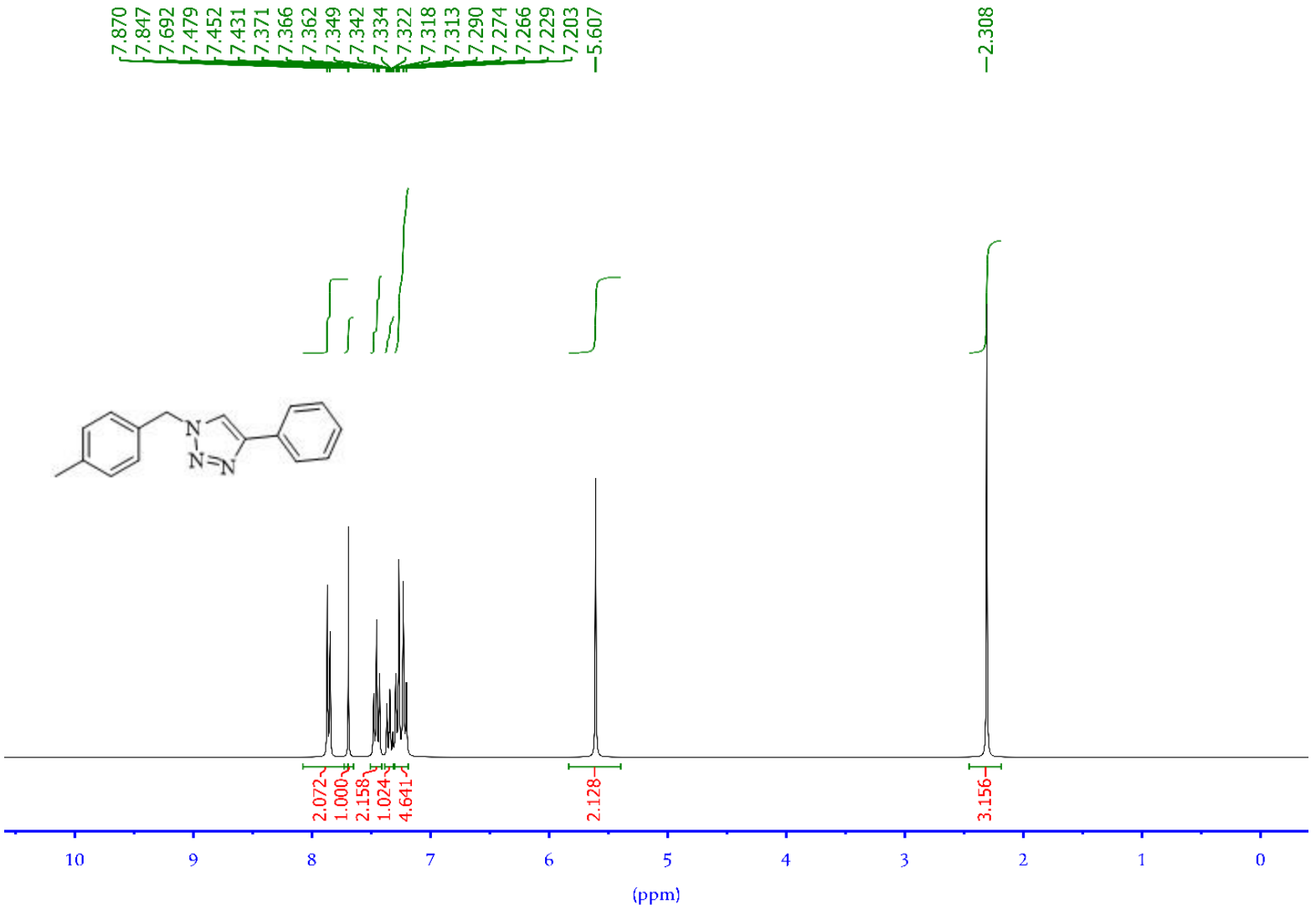


Figure S3: ^{1}H-NMR of 1-(4-methylbenzyl)-4-phenyl-1H-1,2,3-triazole

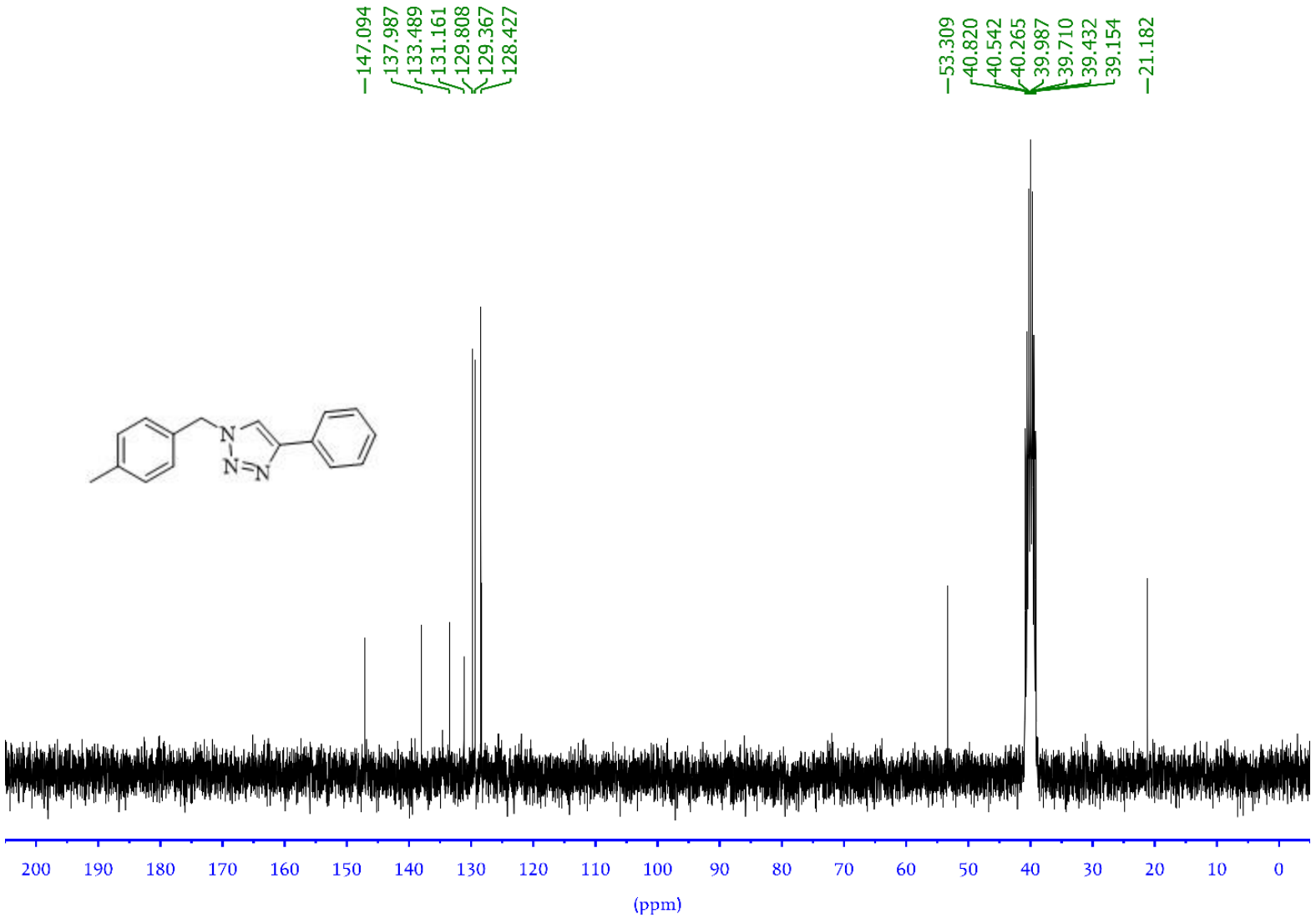


Figure S4: ^{13}C-NMR of 1-(4-methylbenzyl)-4-phenyl-1H-1,2,3-triazole

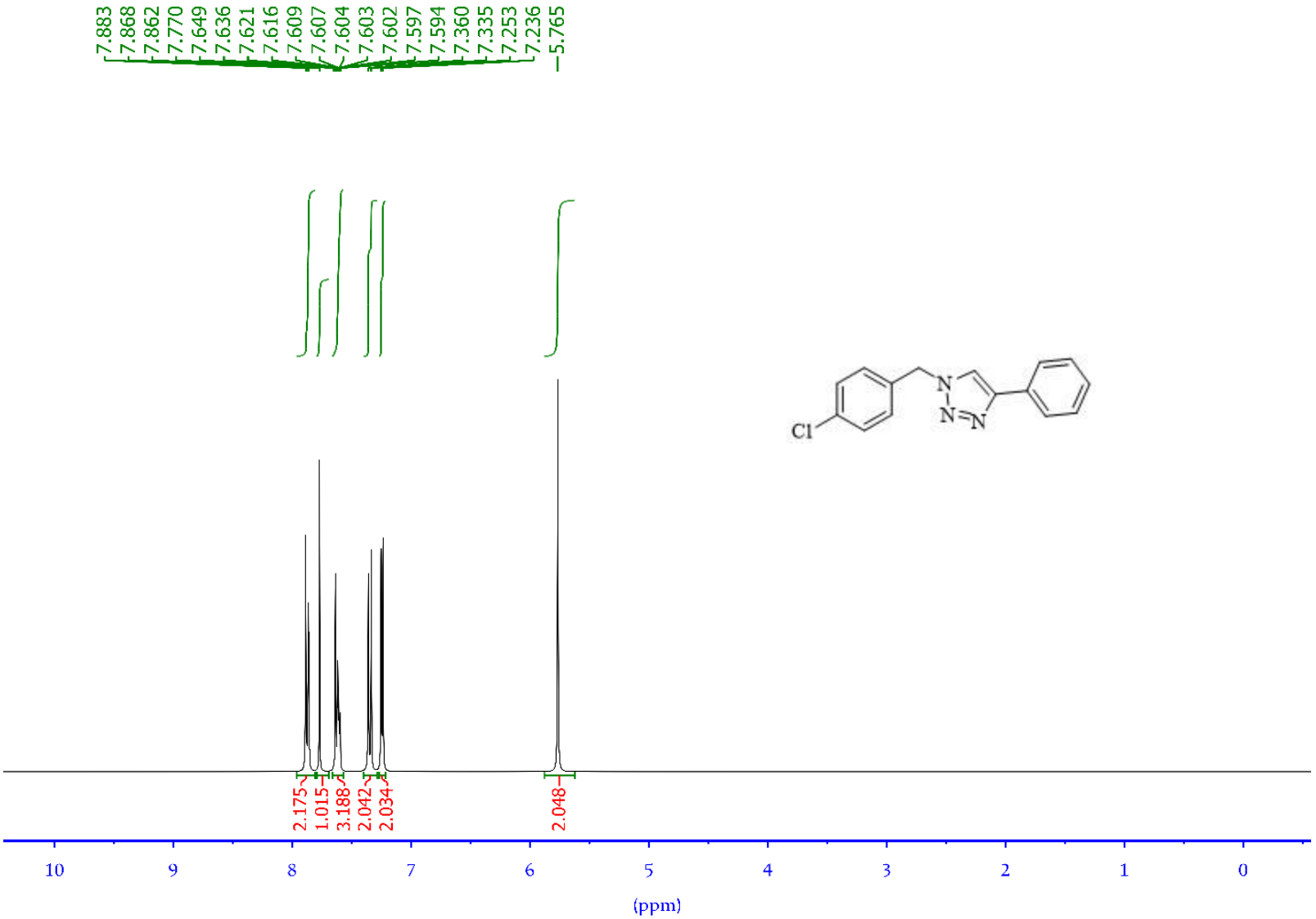


Figure S5: ^{1}H-NMR of 1-(4-chlorobenzyl)-4-phenyl-1H-1,2,3-triazole

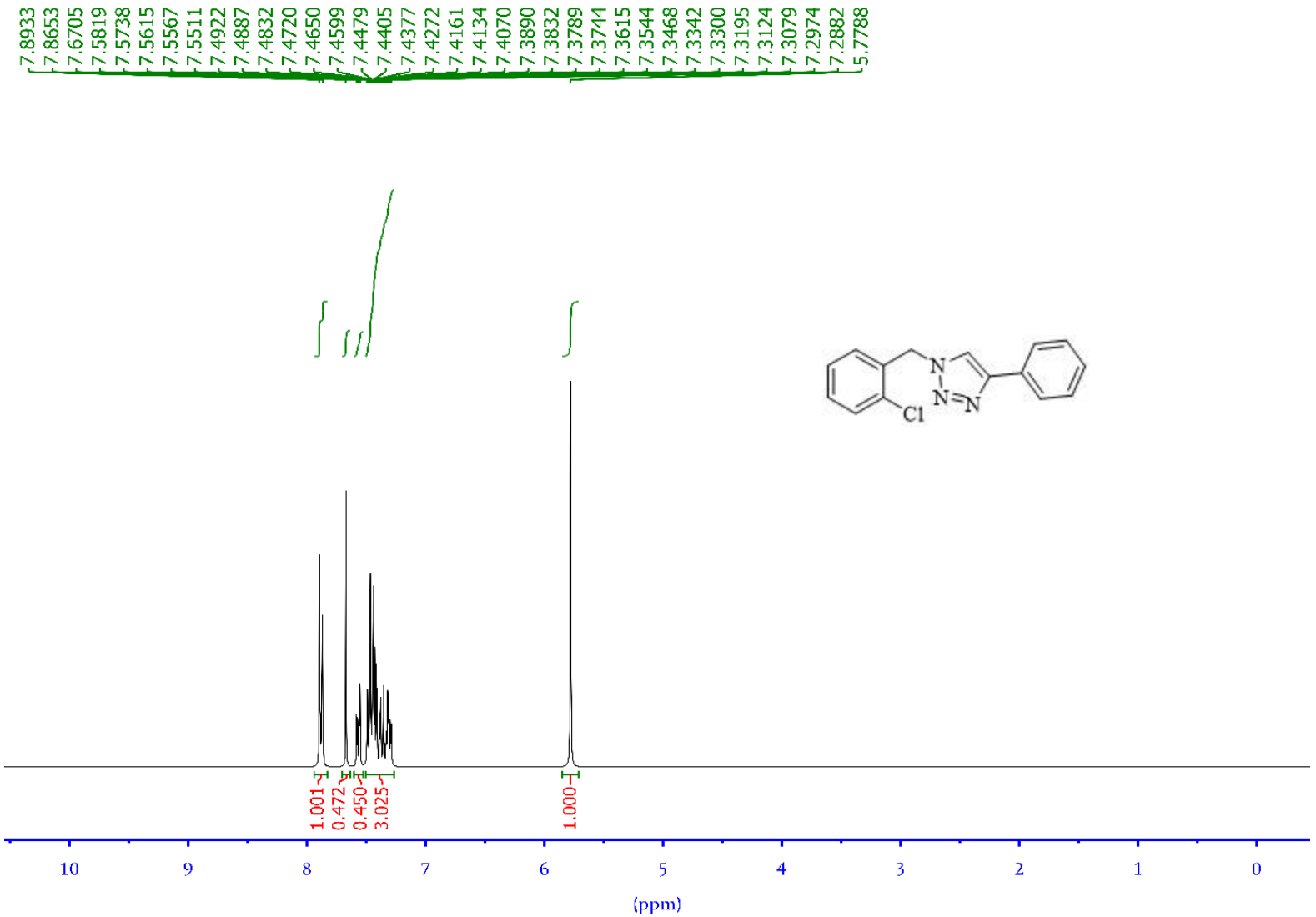


Figure S6: ^{1}H-NMR of 1-(2-chlorobenzyl)-4-phenyl-1H-1,2,3-triazole

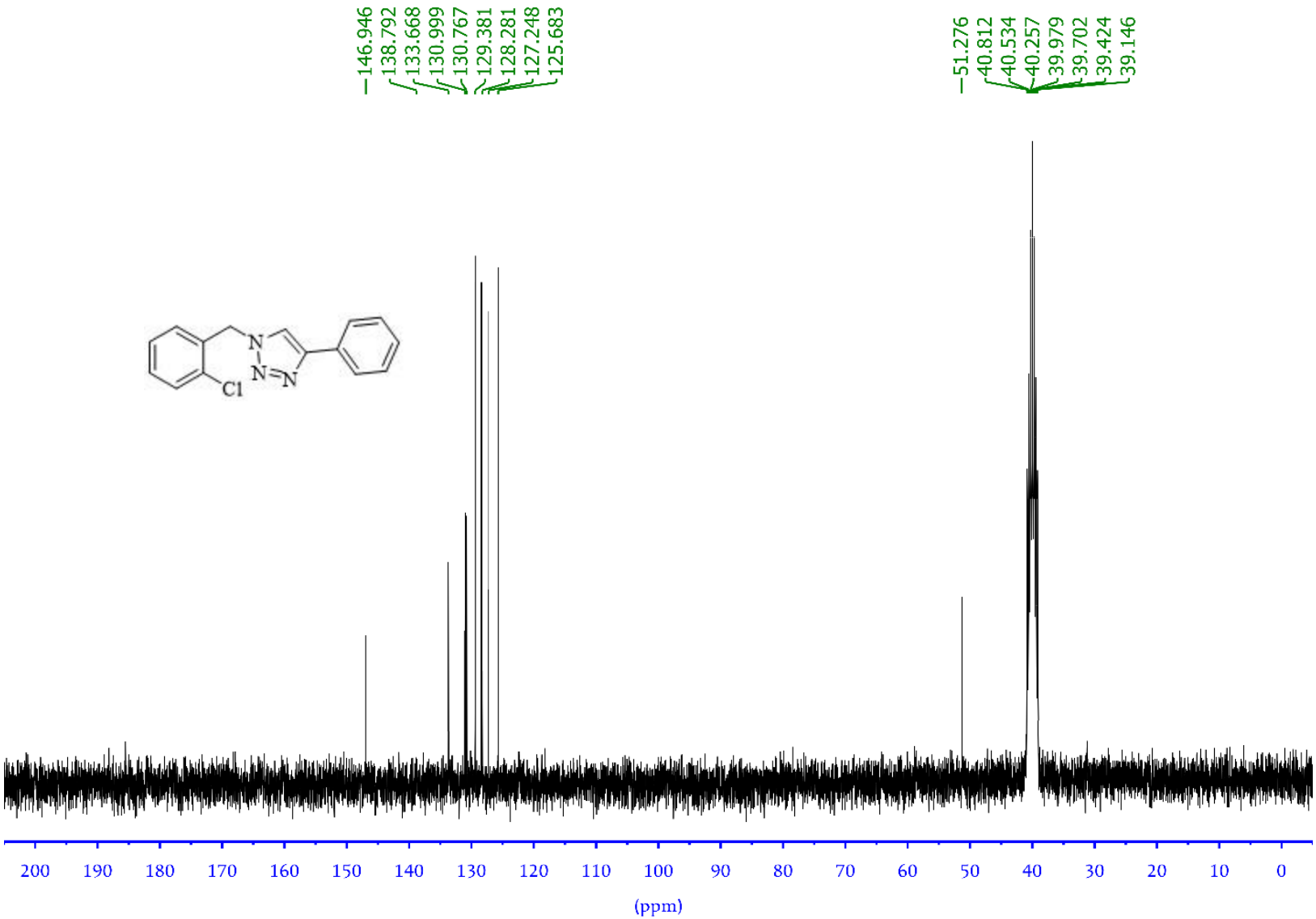


Figure S7: ^{13}C-NMR of 1-(2-chlorobenzyl)-4-phenyl-1H-1,2,3-triazole

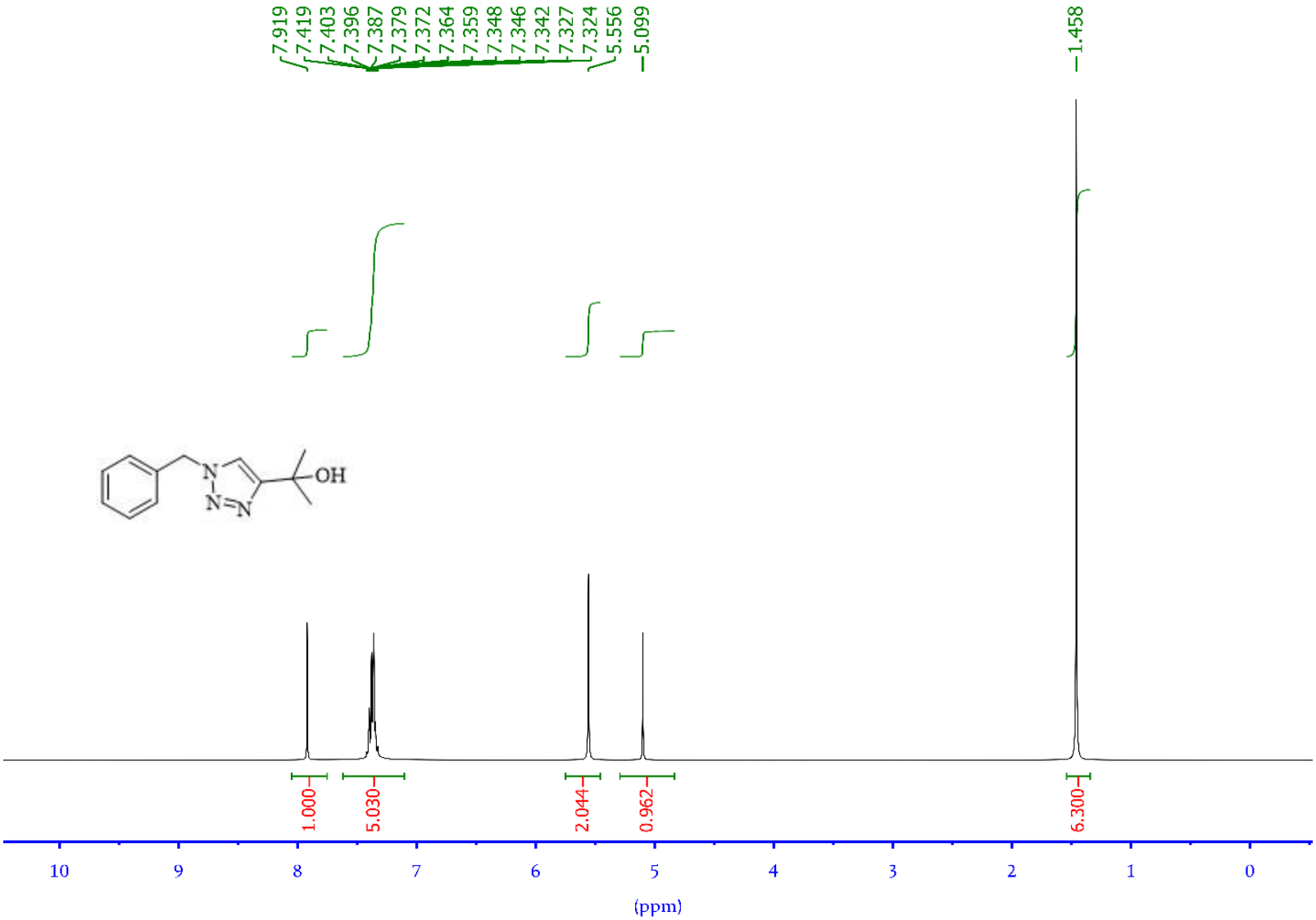


Figure S8: ^{1}H-NMR of 2-(1-benzyl-1H-1,2,3-triazol-4-yl)propan-2-ol

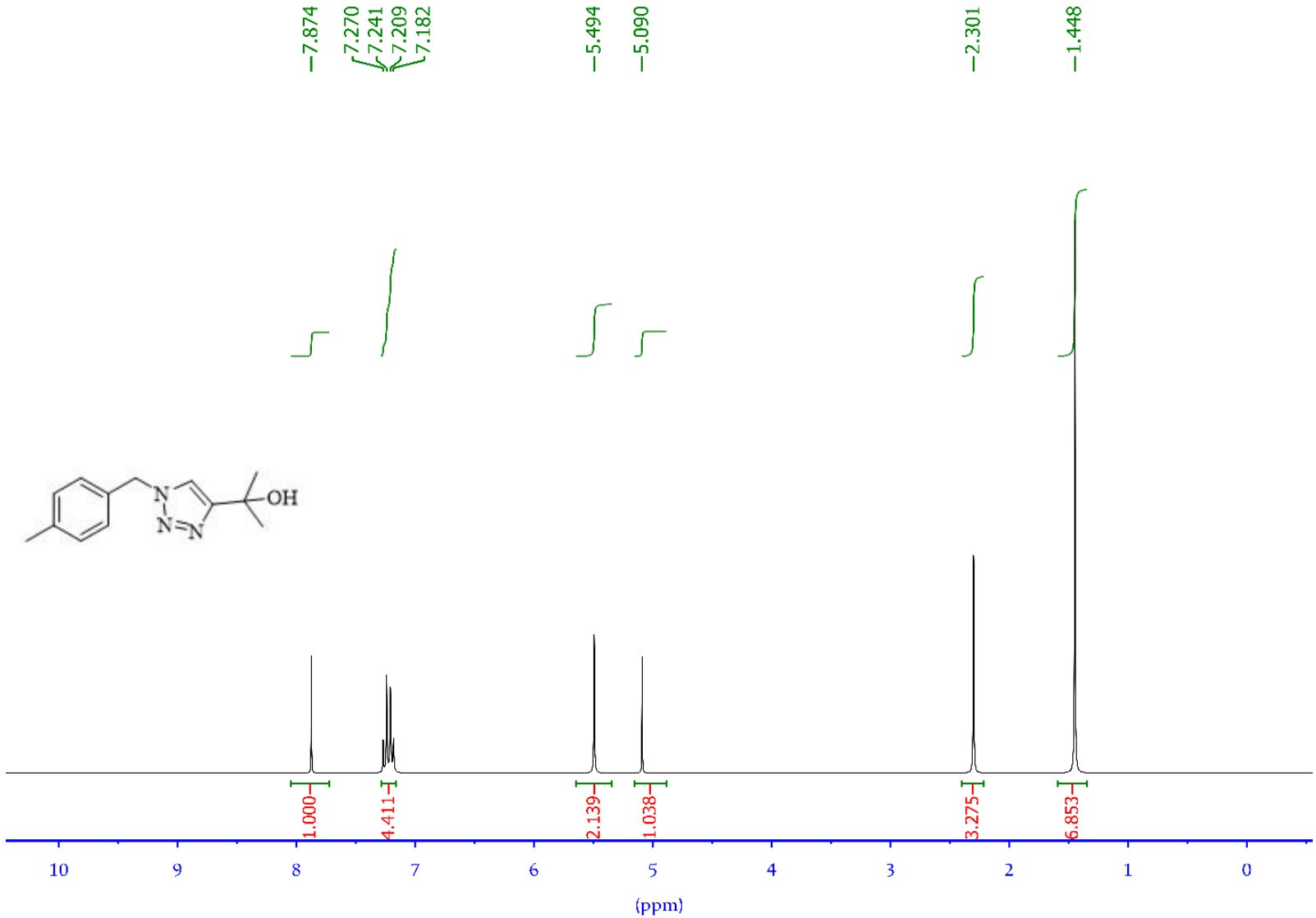


Figure S9: ^{1}H-NMR of 2-(1-(4-methylbenzyl)-1H-1,2,3-triazol-4-yl)propan-2-ol

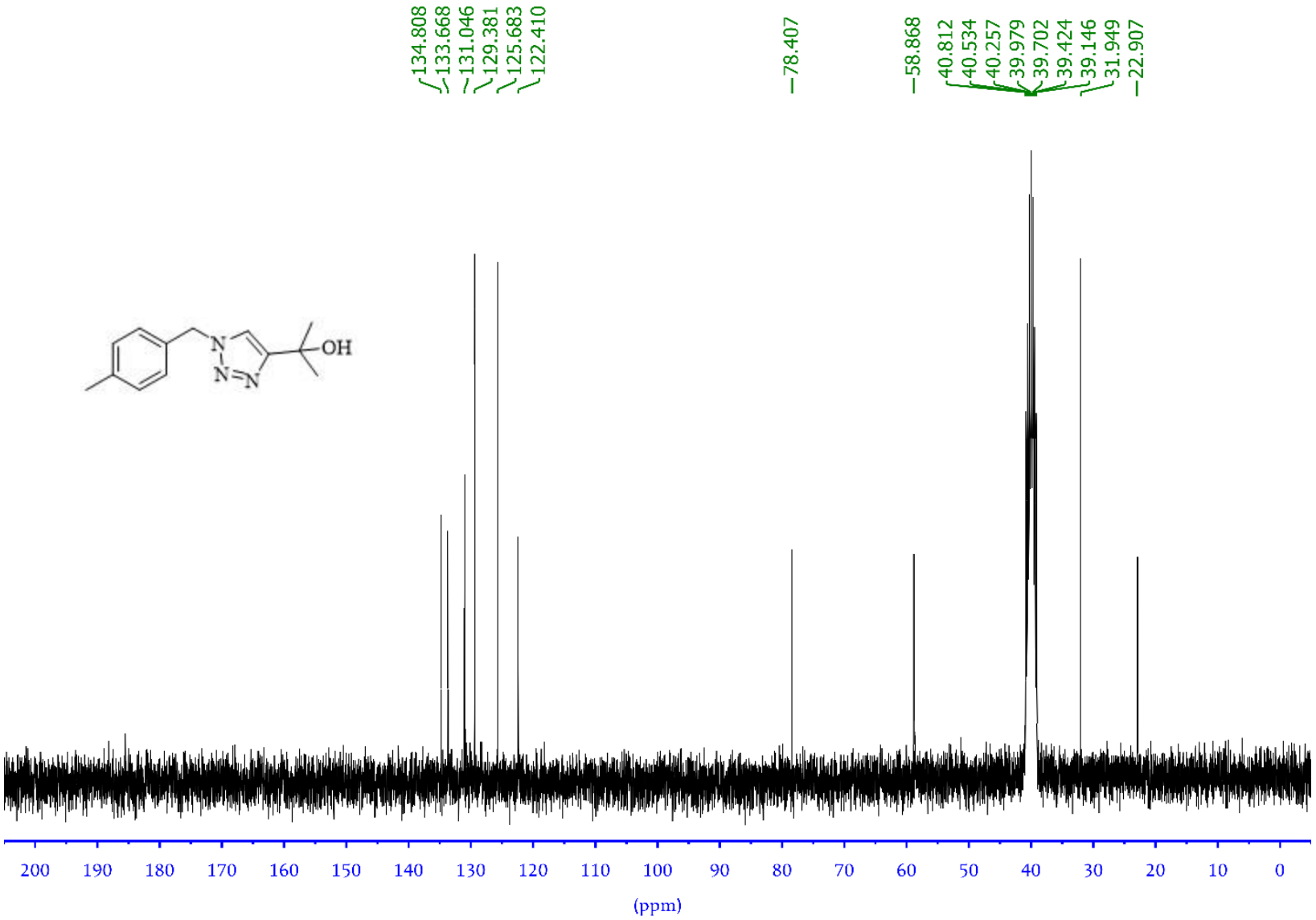


Figure S10: ^{13}C-NMR of 2-(1-(4-methylbenzyl)-1H-1,2,3-triazol-4-yl)propan-2-ol

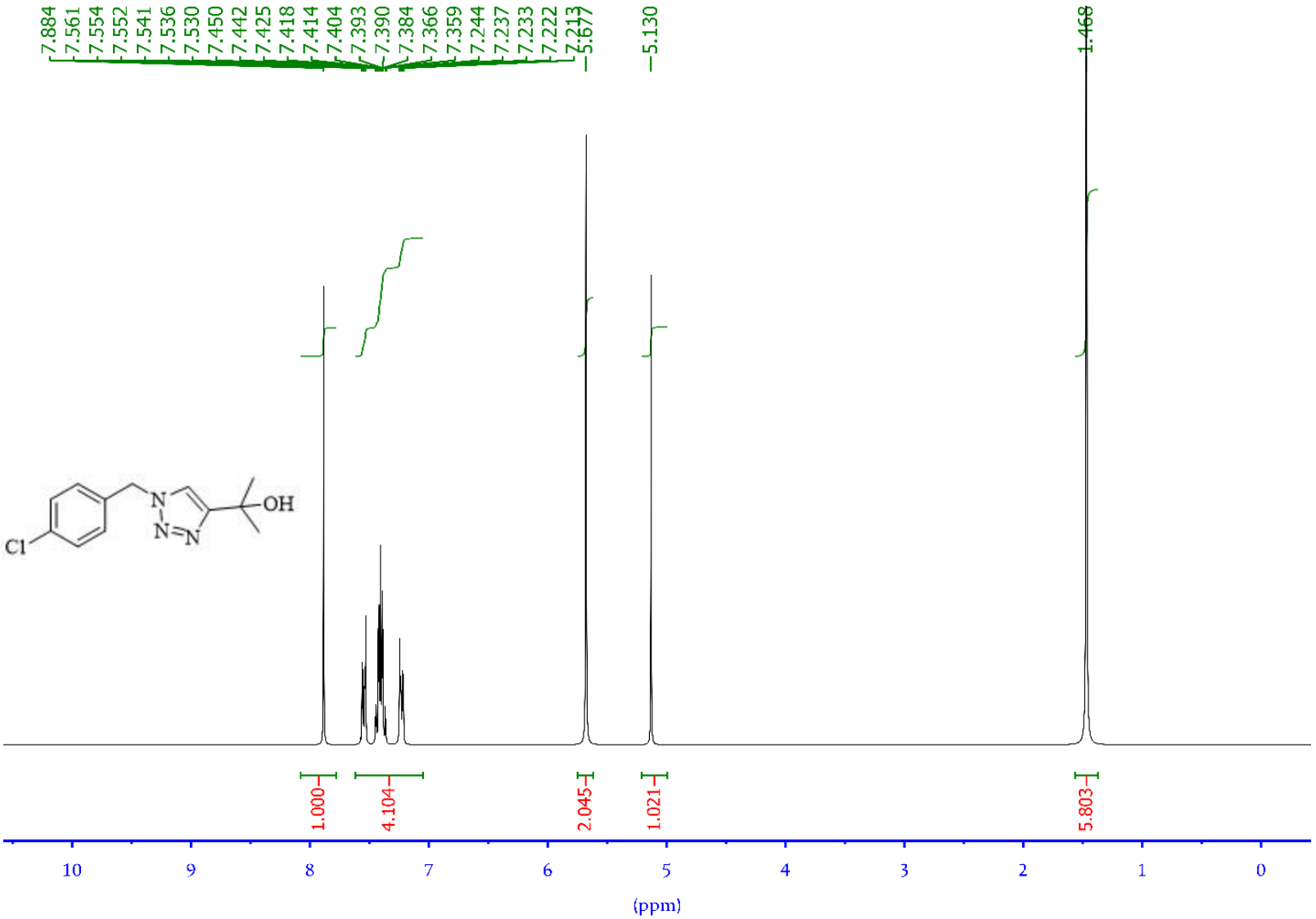


Figure S11: ^{1}H-NMR of 2-(1-(4-chlorobenzyl)-1H-1,2,3-triazol-4-yl)propan-2-ol

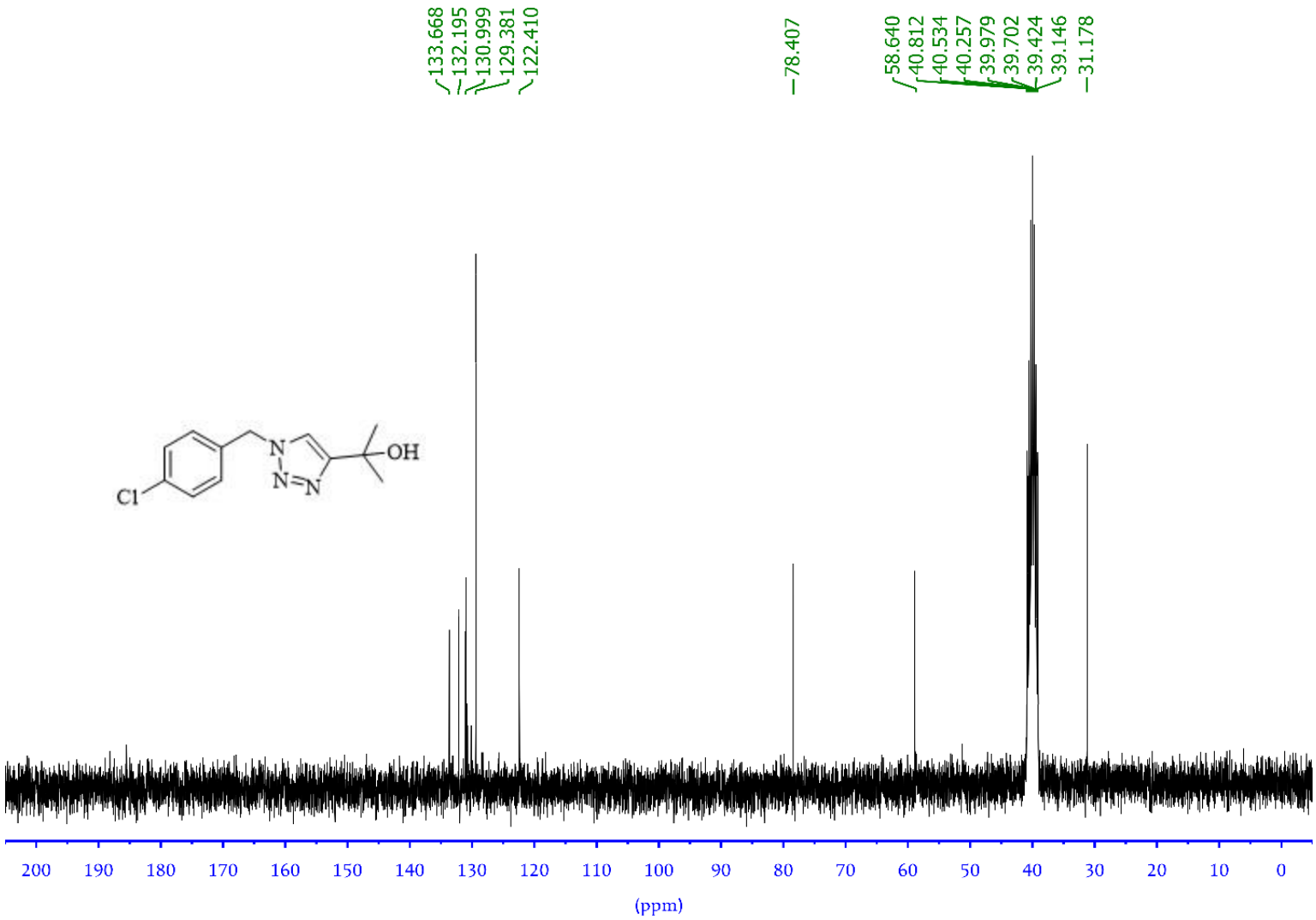


Figure S12: ^{13}C-NMR of 2-(1-(4-chlorobenzyl)-1H-1,2,3-triazol-4-yl)propan-2-ol

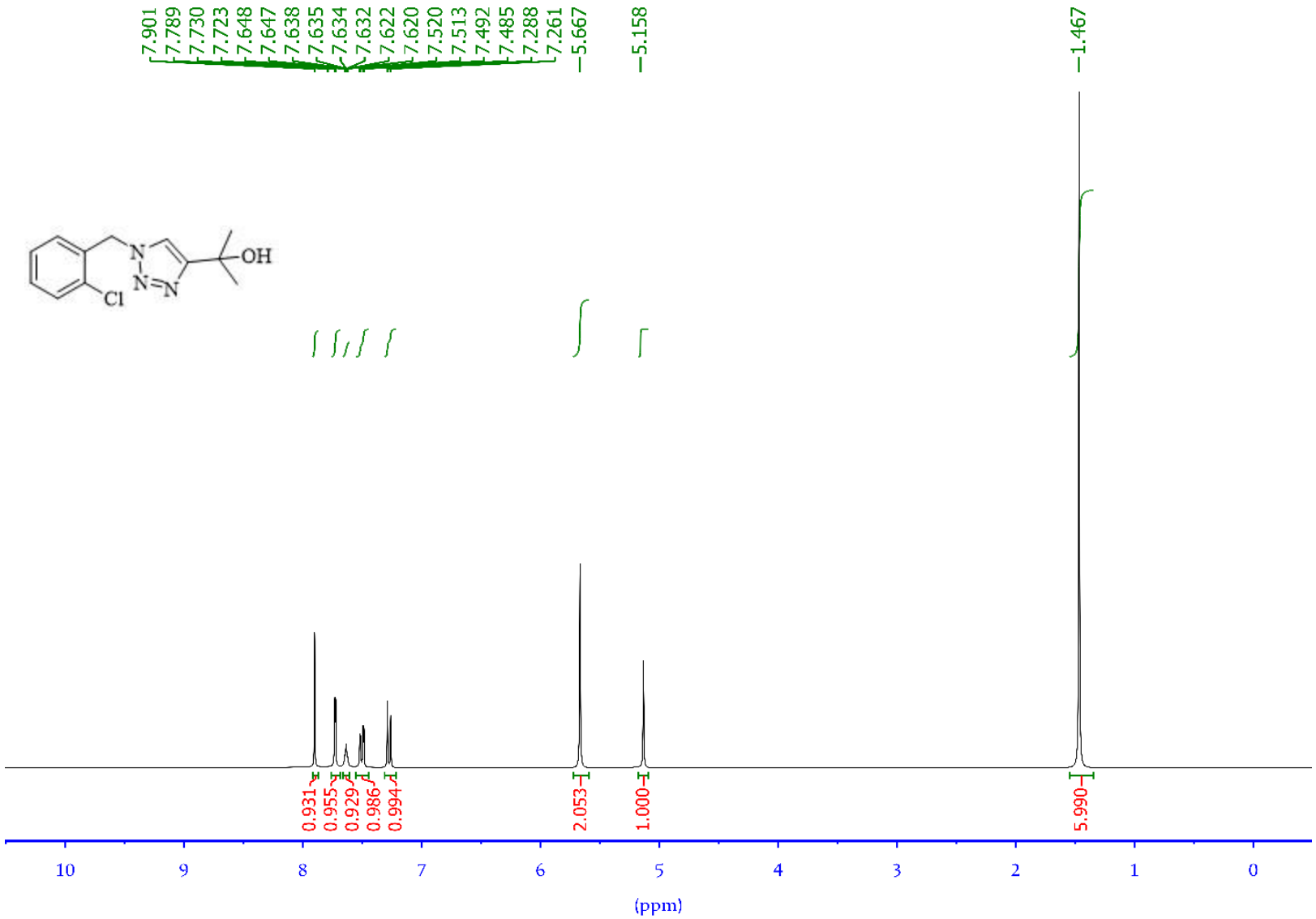


Figure S13: ^{1}H-NMR of 2-(1-(2-chlorobenzyl)-1H-1,2,3-triazol-4-yl)propan-2-ol

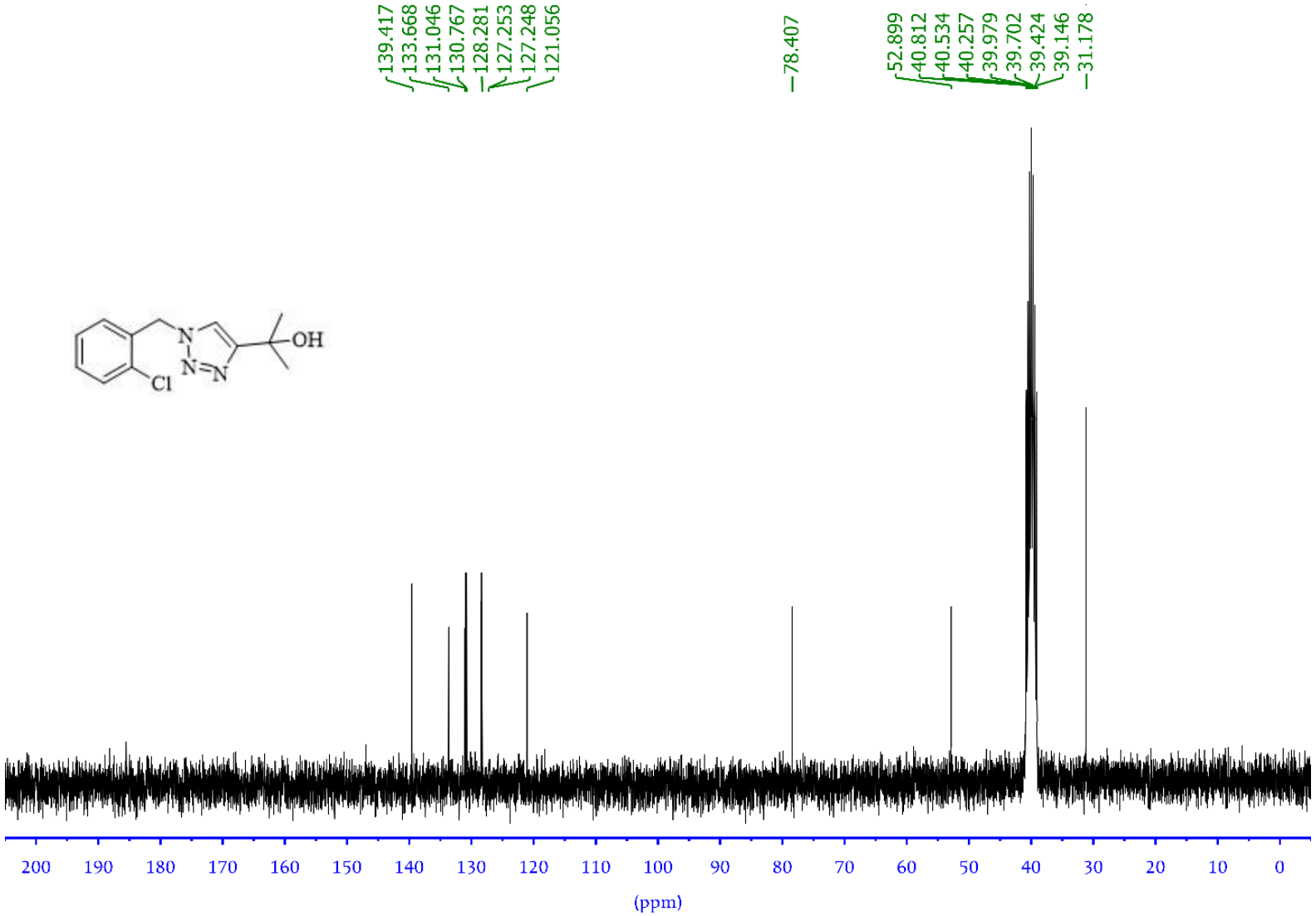


Figure S14: ^{13}C-NMR of 2-(1-(2-chlorobenzyl)-1H-1,2,3-triazol-4-yl)propan-2-ol

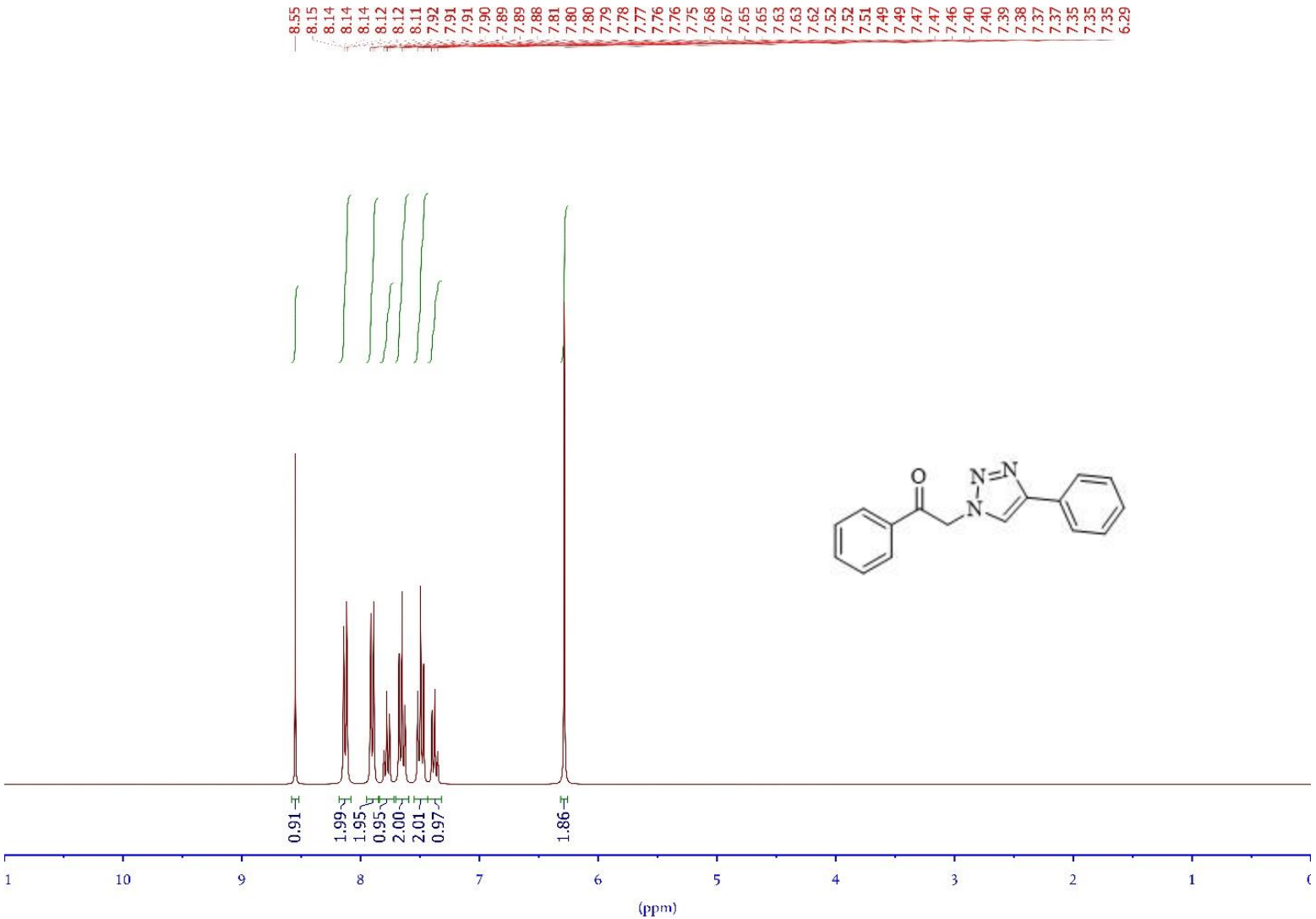


Figure S15: ^{1}H-NMR of 1-Phenyl-2-(4-phenyl-1H-1,2,3-triazol-1-yl)ethanone

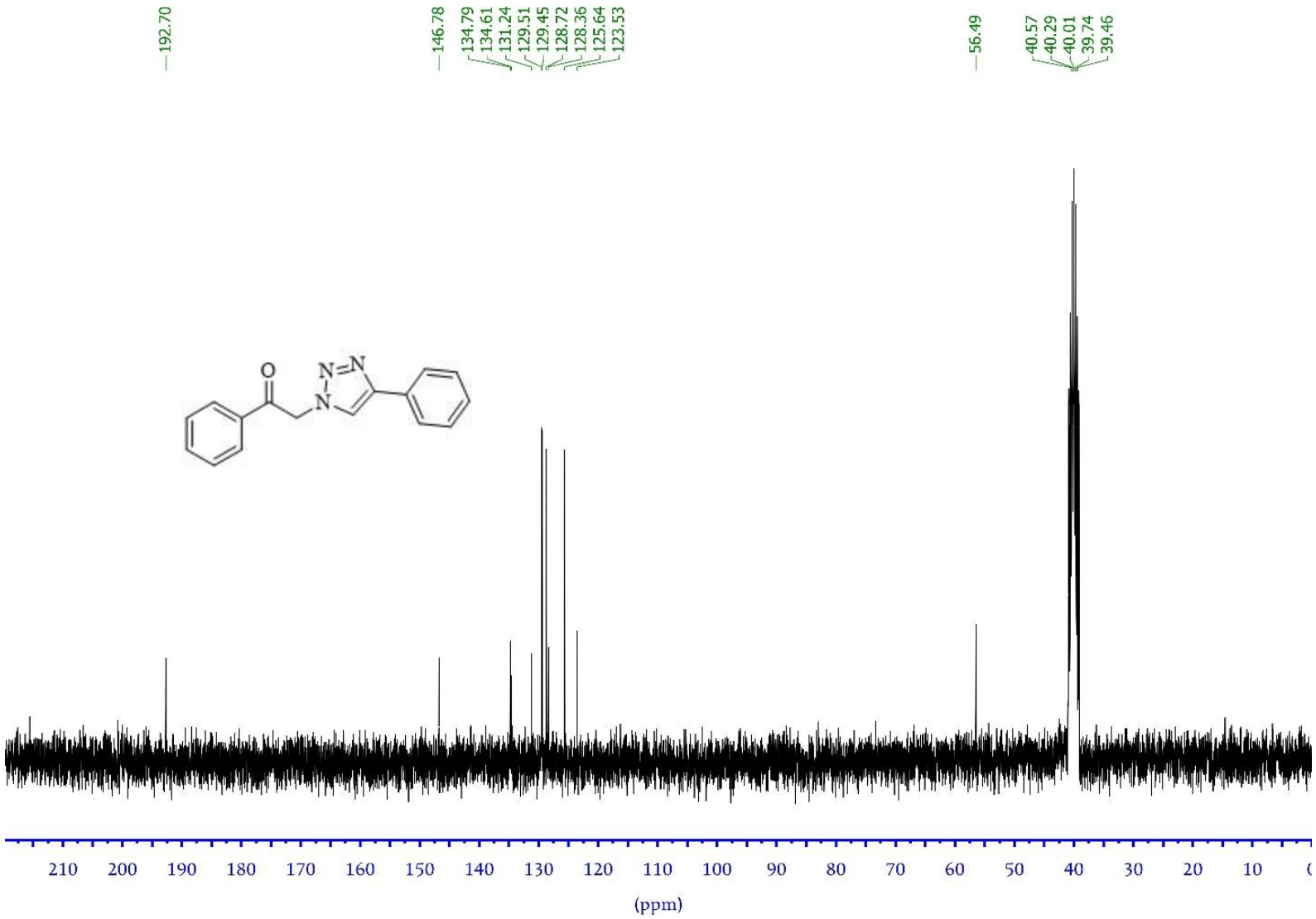


Figure S16: ^{13}C-NMR of 1-Phenyl-2-(4-phenyl-1H-1,2,3-triazol-1-yl)ethenone

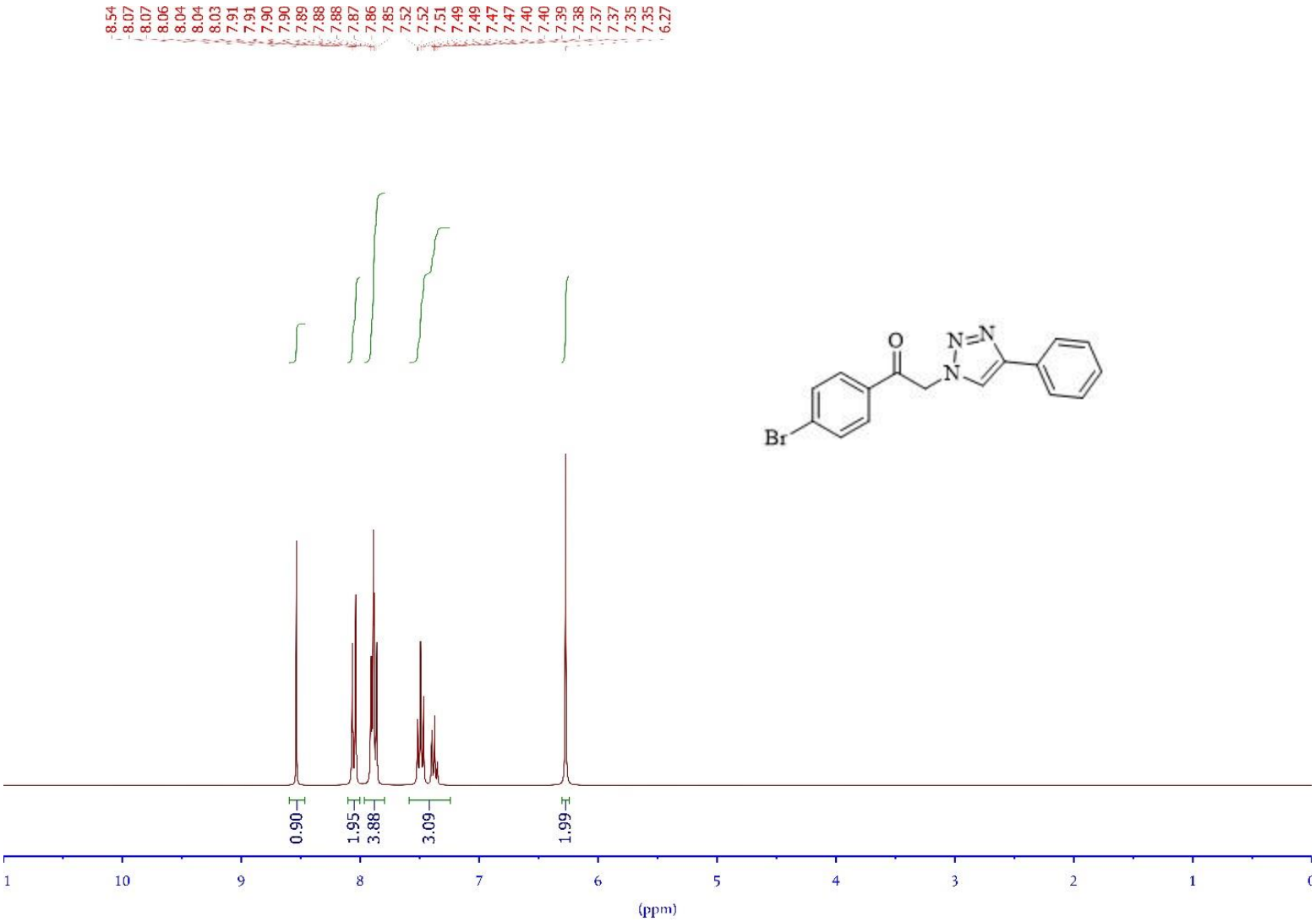


Figure S17: ^{1}H-NMR of 1-(4-Bromophenyl)-2-(4-phenyl-1H-1,2,3-triazol-1-yl) ethanone

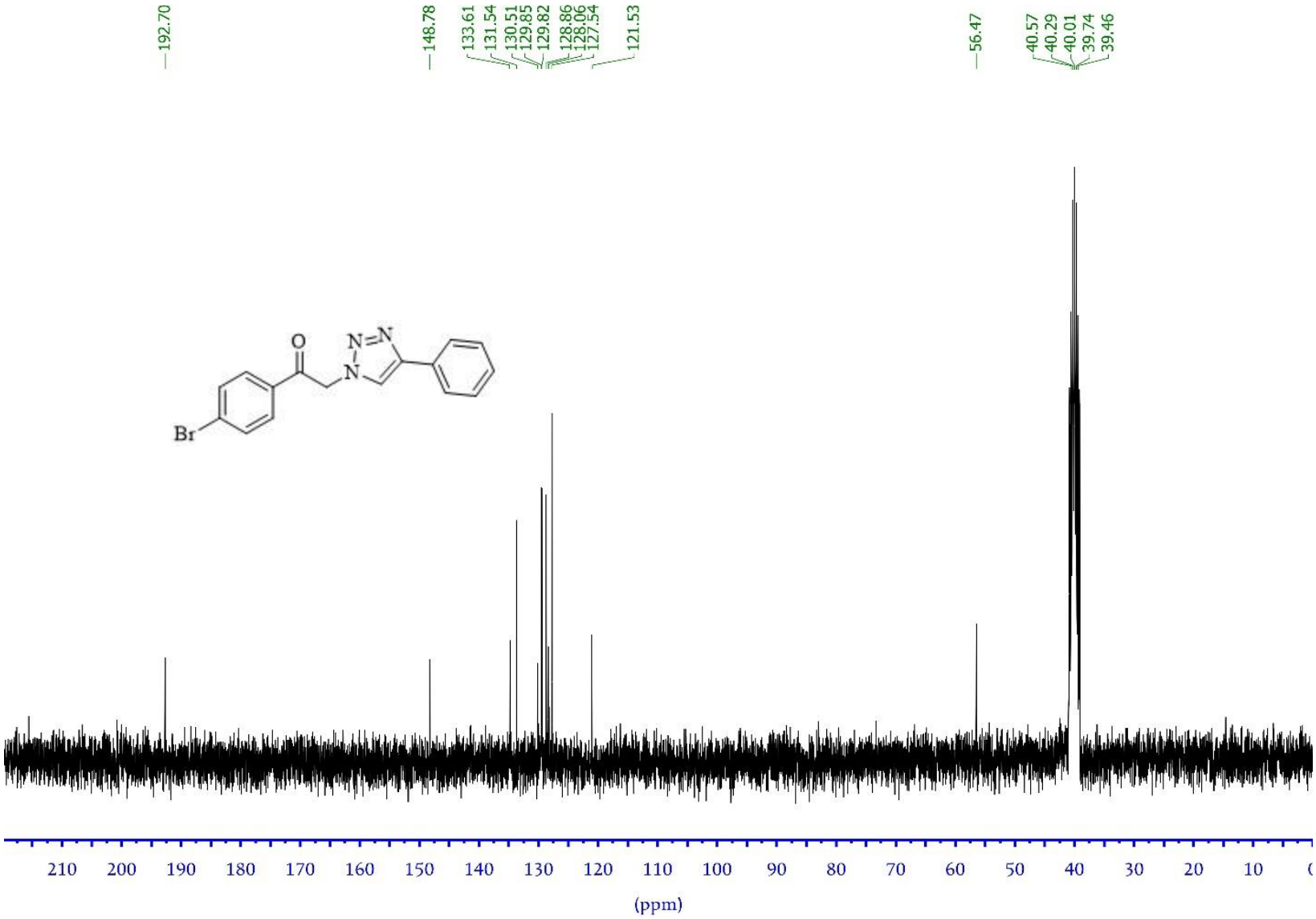


Figure S18: ^{13}C-NMR of 1-(4-Bromophenyl)-2-(4-phenyl-1H-1,2,3-triazol-1-yl) ethanone

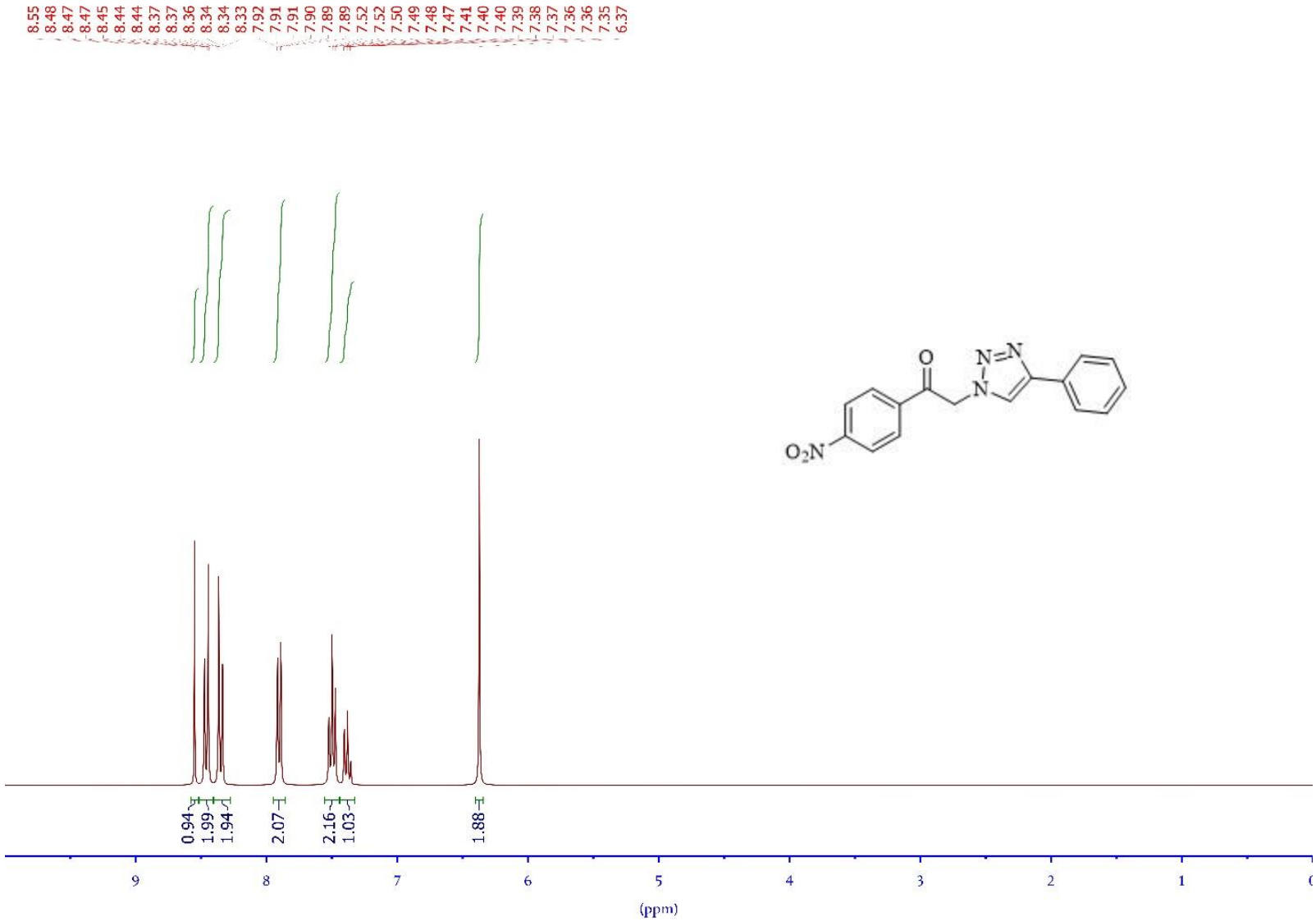


Figure S19: ^{1}H-NMR of 1-(4-Nitro phenyl)-2-(4-phenyl-1H-1,2,3-triazol-1-yl)ethanone

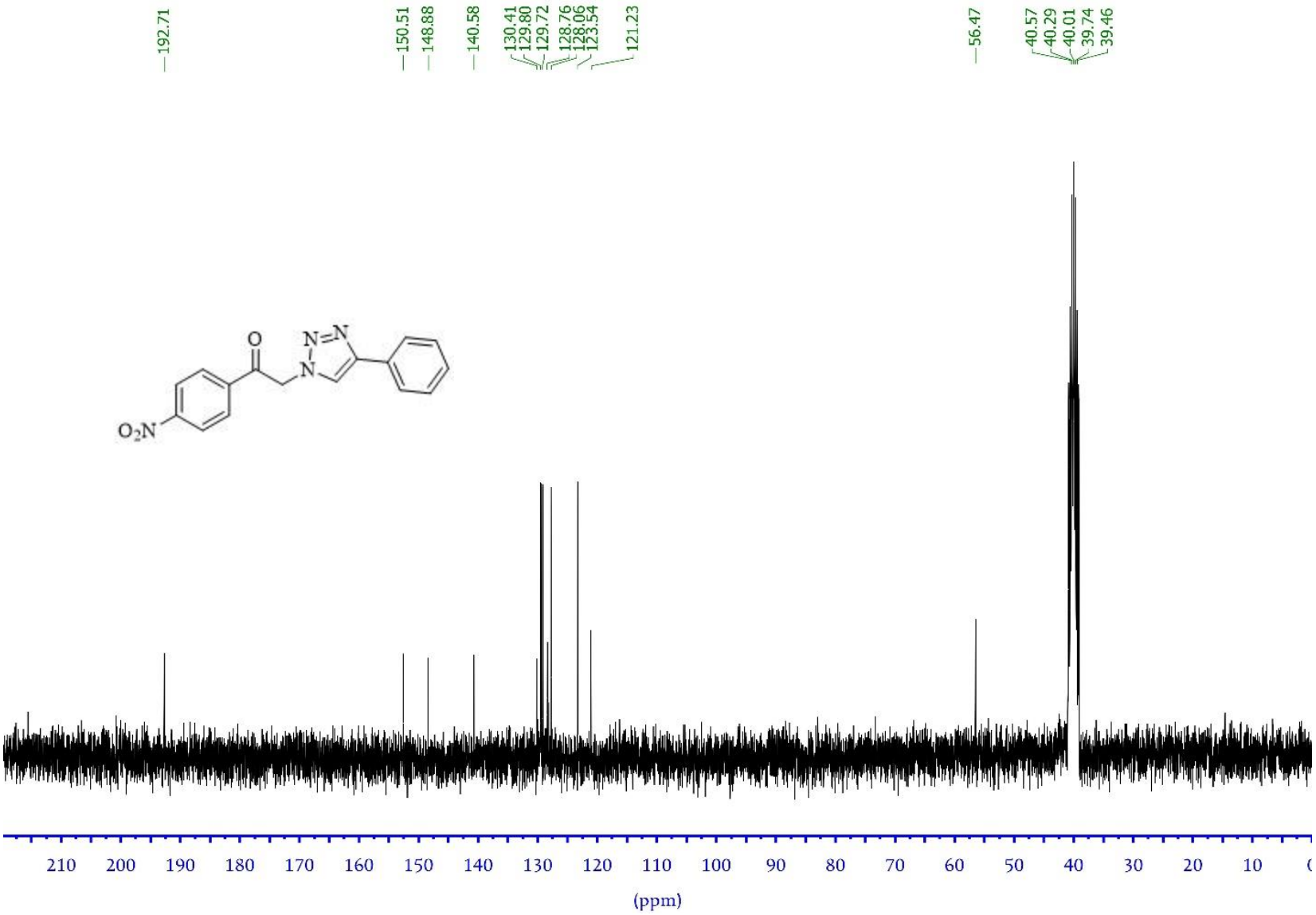


Figure S20: ^{13}C-NMR of 1-(4-Nitro phenyl)-2-(4-phenyl-1H-1,2,3-triazol-1-yl)ethanone

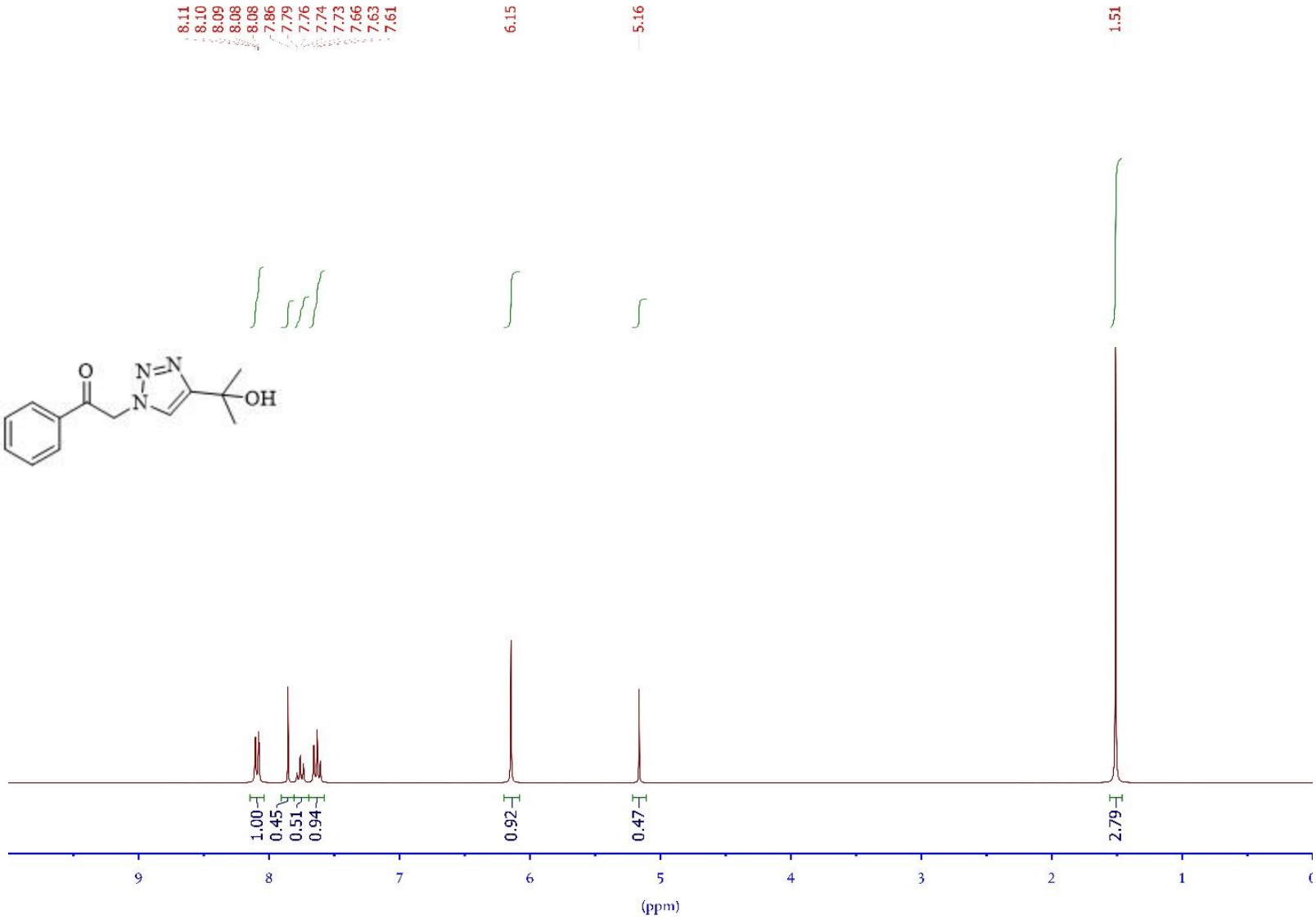


Figure S21: ^{1}H-NMR of 2-(4-(2-Hydroxypropan-2-yl)-1H-1,2,3-triazol-1-yl)-1-phenylethanone

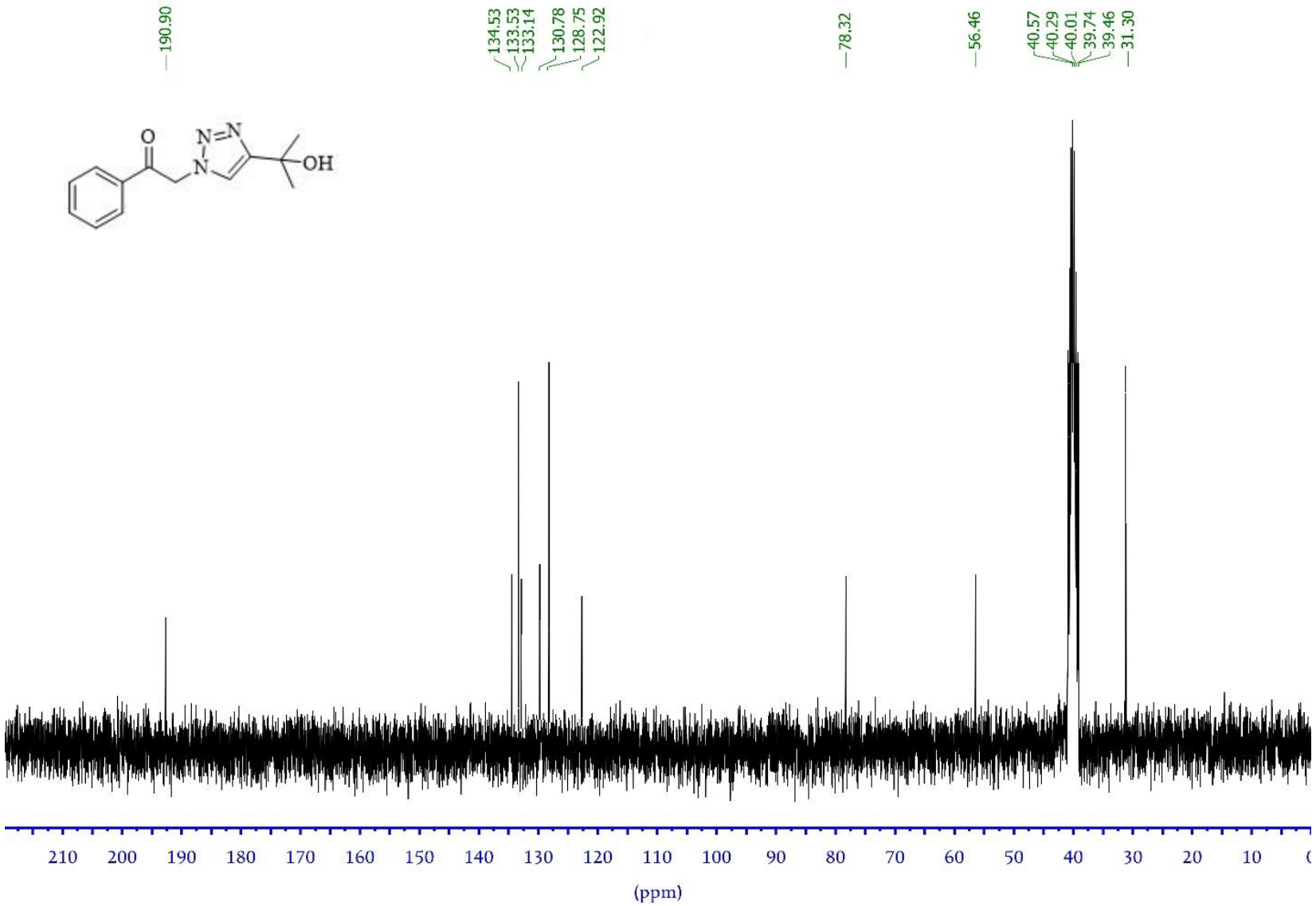


Figure S22: ^{13}C-NMR of 2-(4-(2-Hydroxypropan-2-yl)-1H-1,2,3-triazol-1-yl)-1-phenylethanone

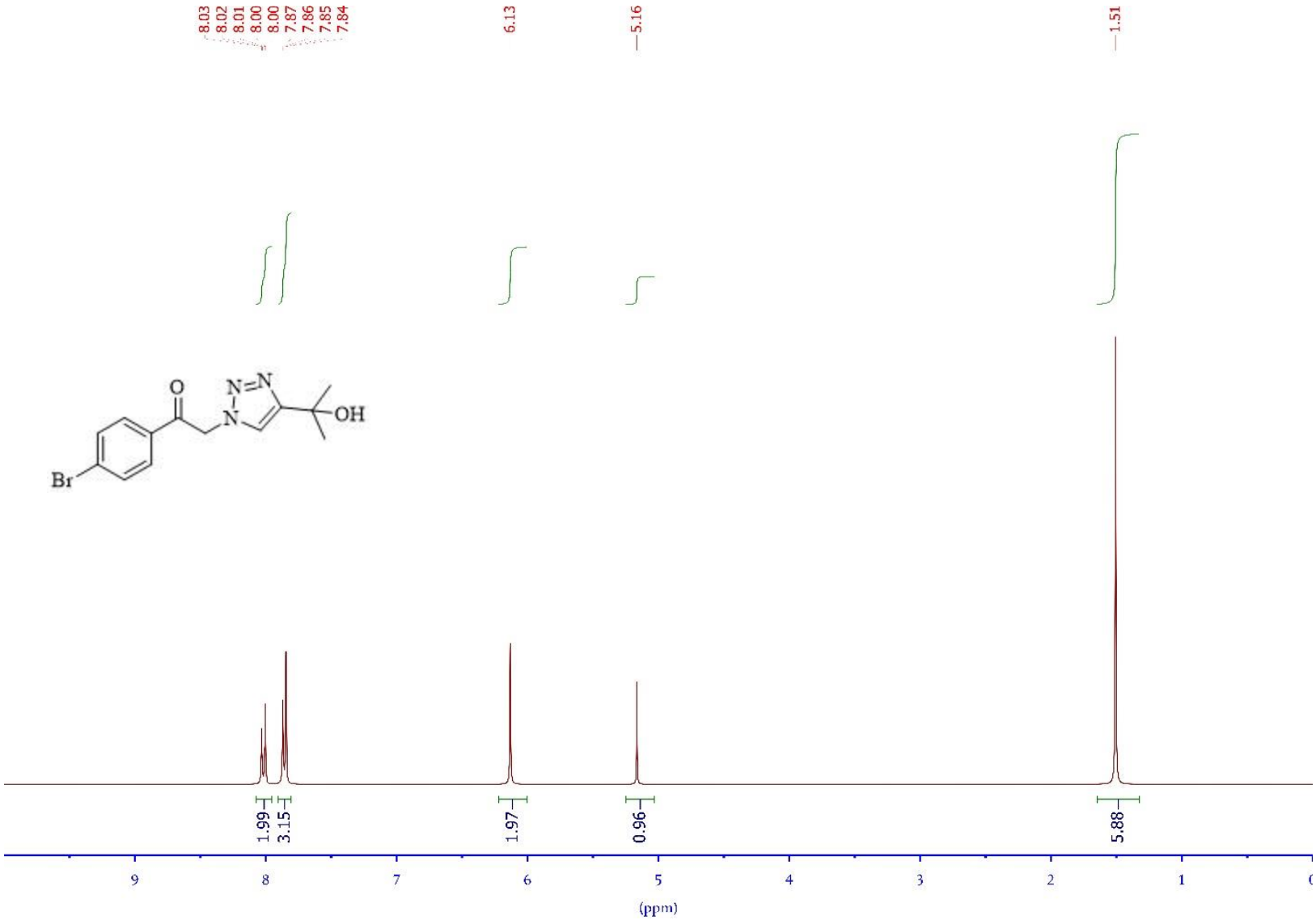


Figure S23: ^{1}H-NMR of 1-(4-Bromophenyl)-2-(4-(2-hydroxypropan-2-yl)-1H-1,2,3-triazol-1-yl)ethanone

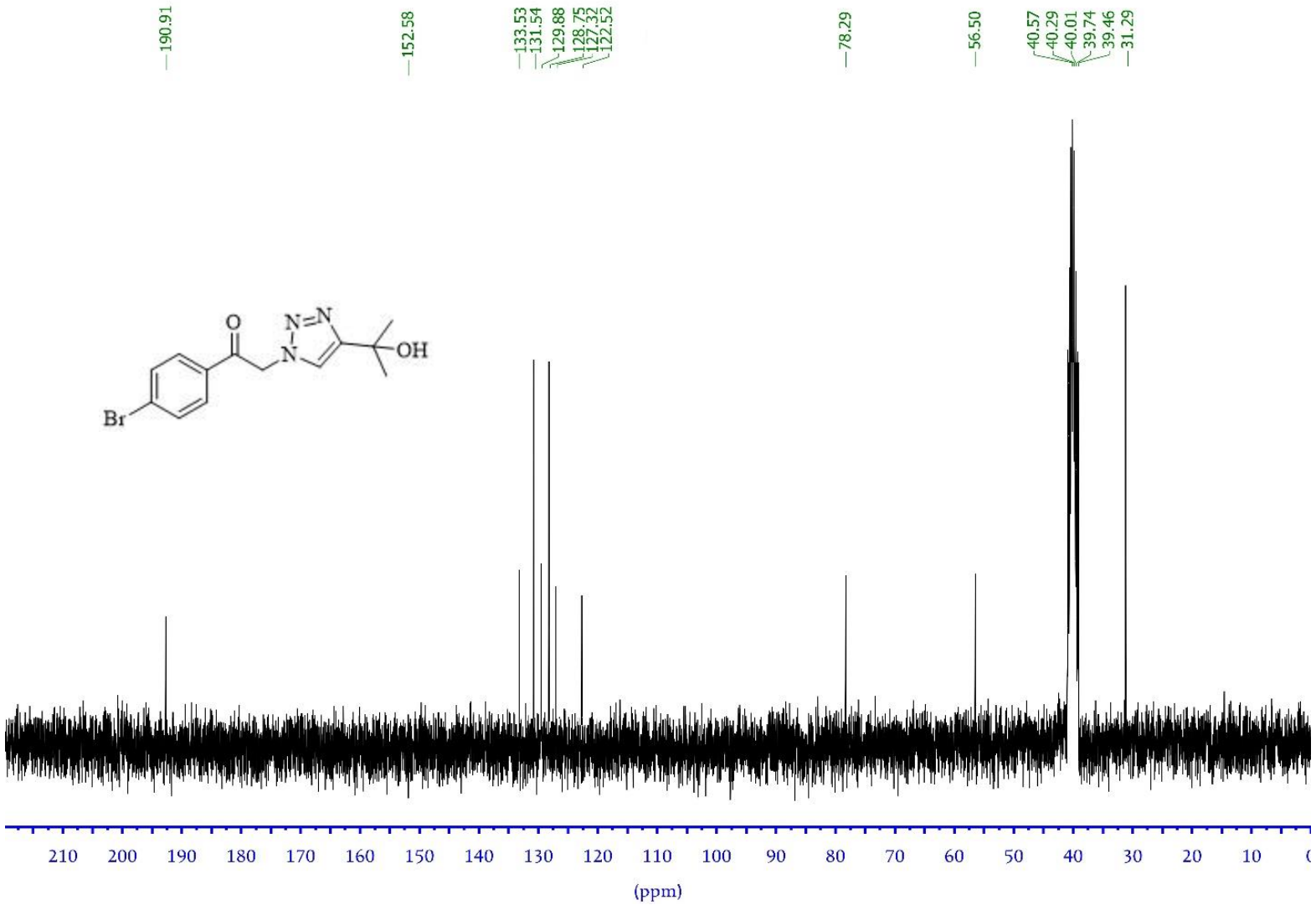


Figure S24: ^{13}C-NMR of 1-(4-Bromophenyl)-2-(4-(2-hydroxypropan-2-yl)-1H-1,2,3-triazol-1-yl)ethanone

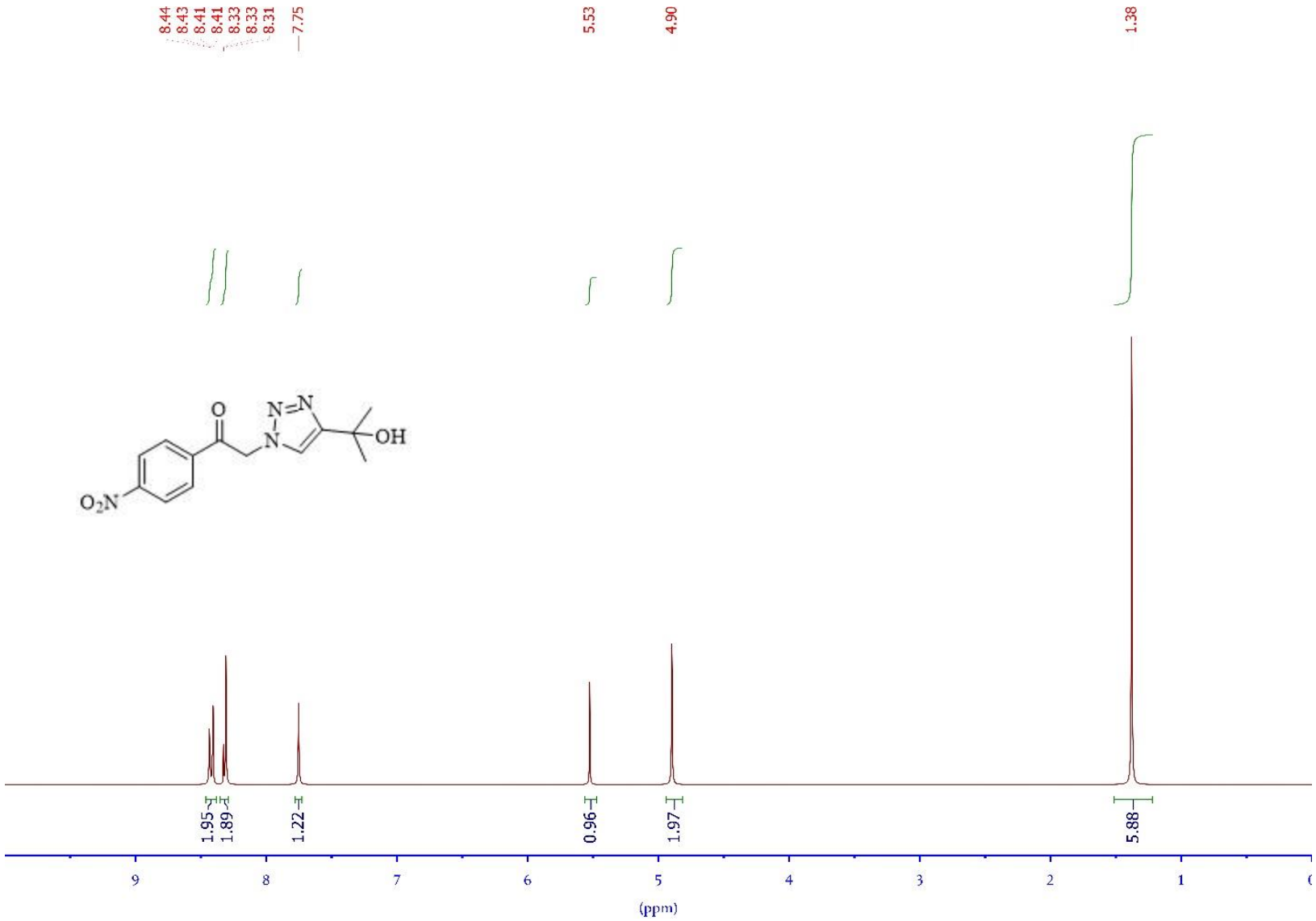


Figure S25: ^{1}H-NMR of 2-(4-(2-Hydroxypropan-2-yl)-1H-1,2,3-triazol-1-yl)-1-(4-nitrophenyl)ethanone

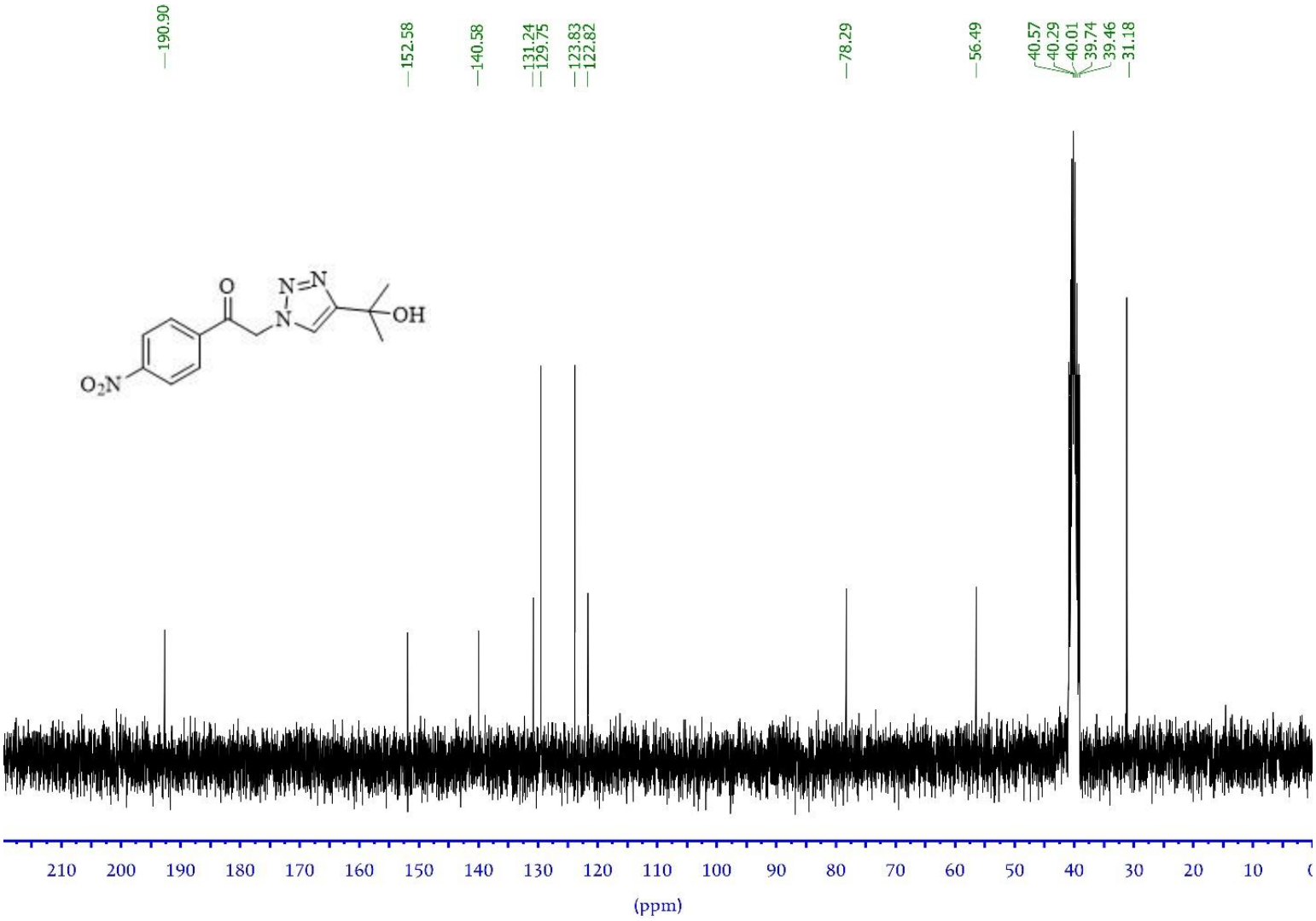


Figure S26: ^{13}C-NMR of 2-(4-(2-Hydroxypropan-2-yl)-1H-1,2,3-triazol-1-yl)-1-(4-nitrophenyl)ethanone

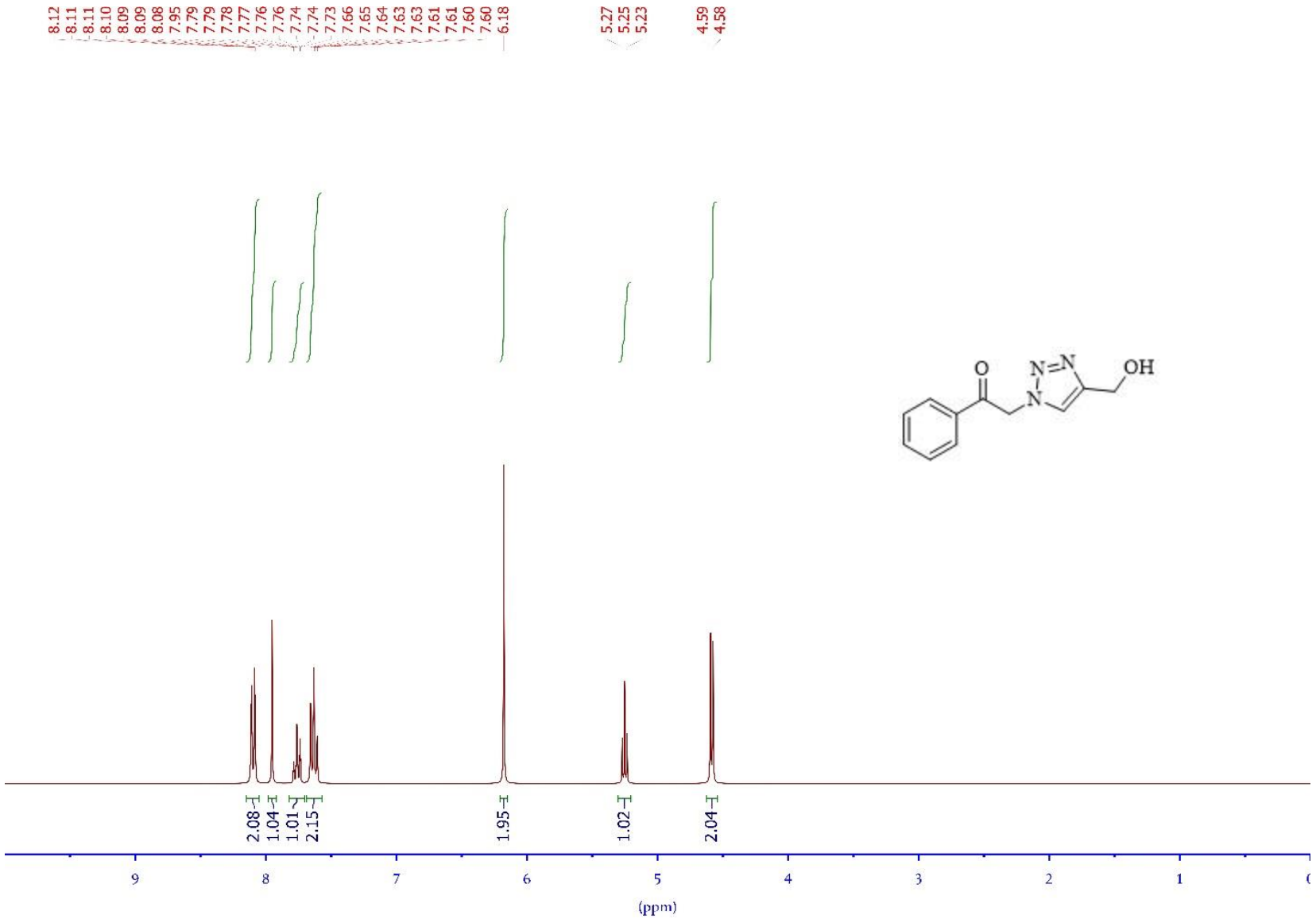


Figure S27: ^{1}H-NMR of 2-(4-(Hydroxymethyl)-1H-1,2,3-triazol-1-yl)-1- phenylethanone

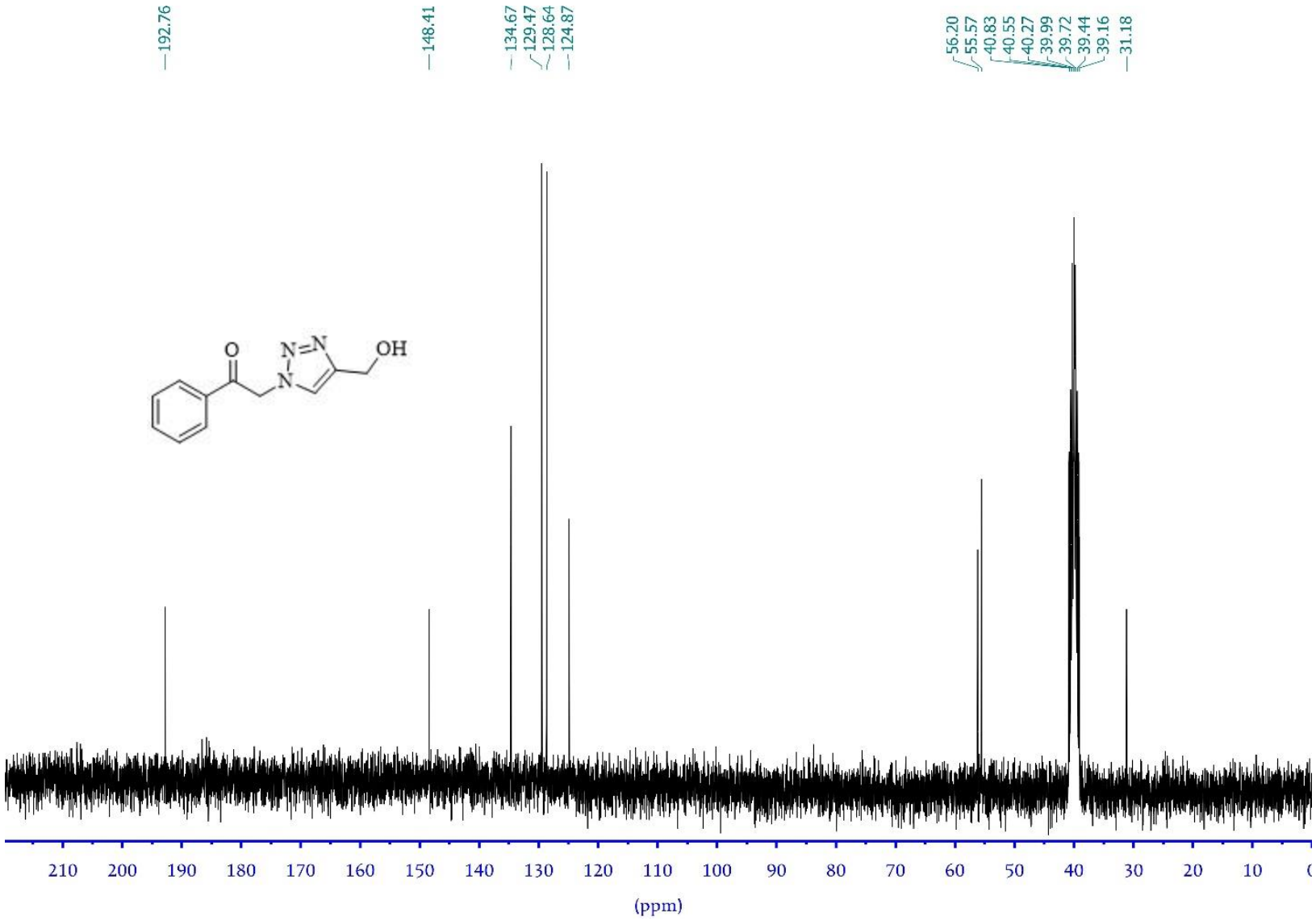


Figure S28: ^{13}C-NMR of 2-(4-(Hydroxymethyl)-1H-1,2,3-triazol-1-yl)-1- phenylethanone

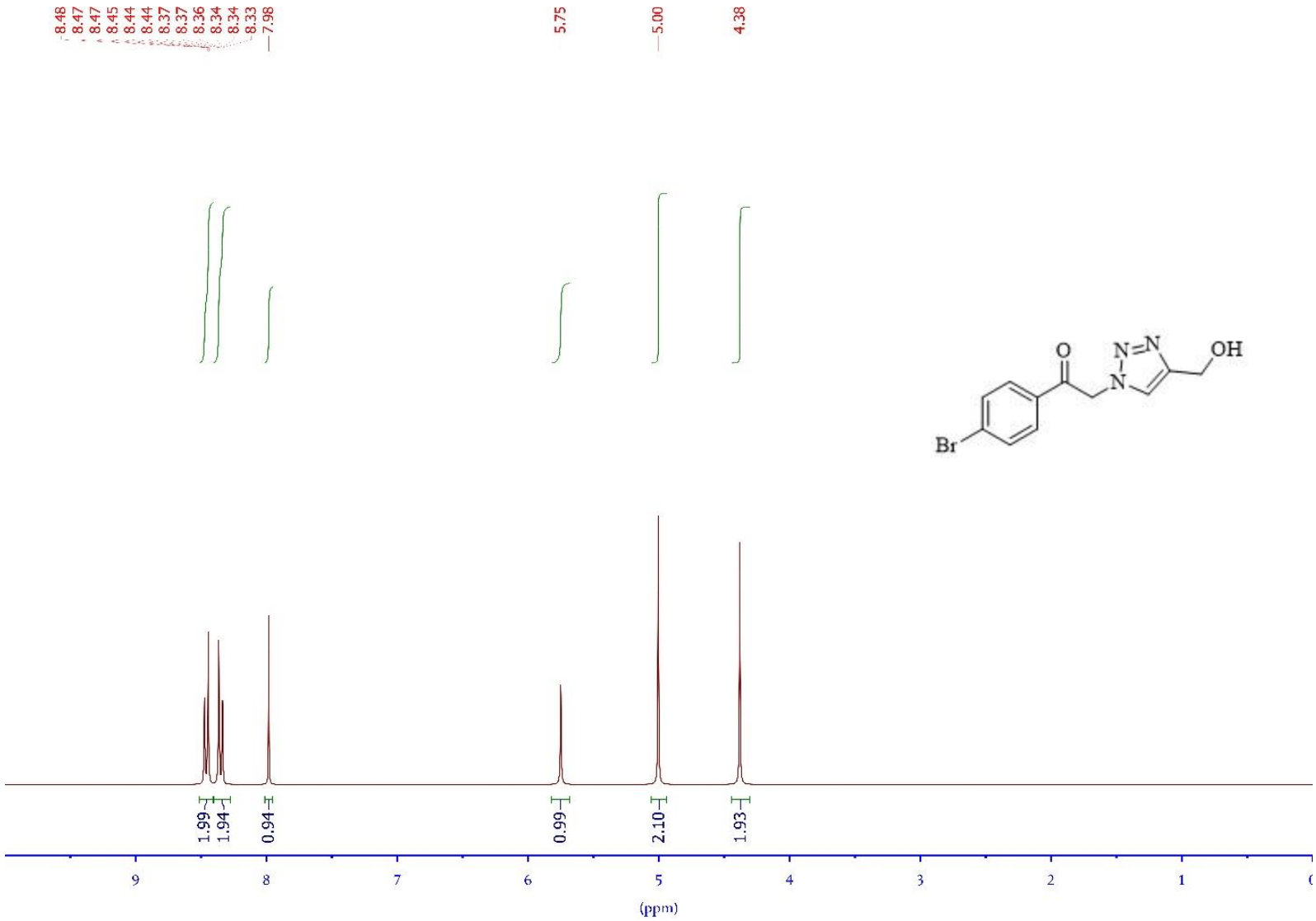


Figure S29: ^{1}H-NMR of 1-(4-Bromophenyl)-2-(4-(hydroxymethyl)-1H-1,2,3-triazol-1-yl)ethanone

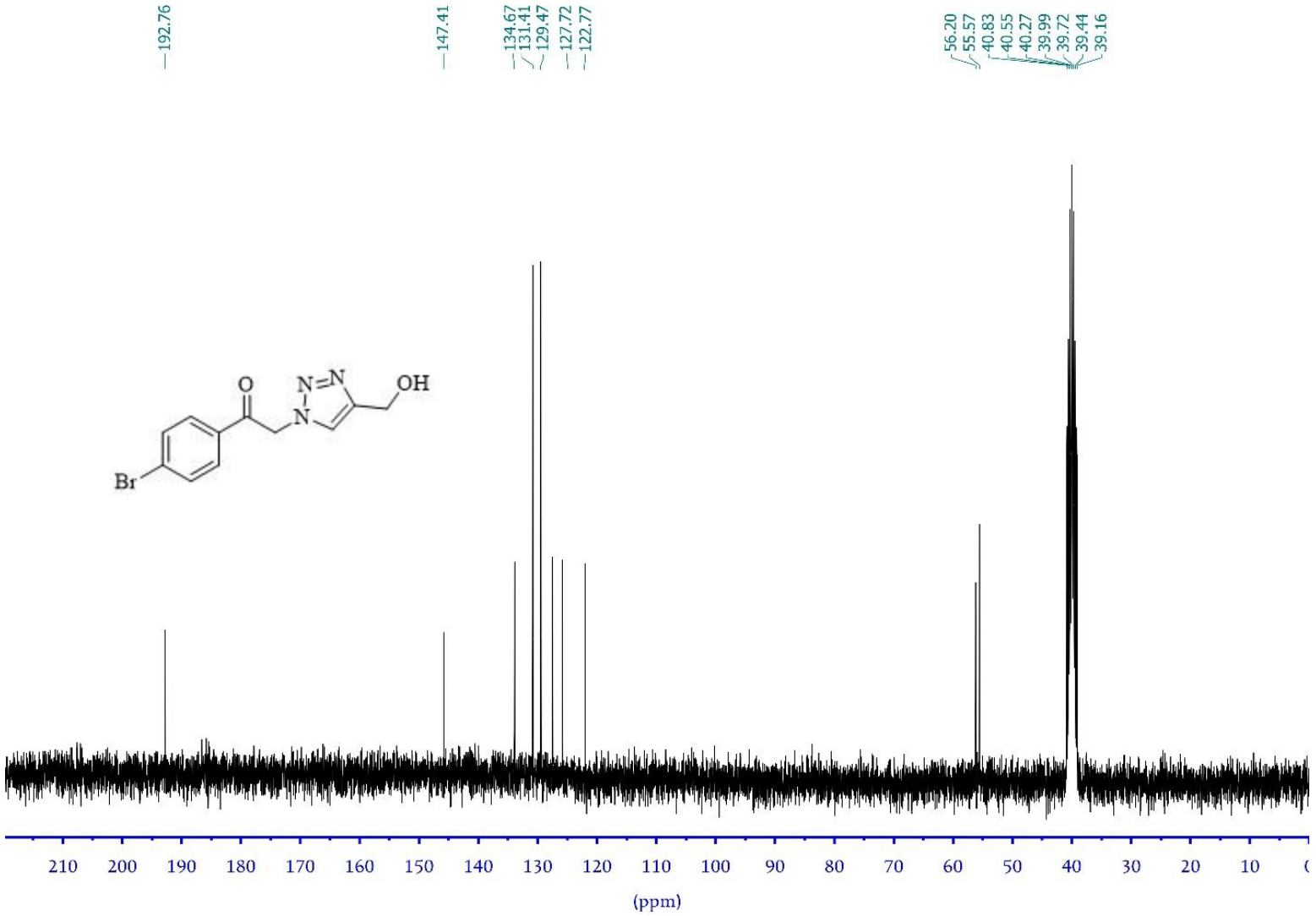


Figure S30: ^{13}C-NMR of 1-(4-Bromophenyl)-2-(4-(hydroxymethyl)-1H-1,2,3-triazol-1-yl)ethanone