PCy_3 assisted Ag(I) catalyzed click reaction for regioselective synthesis of 1,4-disubstituted 1,2,3-triazoles at room temperature

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Supporting Information

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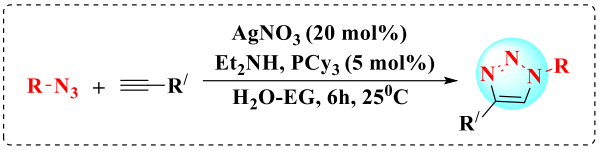
General Information:

All reactions were performed under atmospheric conditions using oven dried glassware. All the glassware, magnetic bead and the spatulas are subjected to acid wash to ensure a copper free environment. All reagents and solvents were purchased from common commercial sources and used without further purification unless otherwise stated. All reported yields are isolated yields. Thin layer chromatography (TLC) was carried out using aluminium sheets pre-coated with silica gel $60F_{254}$ (Merck) and was visualized under 254 nm UV light. Column chromatography was performed on silica gel (120–230 mesh). ^{1}H-NMR spectra were recorded on 500 MHz and ^{13}C on 125 MHz spectrometer using TMS as an internal standard. Chemical shifts are reported in parts per million (ppm, δ).

General procedure for the synthesis of 1,4-disubstituted 1,2,3-triazoles:



In a round bottom flask, a mixture of alkyne derivative (1.2 mmol), diethyl amine (1.2 mmol) and azide (1 mmol) was taken and silver nitrate (20 mol%) and tricyclohexylphosphine (5 mol%) were added to it and then allowed to stir at 25°C for the given time period as mentioned in **Figure 1** of the manuscript. Further in one pot protocol, instead of azide, organic bromide (1 mmol) as well as sodium azide (2 mmol) were employed keeping the other reactants intact (**Table 2** in the manuscript). For the $[Ag(PCy_3)_2]NO_3$ catalyzed reaction, the reactants were added in the similar fashion as mentioned earlier but in this reaction, both silver nitrate and tricyclohexylphosphine were replaced by 10 mol% of the synthesized complex (**Table 3** in the manuscript). The progress of the reaction was monitored by TLC. After completion of the reaction, it was extracted with ethyl acetate (3x10 mL), washed with distilled water and brine solution, dried over anhydrous sodium sulfate and

concentrated under reduced pressure. The resulting residue was purified through silica gel column chromatography to get the desired product.

Complex preparation and characterization

From literature, it was found that silver nitrate can bind with one, two and three molecules of the PCy_3 ligand respectively, we have opted for the synthesis of all the three plausible complexes by the following procedure:

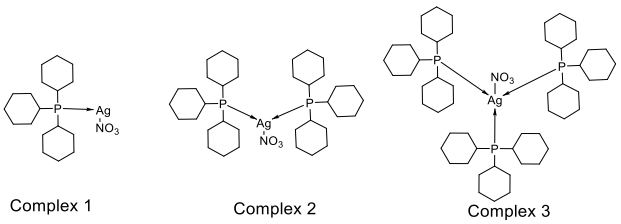
Preparation of $Ag(PCy_3)_2NO_3$: $AgNO_3$ solution (1 mmol) in 5 ml acetonitrile was slowly added to a solution of tricyclohexylphophine (2 mmol) in DCM and the mixture was stirred in room temperature. The clear solution obtained was filtered to remove any impurity present and the filtrate was kept undisturbed for slow evaporation. The white shining crystal obtained, analysed and subjected in the desired reaction as catalyst.

Similarly, $Ag(PCy_3)NO_3$ and $Ag(PCy_3)_3NO_3$ were prepared by varying the molar ratio of $AgNO_3$ and PCy_3 as 1:1 and 1:3 unaltering the remaining conditions.

Table S1: Synthesis of $AgNO_3$-PCy_3 complexes

Ratio	$AgNO_3$	PCy_3	Physical State
1:1	0.200 gm (1.177 mmol)	0.330g (1.177 mmol)	Grey Crystal
1:2	0.200 gm (1.177 mmol)	0.660g (2.354 mmol)	White Crystal
1:3	0.200 gm (1.177 mmol)	0.990g (3.531 mmol)	White Crystal

The possible structures of the compounds are:



Complex 1 Complex 2 Complex 3

We have develop single crystal for $Ag(PCy_3)_2NO_3$ which clearly suggests the discrete formation of the complex.

Crystal structures of the complex was solved and refined in triclinic space group *P*-1 with one symmetry independent molecule in the lattice. The crystal data parameter is available in Table 1 (MS). The ORTEP with 50% probability ellipsoid is displayed in Figure 1. One of the PCy_3 groups is positional disordered and resolved in eight locations with site occupancies 1, 0.5, 0.5, 1, 1, 0.5, 0.5, 1 in each atom. Experimental section is referred for the details of the Single crystal X-ray data collection methods; CIF and CheckCIF report (File name: BS_RN_Ag_1_0m_a) are attached in this supplementary file.

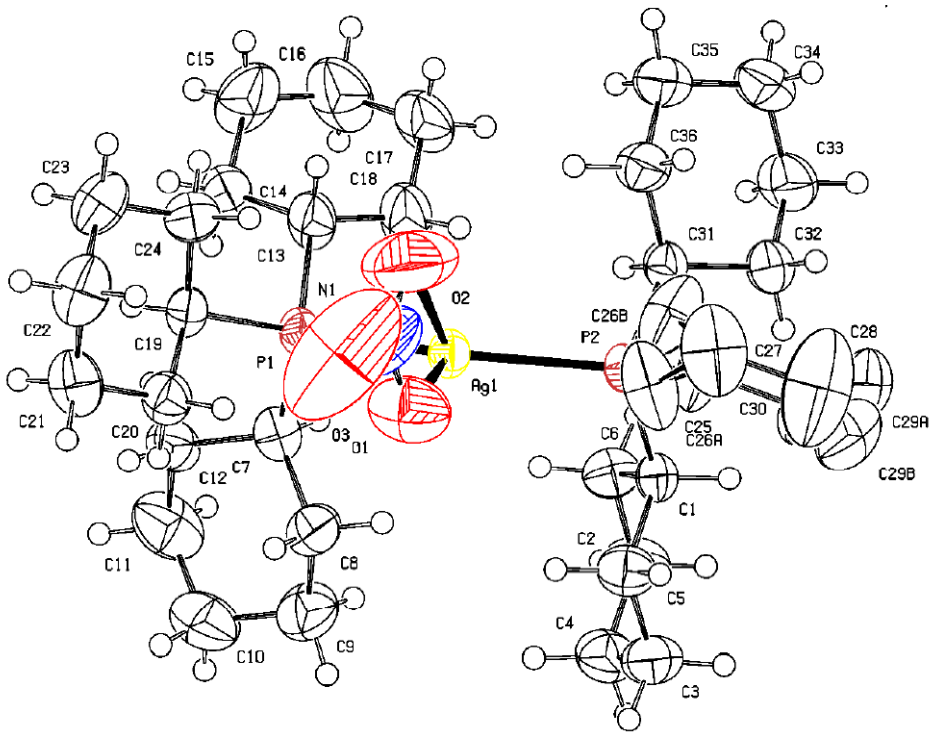


Figure S1: ORTEP of the complex $[Ag(PCy_3)_2]NO_3$ with 50% probability ellipsoid

Single crystal for product molecule 1-benzyl-4-(3,5-bis(trifluoromethyl)phenyl)-1H-1,2,3-triazole(3c):

Crystal structures of one of the synthesized molecules (**3c**) was solved and refined in monoclinic space group $P2_1/n$ with one symmetry independent molecule in the lattice. The

crystal data parameter is available in Table 1 (MS). The ORTEP with 50% probability ellipsoid is displayed in Figure 2 (MS). One of the CF_3 groups in the molecule is positional disordered and resolved in five locations with 0.60 site occupancies in each atom; whereas, the other CF_3 group is resolved in six locations with site occupancies viz. 0.75, 0.25, 0.75, 0.25, 0.60 and 0.40. Experimental section is referred for the details of the Single crystal X-ray data collection methods; CIF and CheckCIF (File name: BS_RHP289) report are attached in this supplementary file.

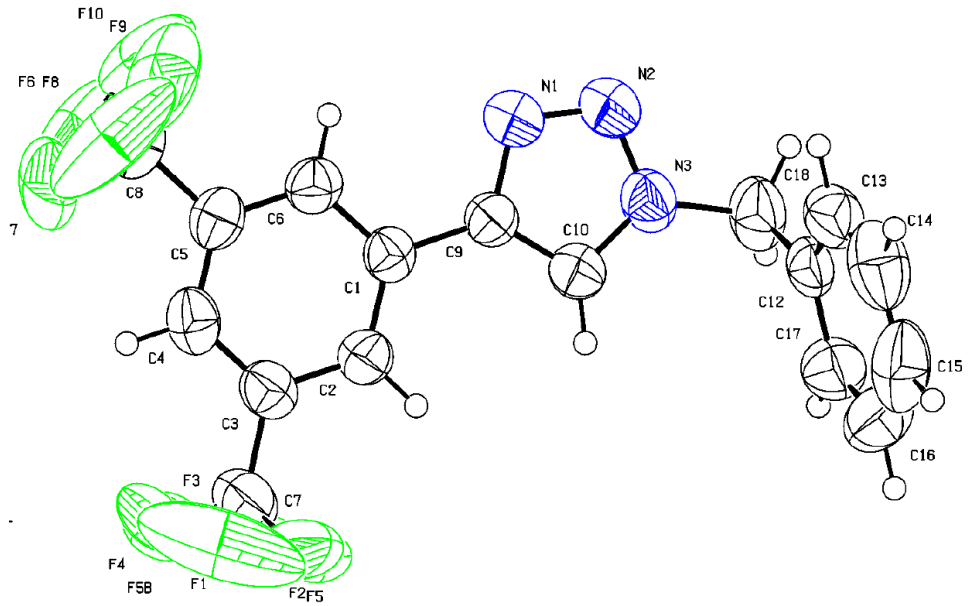


Figure S2: ORTEP of the synthesized molecule $C_{17}H_{11}F_6N_3$ with 50% probability ellipsoid

Table S2: Crystallographic parameters

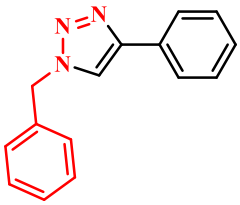
Crystal data	$[Ag(PCy_3)_2]NO_3$	**$C_{17}H_{11}F_6N_3$**
Formula unit	$C_{36}H_{55}AgNO_3P_2$	$C_{17}H_{11}F_6N_3$
Formula weight ($gmol^{-1}$)	719.62	371.29
Crystal system	Triclinic	Monoclinic
T [K]	100	100
a [Å]	9.262(2)	12.664(6)
b [Å]	9.837(2)	4.767(2)
c [Å]	23.332(5)	27.831(13)
α [°]	94.658(6)	90
β [°]	96.469(6)	103.124(11)

γ [°]	116.368(6)	90
Volume [Å^3]	1871.8(7)	1636.3(13)
Space group	*P*-1	$P2_1/n$
Z	2	4
D_{cal} [g/cm^3]	1.277	1.507
R_1, *w*R2	0.0511, 0.1284	0.0458, 0.0960
GOOF	1.067	1.003
Instrument	Bruker CCD Apex II	Bruker CCD Apex II
CCDC No	2254372	2254371

Table S3: Comparable study of the present work with some of the existing works

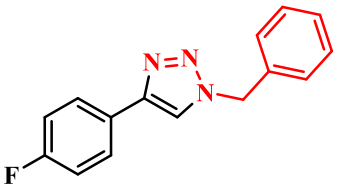
Literature	Catalyst	Catalyst preparation required	Reaction conditions	Yield (%)	Substrate scope
Zhao *et. al.* (2016)[1]	Silver–polyamine nanocomposite	Yes	$H_2O/80^0C/8h$	92	10 examples
McNulty *et. al.* (2011)[2]	N,N-diisopropyl(2-diphenylphosphanyl)benzamide: AgOAc	Yes	Toluene/caprylic acid (20 mol%)/ RT/ 48 h	98	19 examples
Ortega-Arizmendi *et. al.* (2013)[3]	AgCl (5 mol%)	No	H_2O/acetone/RT/24 h	64	20 examples
El Ayouchia *et. al.* (2020)[4]	AgCl (10 mol%)	No	H_2O/RT/24 h	92	9 examples
McNulty *et. al.* (2012)[5]	$Ag(OOCCH_3)$ (2 mol%)/ N,N-diisopropylamide substituent ligand	Yes	Toluene/90^0C/Caprylic acid/24 h	98	16 examples
Garg *et. al.* (2019)[6]	Ag–NHC@SiO_2	Yes	H_2O/quinine/60^0C/6h	98	22 examples
This work	$AgNO_3$ (20 mol%)	No	H_2O-EG/diethyl amine/PCy_3/RT/6h	95	50 examples

Characterization of the compounds:



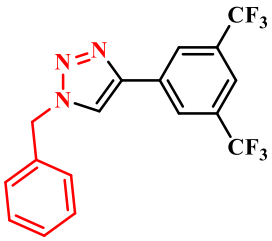
1-benzyl-4-phenyl-1H-1,2,3-triazole[7] (3a): White solid, mp 128-130°C, ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 (d, *J* = 7.6 Hz, 2H), 7.61 (s, 1H), 7.30 (ddd, *J* = 30.0, 11.0, 6.7 Hz, 8H), 5.51 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 147.21 (s), 133.67 (s), 129.50 (s), 128.13 (s), 127.77 (d, *J* = 2.2 Hz), 127.09 (d, *J* = 13.2 Hz), 124.69 (s), 118.49 (s), 53.21 (s). MS (ESI) m/z: $[M+H]^+$ calcd for $C_{15}H_{13}N_3$ 236.11; Found 236.10



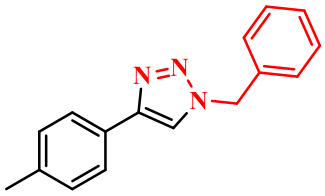
1-benzyl-4-(4-fluorophenyl)-1H-1,2,3-triazole[8] (3b): White solid, mp 109-110°C, ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.71 (d, *J* = 3.2 Hz, 2H), 7.58 (s, 1H), 7.37–7.18 (m, 5H), 7.03 (t, *J* = 8.6 Hz, 2H), 5.51 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 162.77 (d, *J* = 247.2 Hz).134.71 (s), 129.32 (s), 128.98 (s), 128.23 (s), 127.56 (d, *J* = 8.2 Hz), 126.88 (s), 119.45 (s), 116.01 (s), 115.84 (s), 54.40 (s). MS (ESI) m/z: $[M+H]^+$ calcd for $C_{15}H_{12}FN_3$ 254.10; Found 254.13



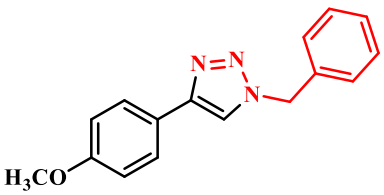
1-benzyl-4-(3,5-bis(trifluoromethyl)phenyl)-1H-1,2,3-triazole(3c): White solids, mp.: 95°C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.27 (s, 2H), 7.85 (s, 1H), 7.82 (s, 1H), 7.47 – 7.38 (m, 3H), 7.38 – 7.32 (m, 2H), 5.63 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 145.65 (s), 134.22 (s), 132.79 (s), 132.32 (q, *J* = 33.5 Hz), 129.45 (s), 129.22 (s), 128.30 (s), 125.70 (s), 124.38 (s), 122.22 (s), 121.65 (q), 120.62 (s), 54.64 (s). MS (ESI) m/z: $[M+H]^+$ calcd for $C_{17}H_{11}F_6N_3$ 372.09; Found 372.10



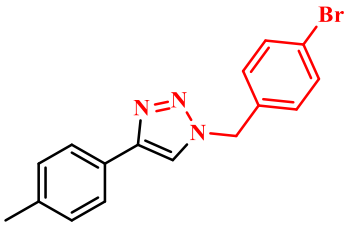
1-benzyl-4-(p-tolyl)-1H-1,2,3-triazole[9] (3d): Pale yellow solid, mp 150-152 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.1 Hz, 2H), 7.63 (s, 1H), 7.37 (dd, *J* = 8.0, 5.8 Hz, 3H), 7.31 (dd, *J* = 7.5, 1.6 Hz, 2H), 7.20 (d, *J* = 8.1 Hz, 2H), 5.56 (s, 2H), 2.36 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 148.39 (s), 138.16 (s), 134.82 (s), 129.61 (s), 129.26 (s), 128.88 (s), 128.19 (s), 127.73 (s), 125.73 (s), 119.33 (s), 54.33 (s), 21.41 (s). MS (ESI) m/z: $[M+H]^+$ calcd for $C_{16}H_{15}N_3$ 250.13; Found 250.10



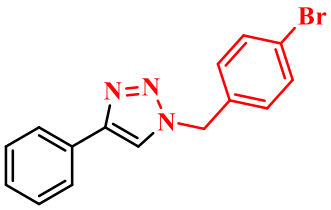
1-benzyl-4-(4-methoxyphenyl)-1H-1,2,3-triazole[10] (3e): Pale yellow solid, mp 142-144 °C. ^{1}H NMR (500 MHz,) δ 7.72 (d, *J* = 8.7 Hz, 2H), 7.57 (s, 1H), 7.43 – 7.34 (m, 3H), 7.34 – 7.27 (m, 2H), 6.93 (d, *J* = 8.8 Hz, 2H), 5.56 (s, 2H), 3.83 (s, 3H).

^{13}C NMR (125 MHz,) δ 159.62 (s), 148.12 (s), 134.79 (s), 129.14 (s), 128.75 (s), 128.06 (s), 127.02 (s), 123.30 (s), 118.68 (s), 114.23 (s), 55.32 (s), 54.21 (s). MS (ESI) m/z: $[M+H]^+$ calcd for $C_{16}H_{15}N_3O$ 266.12; Found 266.11



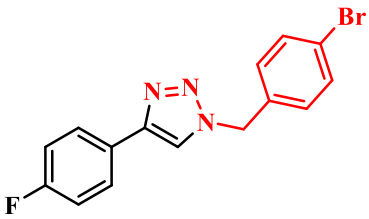
1-(4-bromobenzyl)-4-(p-tolyl)-1H-1,2,3-triazole[11] (3f): Pale yellow solid, m.p 202–204°C: ^{1}H NMR (500 MHz,) δ 7.68 (d, *J* = 7.8 Hz, 2H), 7.62 (s, 1H), 7.51 (d, *J* = 8.1 Hz, 2H), 7.19 (m, 4H), 5.51 (s, 2H), 2.36 (s, 3H).

^{13}C NMR (125 MHz,) δ 148.51 (s), 138.16 (s), 133.78 (s), 132.33 (s), 129.59 (d, *J* = 19.0 Hz), 127.55 (s), 125.63 (s), 122.93 (s), 119.08 (s), 53.51 (s), 21.29 (s). MS (ESI) m/z: $[M+H]^+$ calcd for $C_{16}H_{14}BrN_3$ 328.04; Found 328.07



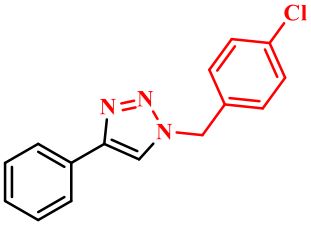
1-(4-bromobenzyl)-4-phenyl-1H-1,2,3-triazole[10] (3g): White solid, mp 150-152°C, ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.3 Hz, 2H), 7.67 (s, 1H), 7.51 (d, *J* = 8.4 Hz, 2H), 7.40 (t, *J* = 7.6 Hz, 2H), 7.32 (t, *J* = 7.4 Hz, 1H), 7.17 (d, *J* = 8.3 Hz, 2H), 5.52 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 148.52 (s), 133.83 (s), 132.45 (s), 130.45 (s), 129.79 (s), 128.99 (s), 128.44 (s), 125.83 (s), 123.08 (s), 119.61 (s), 53.65 (s). MS (ESI) m/z: $[M+H]^+$ calcd for $C_{15}H_{12}BrN_3$ 314.02; Found 314.05



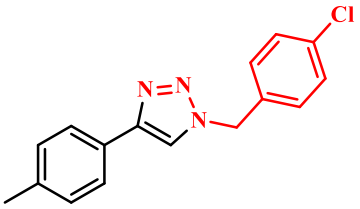
1-(4-bromobenzyl)-4-(4-fluorophenyl)-1H-1,2,3-triazole (3h): Pale yellow solid, ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.72 (dd, *J* = 7.9, 5.6 Hz, 2H), 7.58 (s, 1H), 7.47 (d, *J* = 8.2 Hz, 2H), 7.14 (d, *J* = 8.1 Hz, 2H), 7.05 (dd, *J* = 12.6, 4.7 Hz, 2H), 5.47 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 163.16 (d, *J* = 247.3 Hz), 147.97 (s), 135.63 (s), 134.06 (s), 132.80 (s), 130.12 (s), 127.91 (d, *J* = 8.4 Hz), 125.47 (s), 123.46 (s), 119.64 (s), 116.35 (s), 116.21 (s), 54.01 (s).



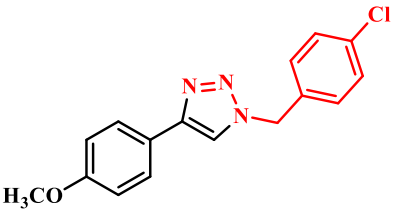
1-(4-chlorobenzyl)-4-phenyl-1H-1,2,3-triazole[2] (3i): White solid, mp 138-140°C, $C_{15}H_{12}ClN_3$;^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.7 Hz, 2H), 7.69 (s, 1H), 7.46 – 7.30 (m, 5H), 7.26 (d, *J* = 8.3 Hz, 2H), 5.55 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 148.79 (s), 135.24 (s), 133.62 (s), 130.78 (s), 129.77 (s), 129.25 (s), 128.69 (s), 126.12 (s), 119.87 (s), 53.87 (s). MS (ESI) m/z: $[M+H]^+$ calcd for $C_{15}H_{12}ClN_3$ 270.07; Found 270.05

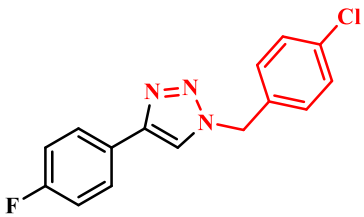


1-(4-chlorobenzyl)-4-(p-tolyl)-1H-1,2,3-triazole[12] (3j): Off-white solid; mp. 140–143^{o}C: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 (d, *J* = 7.6 Hz, 2H), 7.55 (s, 1H), 7.28 (d, *J* = 7.6 Hz, 2H), 7.24 – 7.09 (m, 4H), 5.46 (s, 2H), 2.29 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 148.47(S), 138.19 (s), 134.84 (s), 133.22 (s), 129.53 (s), 129.38 (d, *J* = 3.2 Hz), 127.48 (s), 125.64 (s), 119.13 (s), 53.51 (s), 21.30 (s). MS (ESI) m/z: $[M+H]^+$ calcd for $C_{16}H_{14}ClN_3$ 284.09; Found 284.10

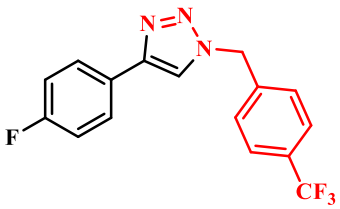


1-(4-chlorobenzyl)-4-(4-methoxyphenyl)-1H-1,2,3-triazole (3k): White solids: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.7 Hz, 2H), 7.58 (s, 1H), 7.36 (d, *J* = 8.4 Hz, 2H), 7.25 (d, *J* = 8.4 Hz, 2H), 6.94 (d, *J* = 8.7 Hz, 2H), 5.54 (s, 2H), 3.84 (s, 3H). MS (ESI) m/z: $[M+H]^+$ calcd for $C_{16}H_{14}ClN_3O$ 300.08; Found 300.10



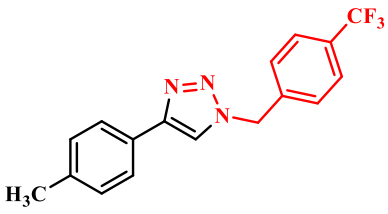
1-(4-chlorobenzyl)-4-(4-fluorophenyl)-1H-1,2,3-triazole (3l): White solids, mp. 105-107^{0}C : ^{1}H NMR (500 MHz,) δ 7.79 – 7.73 (m, 2H), 7.63 (s, 1H), 7.36 (d, *J* = 8.4 Hz, 2H), 7.24 (d, *J* = 8.4 Hz, 2H), 7.09 (t, *J* = 8.6 Hz, 2H), 5.53 (s, 2H).

^{13}C NMR (125 MHz,) δ 162.73 (d, *J* = 247.8 Hz), 147.54 (s), 134.92 (s), 133.11 (s), 129.40 (s), 127.47 (d, *J* = 7.9 Hz), 126.62 (d, *J* = 2.7 Hz), 119.19 (s), 115.91 (s), 115.77 (s), 53.51 (s). MS (ESI) m/z: $[M+H]^+$ calcd for $C_{15}H_{11}ClFN_3$ 288.06; Found 288.05



4-(4-fluorophenyl)-1-(4-(trifluoromethyl)benzyl)-1H-1,2,3-triazole (3m): ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73 (dd, *J* = 8.3, 5.5 Hz, 2H), 7.61 (s, 2H), 7.60 (s, 1H), 7.37 (d, *J* = 8.0 Hz, 2H), 7.05 (t, *J* = 8.6 Hz, 2H), 5.59 (s, 2H)

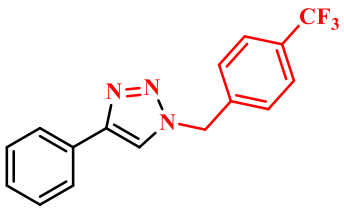
^{13}C NMR (125 MHz, $CDCl_3$) δ 161.64 (d, *J* = 247.7 Hz), 146.58 (s), 137.42 (s), 130.01, 127.07 (s), 126.36 (d, *J* = 8.2 Hz), 125.05 (q), 118.16 (s), 114.81 (s), 114.67 (s), 52.46 (s). MS (ESI) m/z: $[M+H]^+$ calcd for $C_{16}H_{11}F_4N_3$ 322.09; Found 322.12



4-(p-tolyl)-1-(4-(trifluoromethyl)benzyl)-1H-1,2,3-triazole (3n): Off White solids, m.p. 150-152^{0}C: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.72 – 7.61 (m, 5H), 7.40 (d, *J* = 8.1 Hz, 2H), 7.22 (d, *J* = 8.0 Hz, 2H), 5.63 (s, 2H), 2.37 (s, 3H).

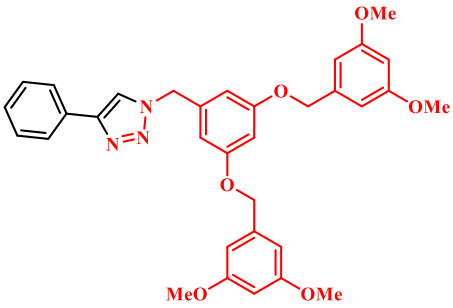
^{13}C NMR (125 MHz, $CDCl_3$) δ 148.67 (s), 138.77 (s), 138.28 (s), 131.07 (q, *J* = 32.7 Hz), 129.58 (s), 128.20 (s), 127.48 (s), 126.16

(q), 125.68 (s), 119.26 (s), 53.54 (s), 21.31 (s). MS (ESI) m/z: $[M+H]^+$ calcd for $C_{17}H_{14}F_3N_3$ 318.11; Found 318.09



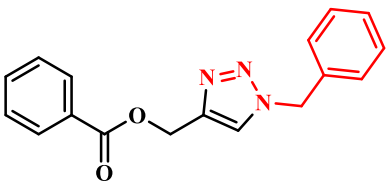
4-phenyl-1-(4-(trifluoromethyl)benzyl)-1H-1,2,3-triazole (3o): White solids, m.p: 117-119^{0}C: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.72 (d, *J* = 7.7 Hz, 2H), 7.64 (s, 1H), 7.55 (d, *J* = 7.9 Hz, 2H), 7.32 (t, *J* = 7.2 Hz, 4H), 7.24 (d, *J* = 7.2 Hz, 1H), 5.55 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 147.77 (s), 137.91 (s), δ 130.29 (q, *J* = 32.7 Hz), 129.47 (s), 128.13 (s), 127.64 (s), 127.44 (s), 125.38 (q), 124.99 (s), 122.12 (s), 118.93 (s), 52.80 (s). MS (ESI) m/z: $[M+H]^+$ calcd for $C_{16}H_{12}F_3N_3$ 304.10; Found 304.09



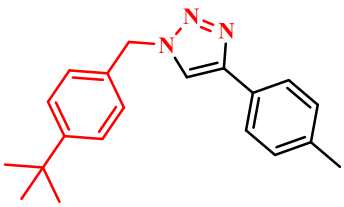
1-(3,5-bis((3,5-dimethoxybenzyl)oxy)benzyl)-4-phenyl-1H-1,2,3-triazole (3p): Pale yellow liquid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.72 (d, *J* = 7.9 Hz, 2H), 7.57 (s, 1H), 7.34– 7.24 (m, 3H), 6.50 (d, *J* = 5.8 Hz, 2H), 6.46 (d, *J* = 4.4 Hz, 5H), 6.32 (s, 2H), 5.40 (s, 2H), 4.87 (s, 4H), 3.70 (s, 12H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 160.99 (s), 160.35 (s), 138.76 (s), 128.80 (s), 125.72 (s), 107.23 (s), 105.21 (s), 99.96 (s), 70.10 (s), 59.75 (s), 55.37 (s). MS (ESI) m/z: $[M+H]^+$ calcd for $C_{33}H_{33}N_3O_6$ 568.24; Found 568.22



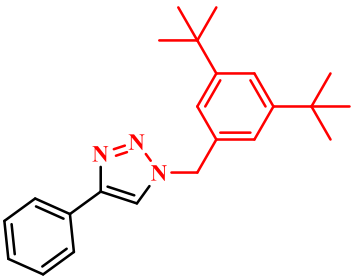
(1-benzyl-1H-1,2,3-triazol-4-yl)methyl benzoate[13] (3q): White solid, mp 84-86^{o}C: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.02 (d, *J* = 7.9 Hz, 2H), 7.61 (s, 1H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.45 – 7.33 (m, 5H), 7.29 – 7.26 (m, 2H), 5.52 (s, 2H), 5.44 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 166.45 (s), 143.36 (s), 134.41 (s), 133.20 (s), 129.76 (s), 129.18 (s), 128.86 (s), 128.40 (s), 128.17 (s), 123.85 (s), 58.10 (s), 54.26 (s). MS (ESI) m/z: $[M+H]^+$ calcd for $C_{17}H_{15}N_3O_2$ 294.12; Found 294.11



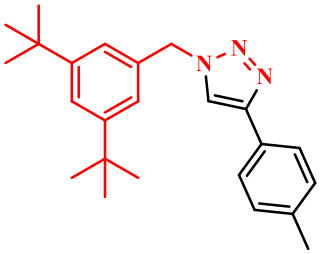
1-(4-(tert-butyl)benzyl)-4-(p-tolyl)-1H-1,2,3-triazole[14] (3r): White solid, mp 109-110 ^{o}C: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.1 Hz, 2H), 7.60 (s, 1H), 7.33-7.39 (m, 4H), 7.18 (d, *J* = 8.0 Hz, 2H), 5.51 (s, 2H), 2.34 (s, 3H), 1.30 (s, 9H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 138.03 (s), 131.79 (s), 129.55 (s), 127.98 (s), 127.57 (s), 125.65 (d, *J* = 8.6 Hz), 119.20 (s), 54.01 (s), 34.73 (s), 31.35 (s), 21.36 (s).



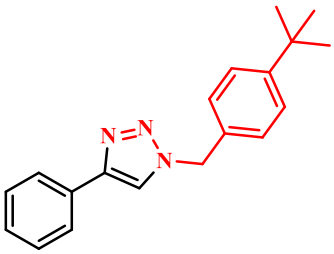
1-(3,5-di-tert-butylbenzyl)-4-phenyl-1H-1,2,3-triazole (3s): white solid: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.6 Hz, 2H), 7.69 (s, 1H), 7.44 (dd, *J* = 16.9, 9.3 Hz, 3H), 7.34 (t, *J* = 7.4 Hz, 1H), 7.19 (d, *J* = 1.4 Hz, 2H), 5.58 (s, 2H), 1.34 (s, 18H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 151.92 (s), 128.80 (s), 128.10 (s), 125.73 (s), 122.87 (s), 122.42 (s), 119.42 (s), 54.90 (s), 34.92 (s), 31.41 (s). MS (ESI) m/z: $[M+H]^+$ calcd for $C_{23}H_{29}N_3$ 348.24; Found 348.22



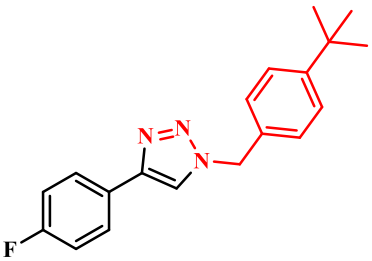
1-(3,5-di-tert-butylbenzyl)-4-(p-tolyl)-1H-1,2,3-triazole (3t): Pale yellow liquid: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.0 Hz, 2H), 7.55 (s, 1H), 7.35 (s, 1H), 7.13 (d, *J* = 7.9 Hz, 2H), 7.08 (s, 2H), 5.47 (s, 2H), 2.29 (s, 3H), 1.23 (s, 18H).

^{13}C NMR (101 MHz, CHLOROFORM-D) δ 151.79 (s), 137.89 (s), 133.82 (s), 129.46 (s), 125.60 (s), 122.79 (s), 122.39 (s), 121.97 (s), 121.29 (s), 119.09 (s), 54.83 (s), 34.88 (s), 31.44 (d, *J* = 7.0 Hz), 21.30 (s). MS (ESI) m/z: $[M+H]^+$ calcd for $C_{24}H_{31}N_3$ 362.25; 362.28



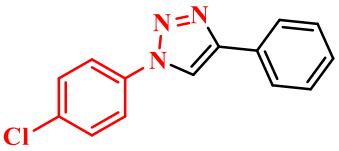
1-(4-(tert-butyl)benzyl)-4-phenyl-1H-1,2,3-triazole (3u):White solid, mp 114-115°C : ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.1 Hz, 2H), 7.58 (s, 1H), 7.31 (t, *J* = 7.7 Hz, 4H), 7.23 – 7.16 (m, 3H), 5.46 (s, 2H), 1.24 (s, 9H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 151.91 (s), 148.10 (s), 131.64 (s), 130.60 (s), 128.78 (s), 128.11 (s), 127.89 (s), 127.46 (s), 126.07 (s), 125.60 (d, *J* = 18.4 Hz), 119.48 (s), 53.94 (s), 34.65 (s), 31.27 (s). MS (ESI) m/z: $[M+H]^+$ calcd for $C_{19}H_{21}N_3$ 292.17; Found 292.15

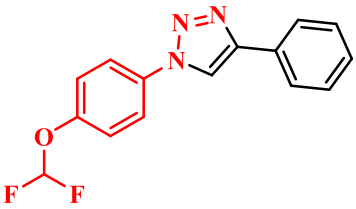


1-(4-(tert-butyl)benzyl)-4-(4-fluorophenyl)-1H-1,2,3-triazole (3v): Pale yellow liquid, ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.71 – 7.65 (m, 2H), 7.53 (s, 1H), 7.33 (d, *J* = 8.2 Hz, 2H), 7.18 – 7.16 (m, 2H), 7.00 (t, *J* = 8.7 Hz, 2H), 5.45 (s, 2H), 1.23 (s, 9H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 162.71 (d, *J* = 247.0 Hz), 152.08 (s), 147.35 (s), 131.63 (s), 127.99 (s), 127.51 (d, *J* = 7.8 Hz), 126.18 (s), 125.11 (s), 119.27 (s), 115.90 (s), 115.76 (s), 54.06 (s), 34.74 (s), 31.33 (s). MS (ESI) m/z: $[M+H]^+$ calcd for $C_{19}H_{20}FN_3$ 310.16; Found 310.15

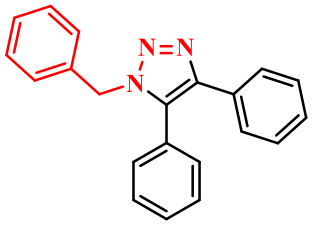


1-(4-chlorophenyl)-4-phenyl-1H-1,2,3-triazole (3w): Yellow liquid, ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.11 (s, 1H), 7.84 (d, *J* = 7.7 Hz, 2H), 7.69 (d, *J* = 8.5 Hz, 2H), 7.47 (d, *J* = 8.3 Hz, 2H), 7.41 (s, 1H), 7.33 (d, *J* = 7.4 Hz, 2H). MS (ESI) m/z: $[M+H]^+$ calcd for $C_{14}H_{10}ClN_3$ 256.06; Found 256.08



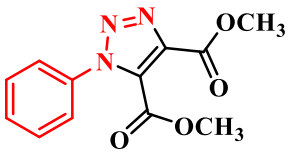
1-(4-(difluoromethoxy)phenyl)-4-phenyl-1H-1,2,3-triazole (3x): Pale yellow solid, ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.10 (s, 1H), 7.84 (d, *J* = 7.5 Hz, 2H), 7.74 (d, *J* = 9.2 Hz, 2H), 7.40 (t, *J* = 7.5 Hz, 2H), 7.31 (t, *J* = 7.4 Hz, 1H), 7.25 (d, *J* = 8.5 Hz, 2H), 6.52 (t, *J* = 72.8 Hz, 1H).

^{13}C NMR (125 MHz, Chloroform-*d*) δ 148.78 (d, *J* = 283.3 Hz), 133.38, 129.09, 128.00, 127.60, 124.91, 121.07, 120.03, 116.63. MS (ESI) m/z: $[M+H]^+$ calcd for $C_{15}H_{11}F_2N_3O$ 288.09; Found 288.08



1-benzyl-4,5-diphenyl-1H-1,2,3-triazole (3y): Brown liquid, ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.49 – 7.45 (m, 2H), 7.40 (t, *J* = 7.4 Hz, 1H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.17 (dd, *J* = 8.8, 4.7 Hz, 6H), 7.06 (d, *J* = 7.4 Hz, 2H), 6.94 (dd, *J* = 6.7, 2.9 Hz, 2H), 5.32 (s, 2H).

^{13}C NMR (125 MHz, Chloroform-*d*) δ 143.44, 134.32, 130.58, 129.06, 128.66, 128.14, 127.67, 127.42, 127.12, 126.46, 125.67, 50.99. MS (ESI) m/z: $[M+H]^+$ calcd for $C_{21}H_{17}N_3$ 312.14; Found 312.10



Dimethyl 1-phenyl-1H-1,2,3-triazole-4,5-dicarboxylate (3z): White solid, ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.63 – 7.59 (m, 5H), 4.07 (s, 3H), 3.97 (s, 3H).

^{13}C NMR (125 MHz, Chloroform-*d*) δ 160.23, 159.49, 138.74, 135.51, 132.53, 130.62, 129.70, 124.30, 52.82. MS (ESI) m/z: $[M+H]^+$ calcd for $C_{12}H_{11}N_3O_4$ 262.07; Found 262.05

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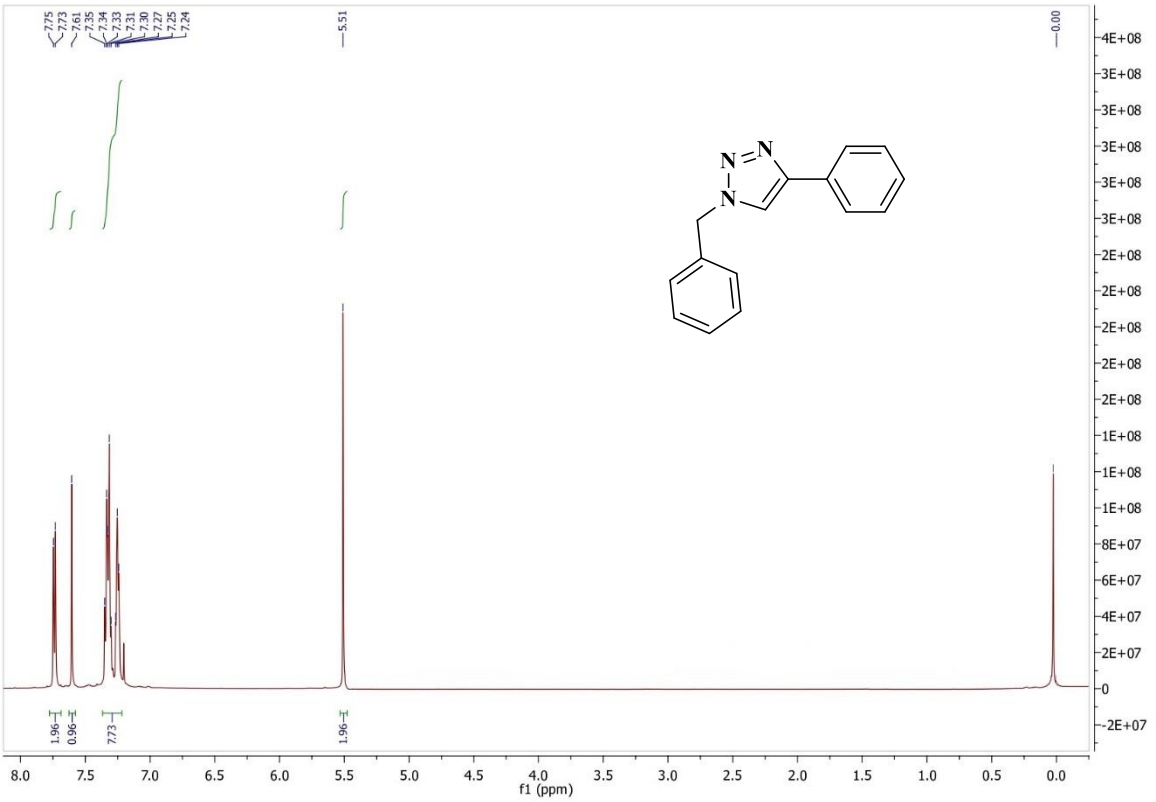
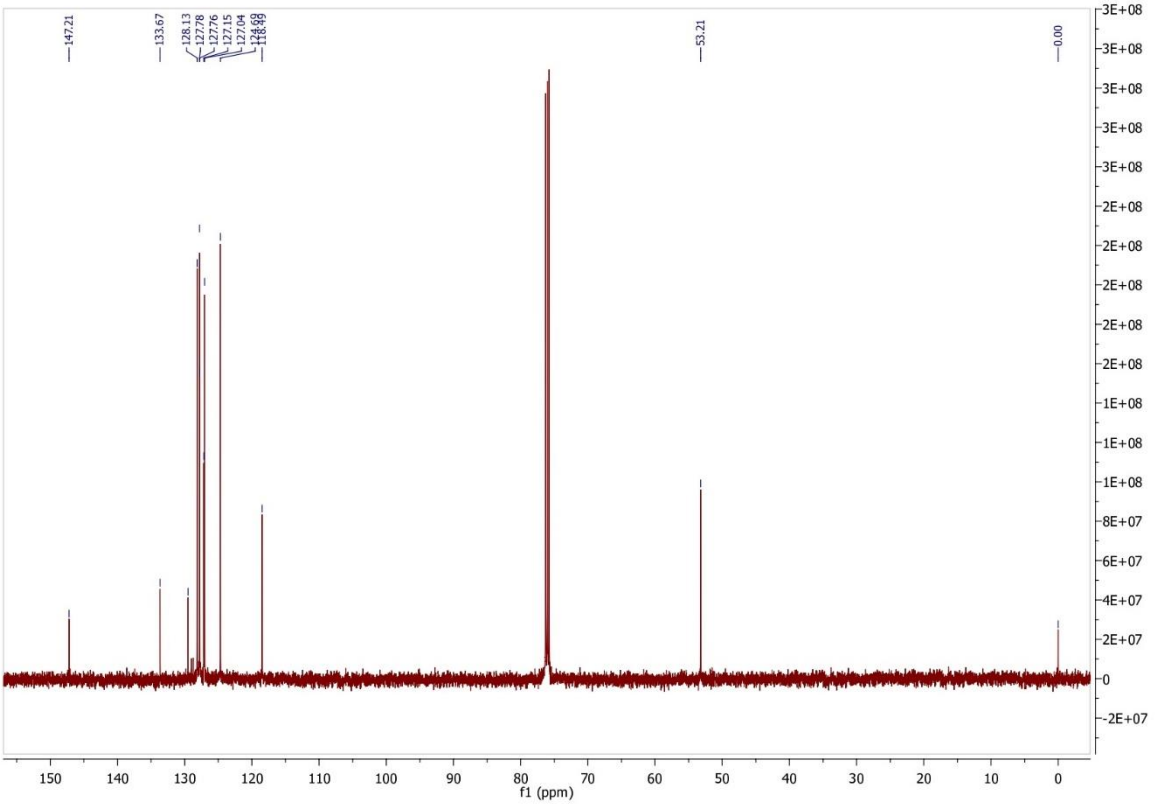
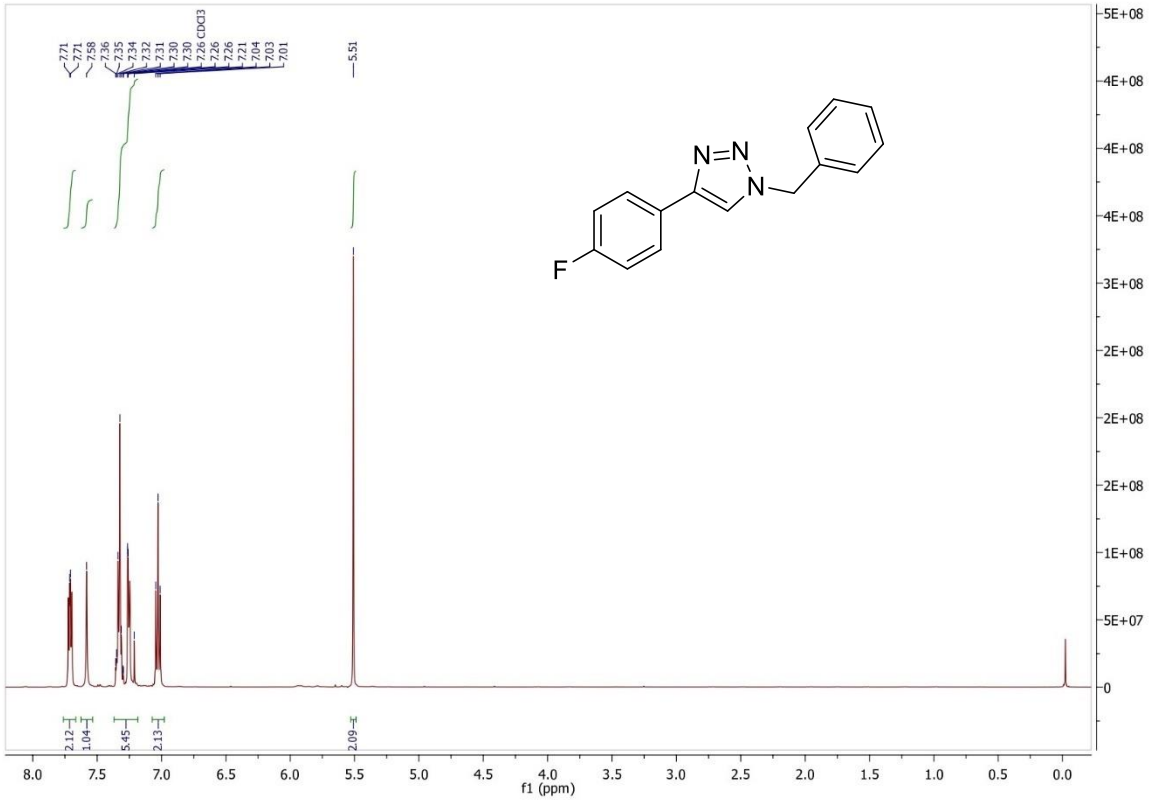
[1]H-NMR spectrum of 1-benzyl-4-phenyl-1H-1,2,3-triazole (3a)



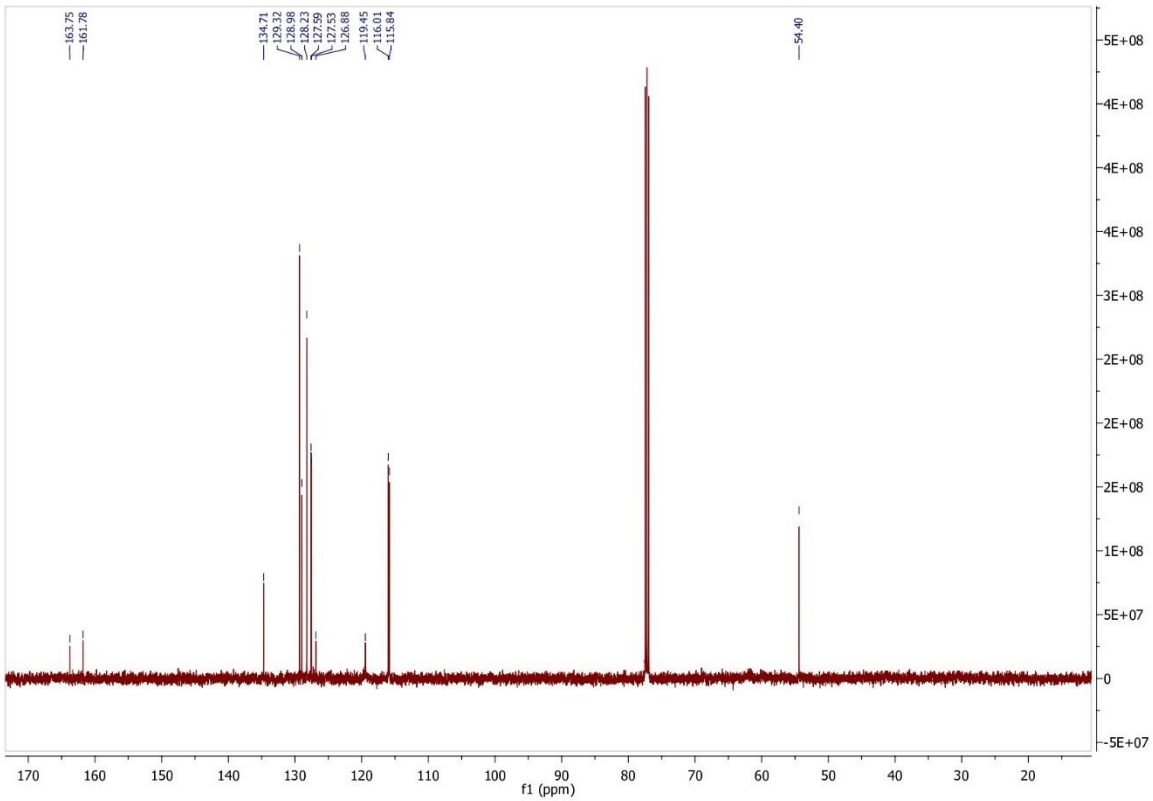
[13]C-NMR spectrum of 1-benzyl-4-phenyl-1H-1,2,3-triazole (3a)



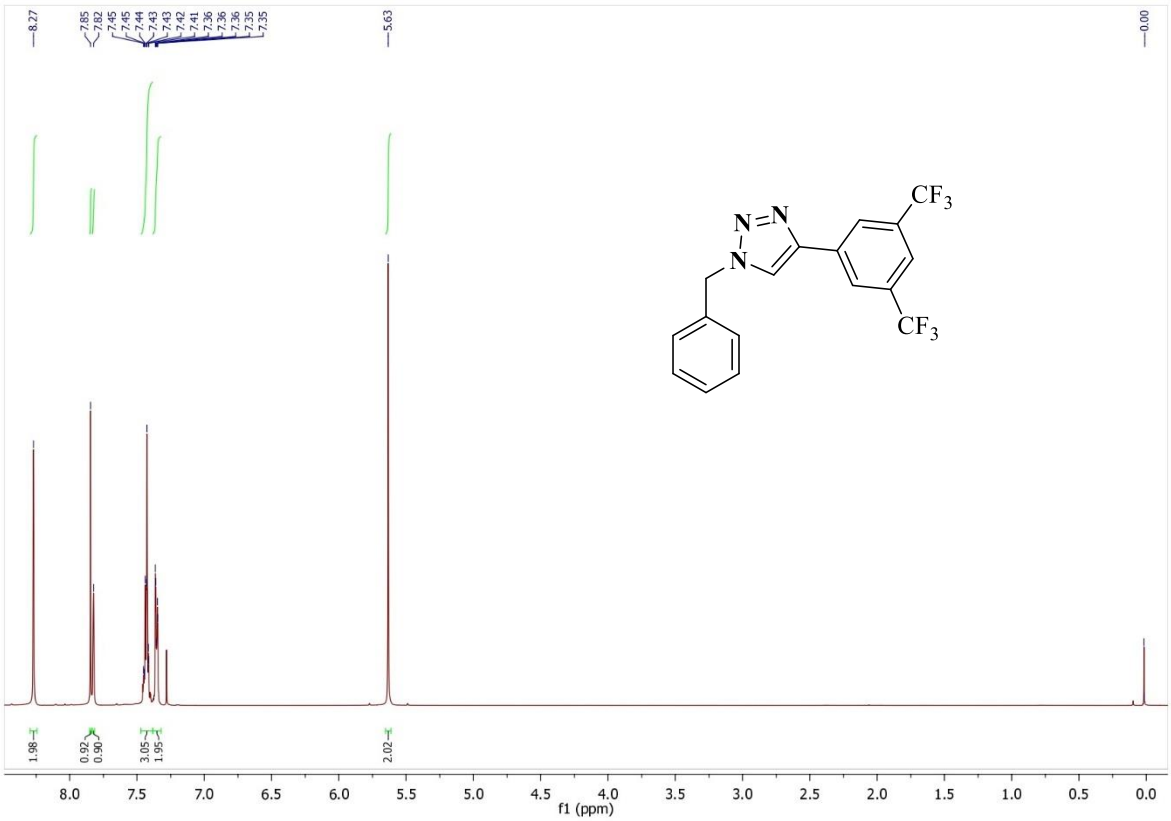
[1]H-NMR spectrum of 1-benzyl-4-(4-fluorophenyl)-1H-1,2,3-triazole (3b)



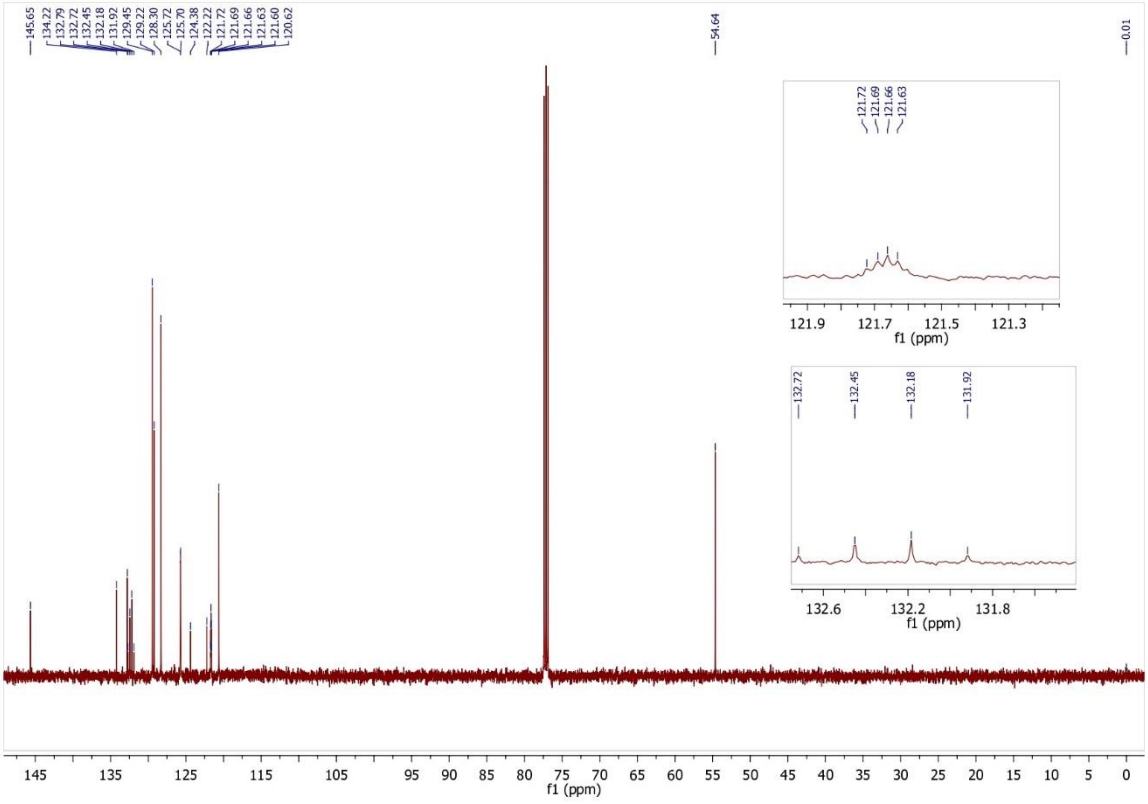
[13]C-NMR spectrum of 1-benzyl-4-(4-fluorophenyl)-1H-1,2,3-triazole (3b)



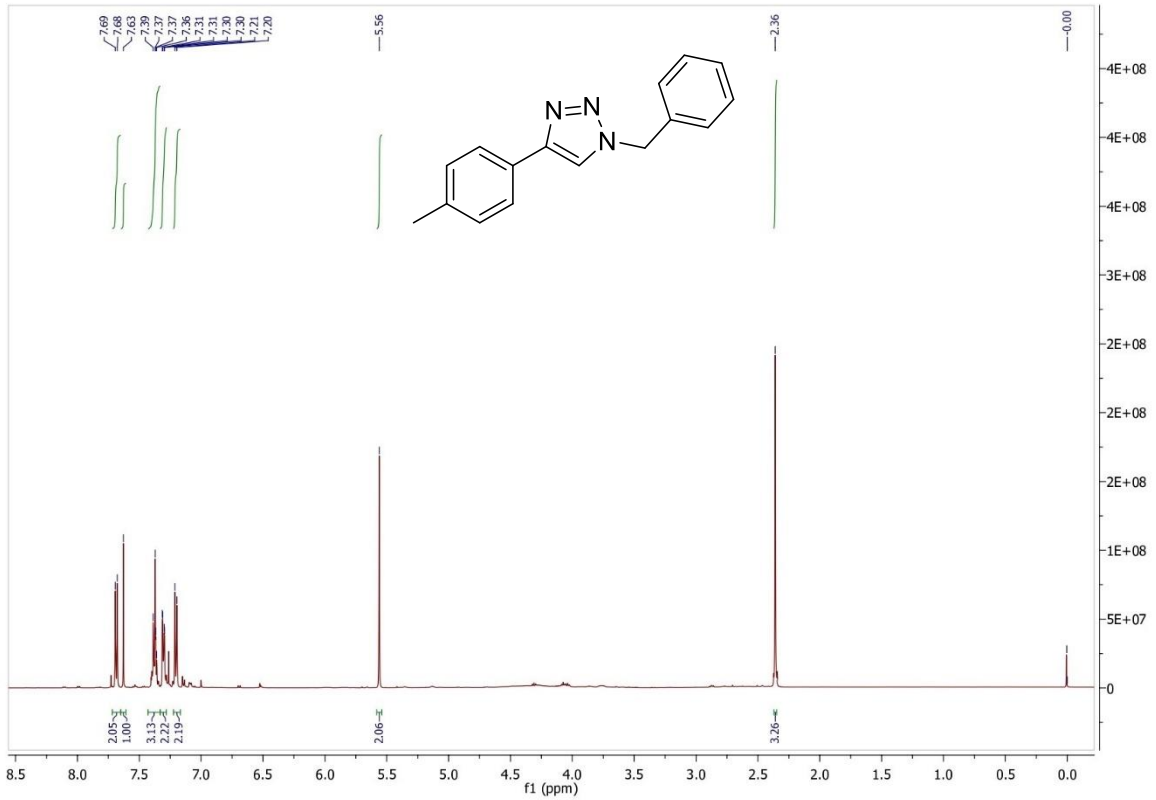
[1]H-NMR spectrum of 1-benzyl-4-(3,5-bis(trifluoromethyl)phenyl)-1H-1,2,3-triazole (3c)



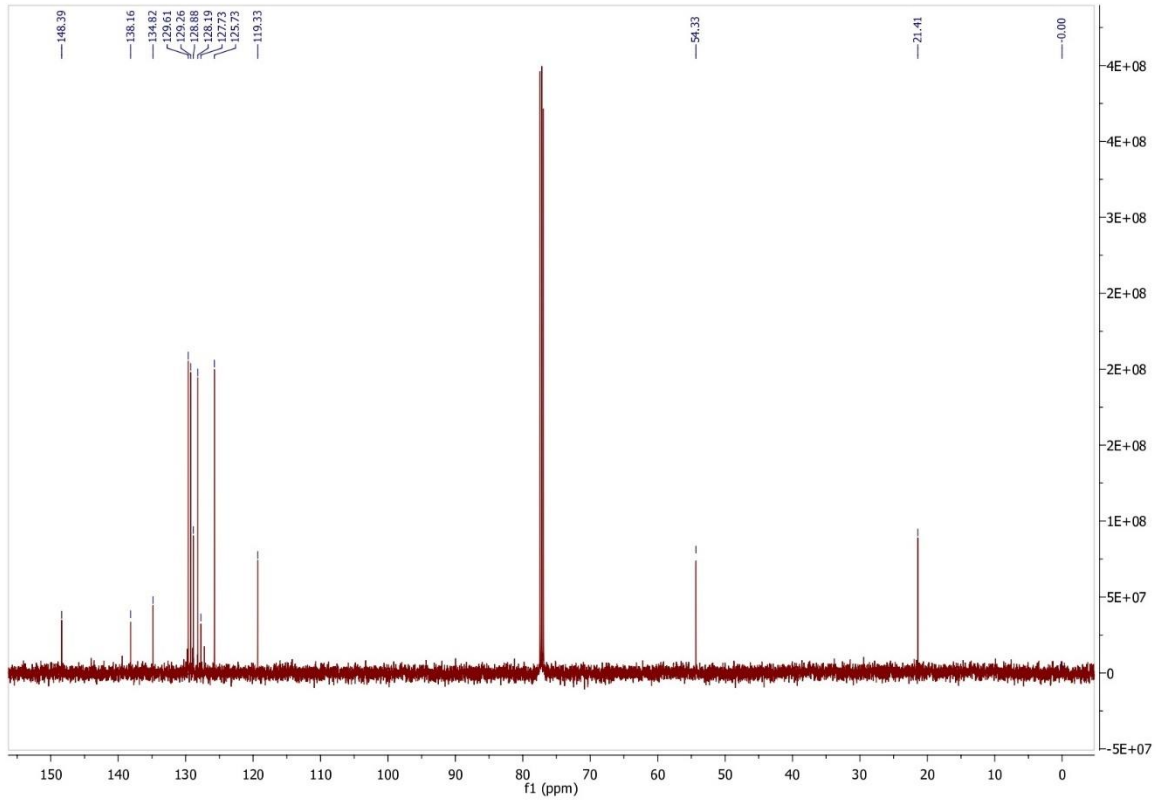
[13]C-NMR spectrum of 1-benzyl-4-(3,5-bis(trifluoromethyl)phenyl)-1H-1,2,3-triazole (3c)



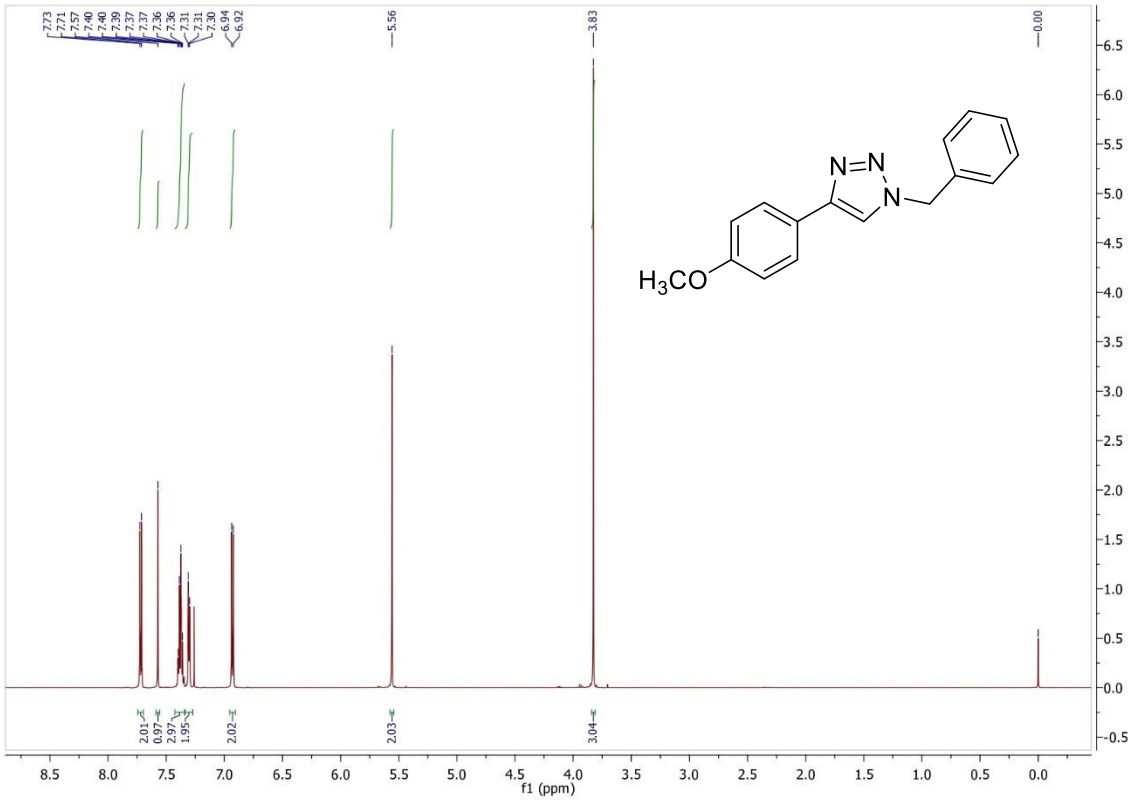
[1]H-NMR spectrum of 1-benzyl-4-(p-tolyl)-1H-1,2,3-triazole (3d)



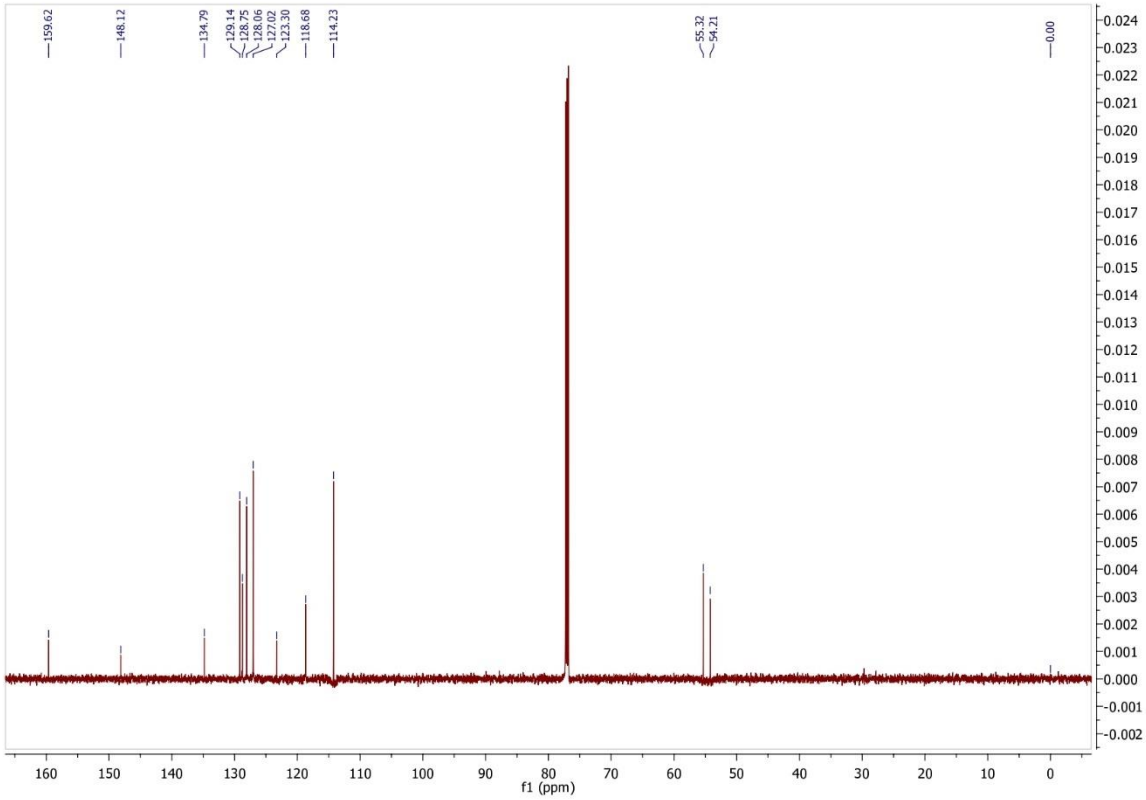
[13]C-NMR spectrum of 1-benzyl-4-(p-tolyl)-1H-1,2,3-triazole (3d)



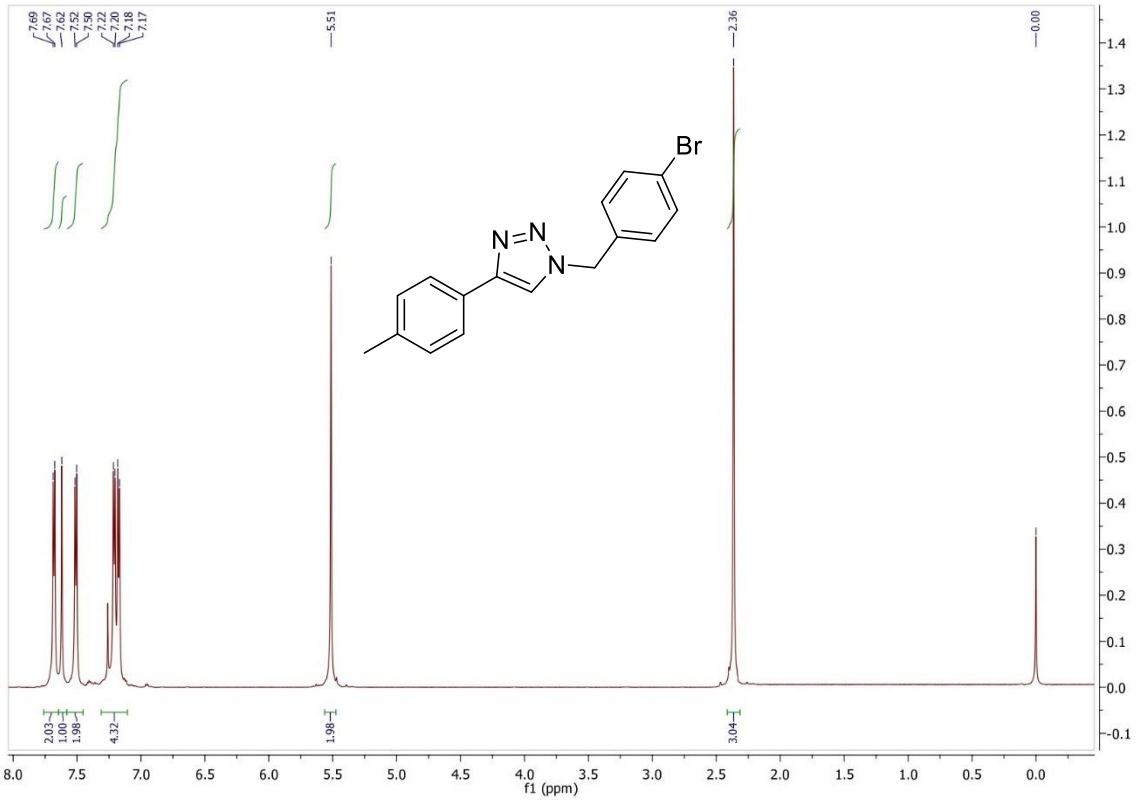
[1]H-NMR spectrum of 1-benzyl-4-(4-methoxyphenyl)-1H-1,2,3-triazole (3e)



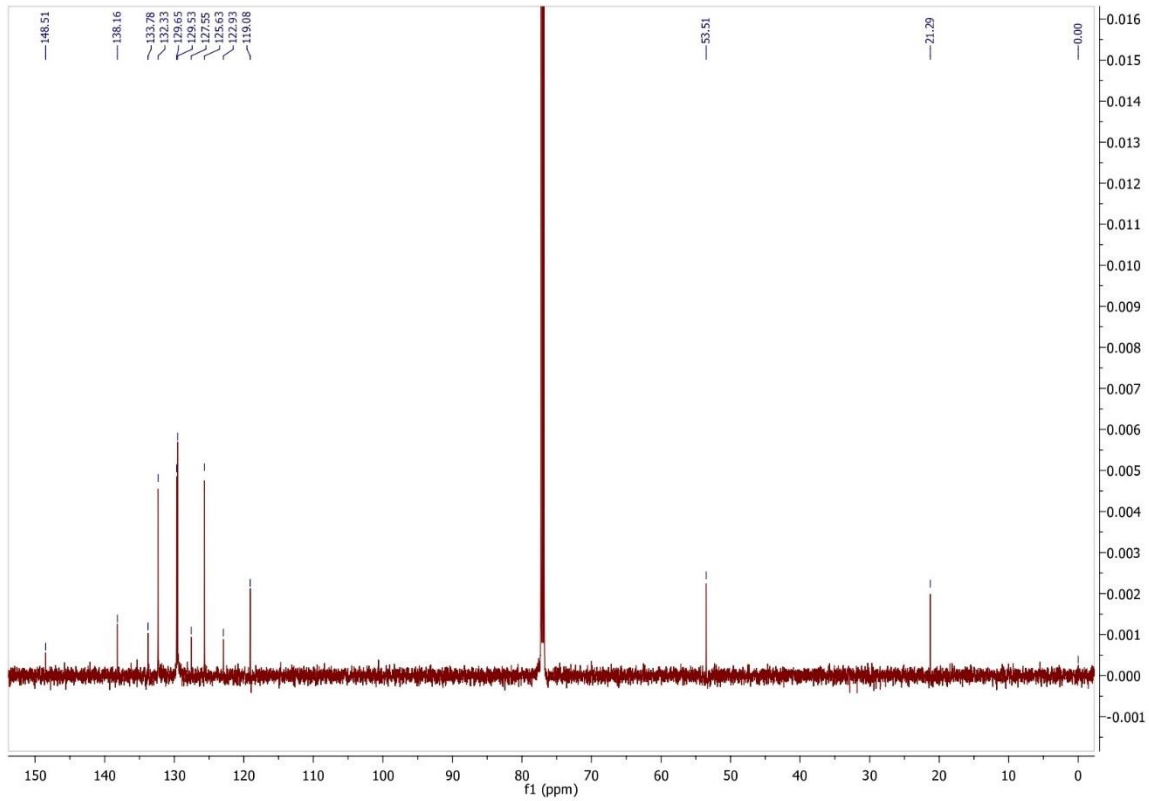
[13]C-NMR spectrum of 1-benzyl-4-(4-methoxyphenyl)-1H-1,2,3-triazole (3e)



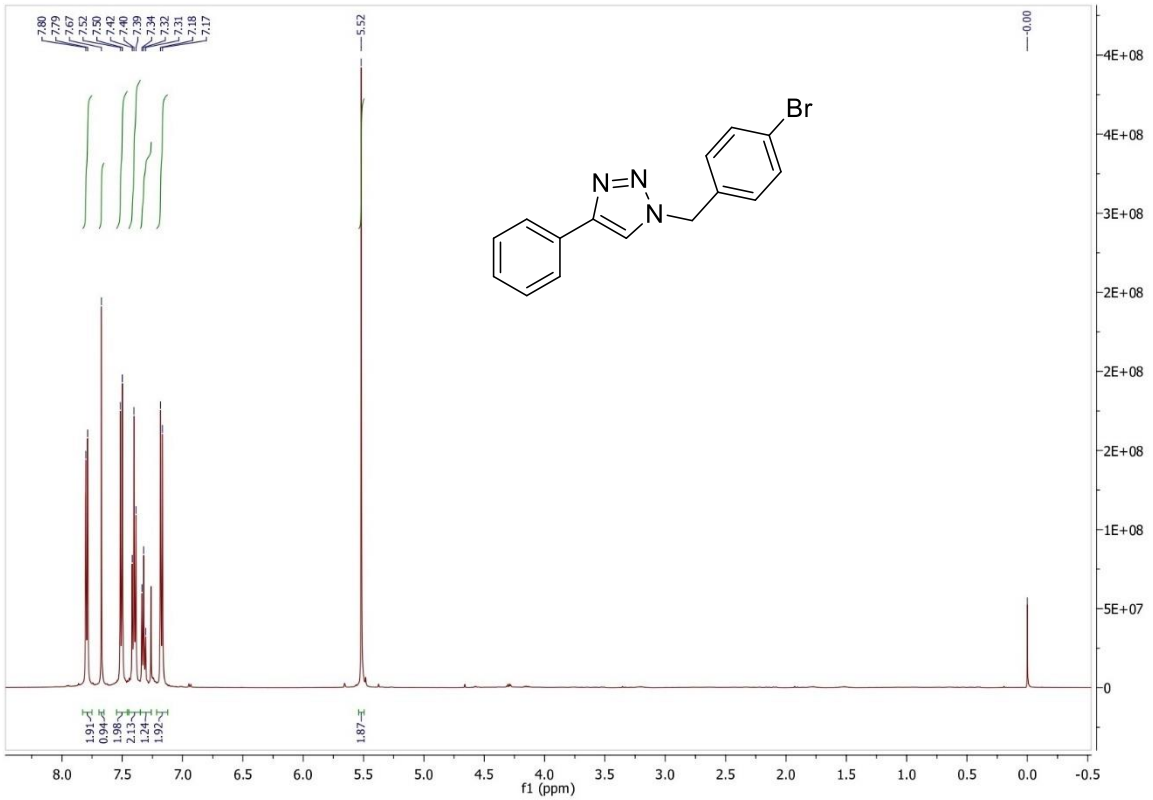
^{1}H-NMR spectrum of 1-(4-bromobenzyl)-4-(p-tolyl)-1H-1,2,3-triazole (3f)



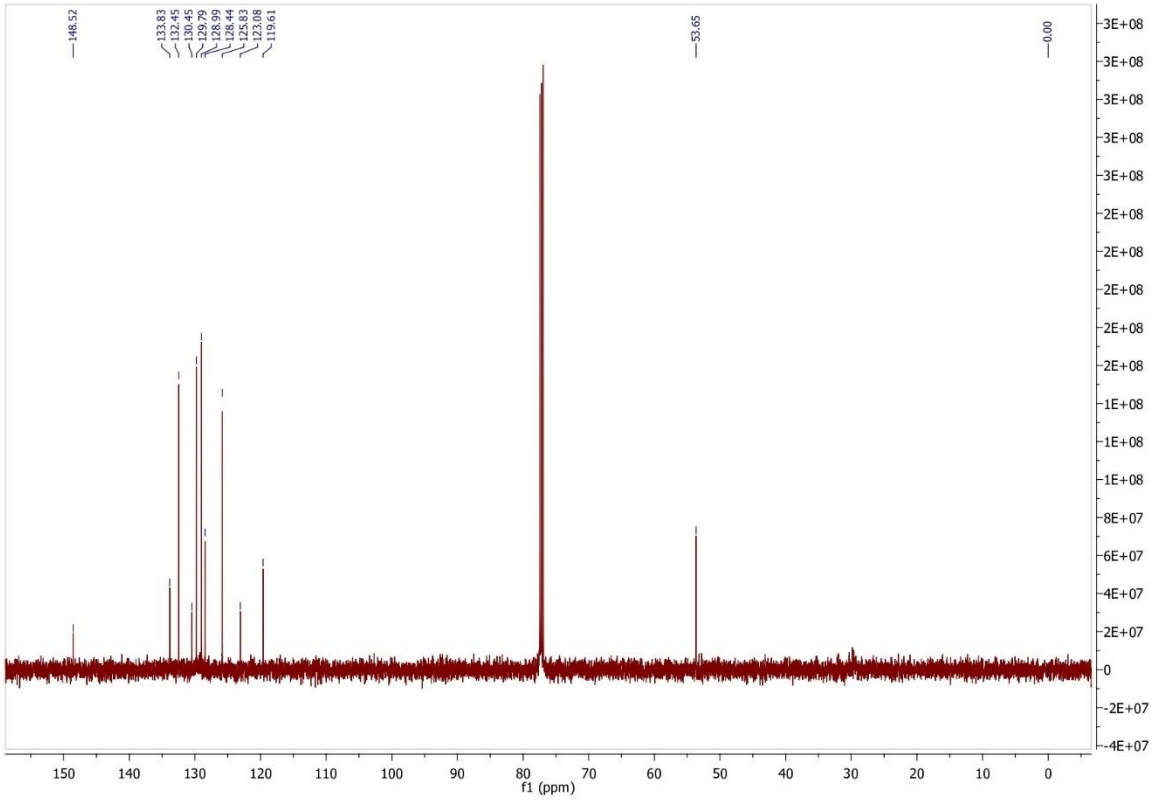
^{13}C-NMR spectrum of 1-(4-bromobenzyl)-4-(p-tolyl)-1H-1,2,3-triazole (3f)



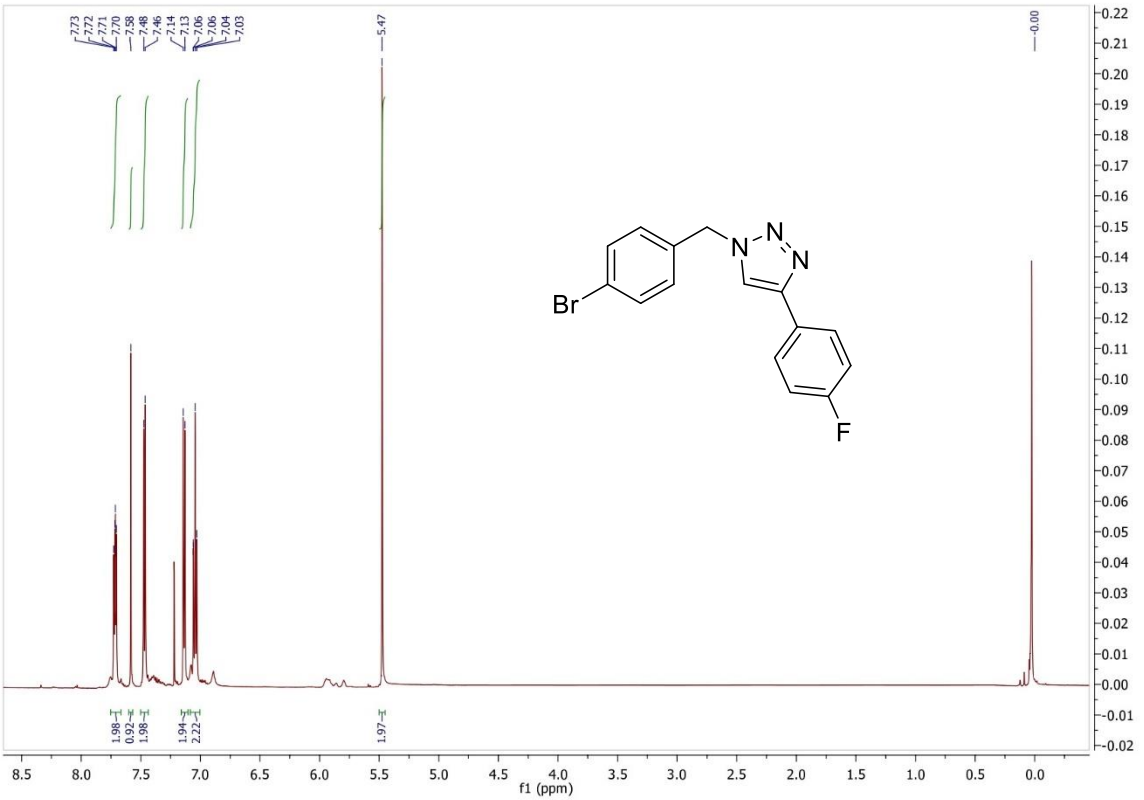
[1]H-NMR spectrum of 1-(4-bromobenzyl)-4-phenyl-1H-1,2,3-triazole (3g)



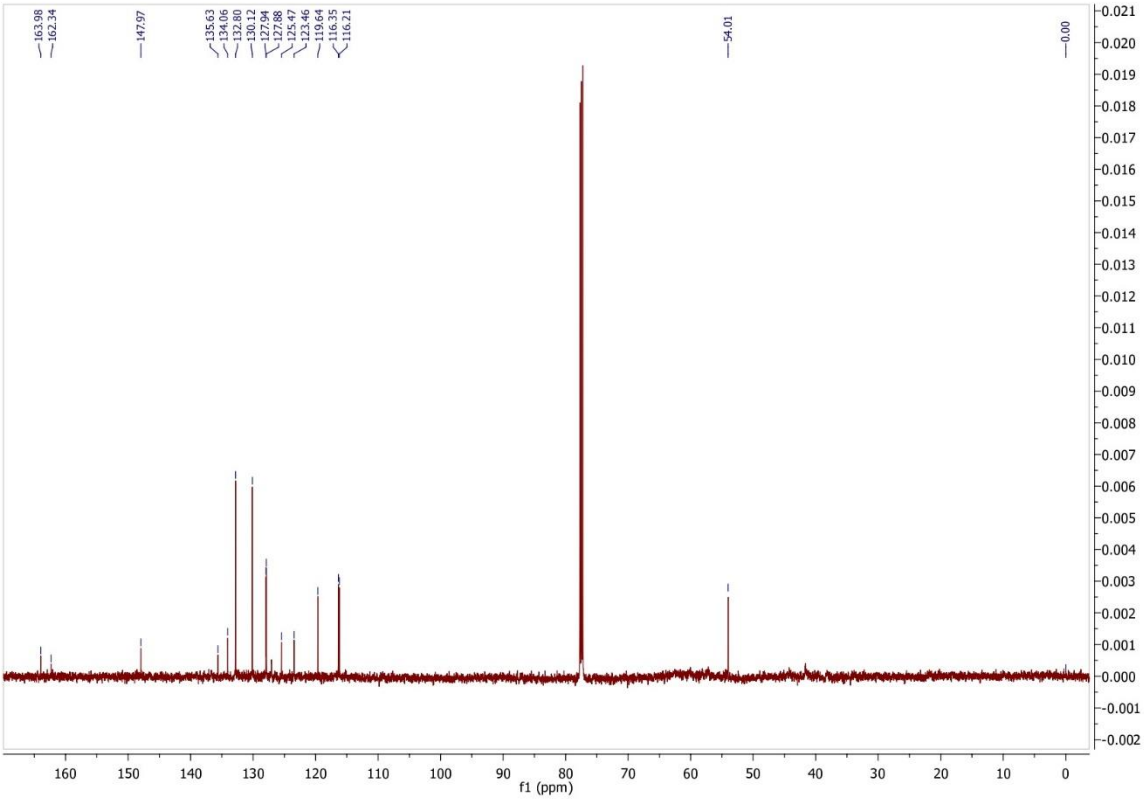
[13]C-NMR spectrum of 1-(4-bromobenzyl)-4-phenyl-1H-1,2,3-triazole (3g)



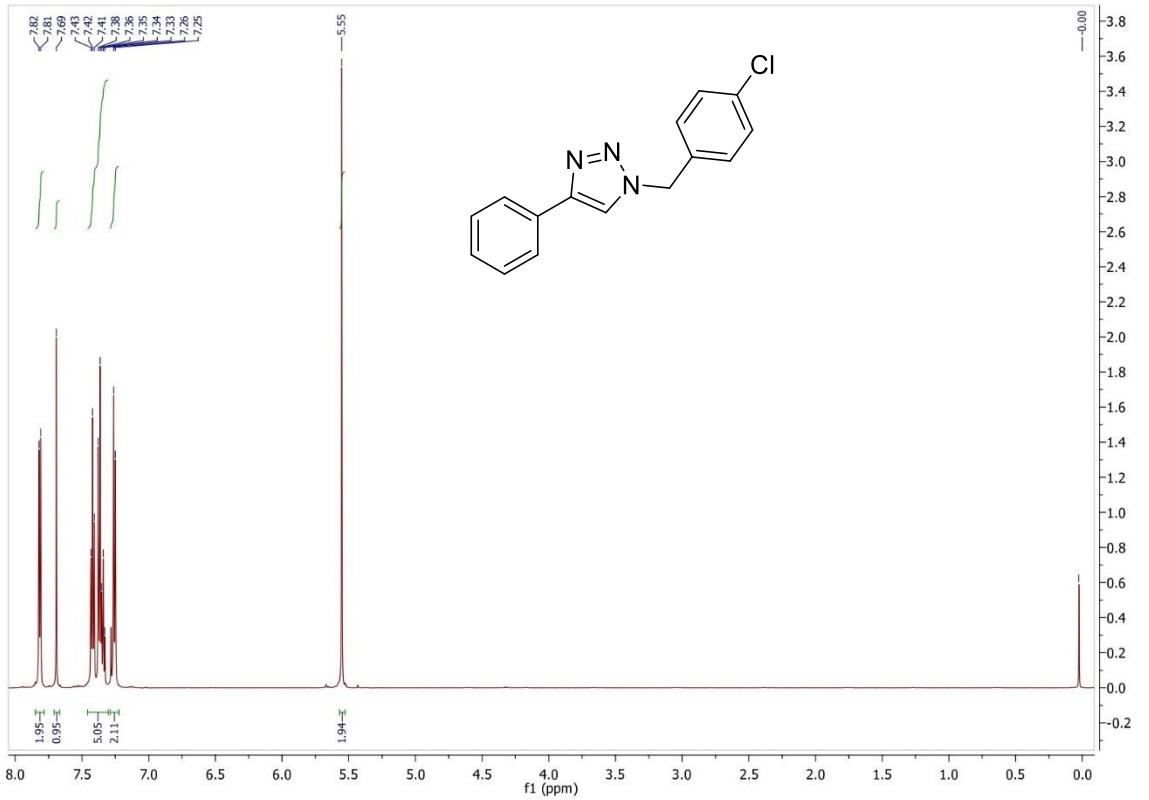
[1]H-NMR spectrum of 1-(4-bromobenzyl)-4-(4-fluorophenyl)-1H-1,2,3-triazole (3h)



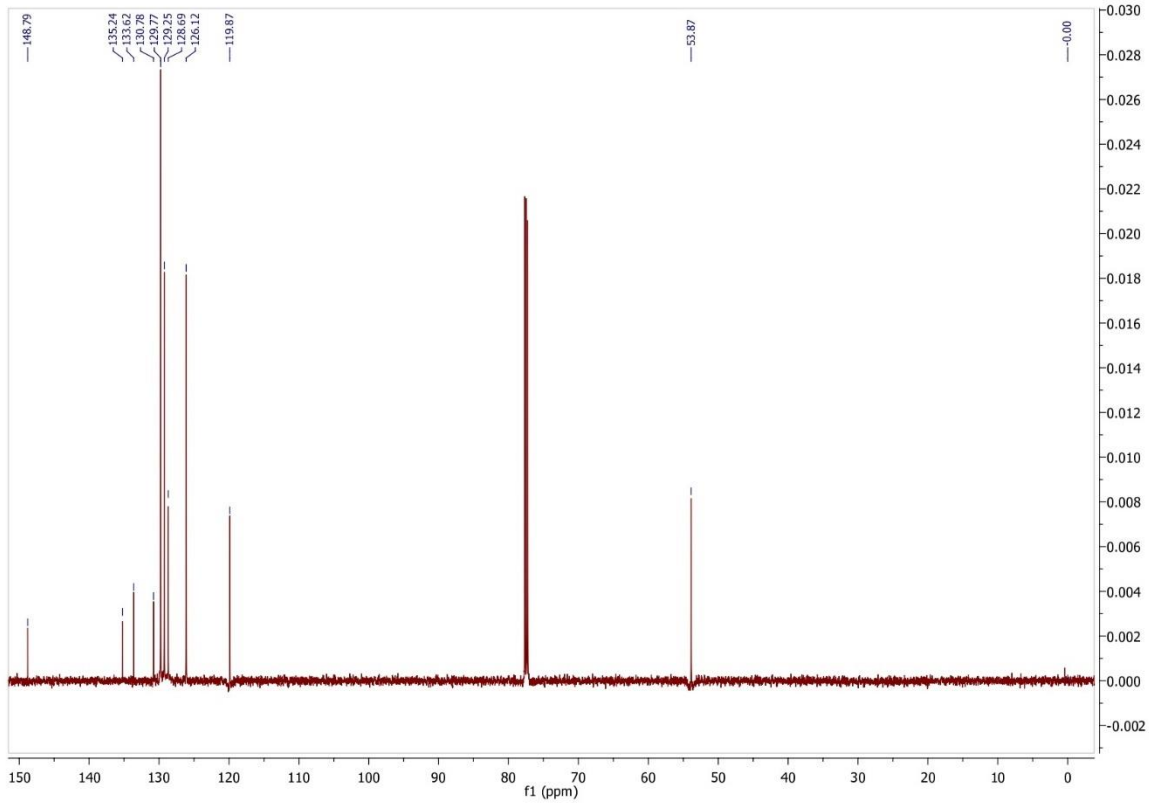
[13]C-NMR spectrum of 1-(4-bromobenzyl)-4-(4-fluorophenyl)-1H-1,2,3-triazole (3h)



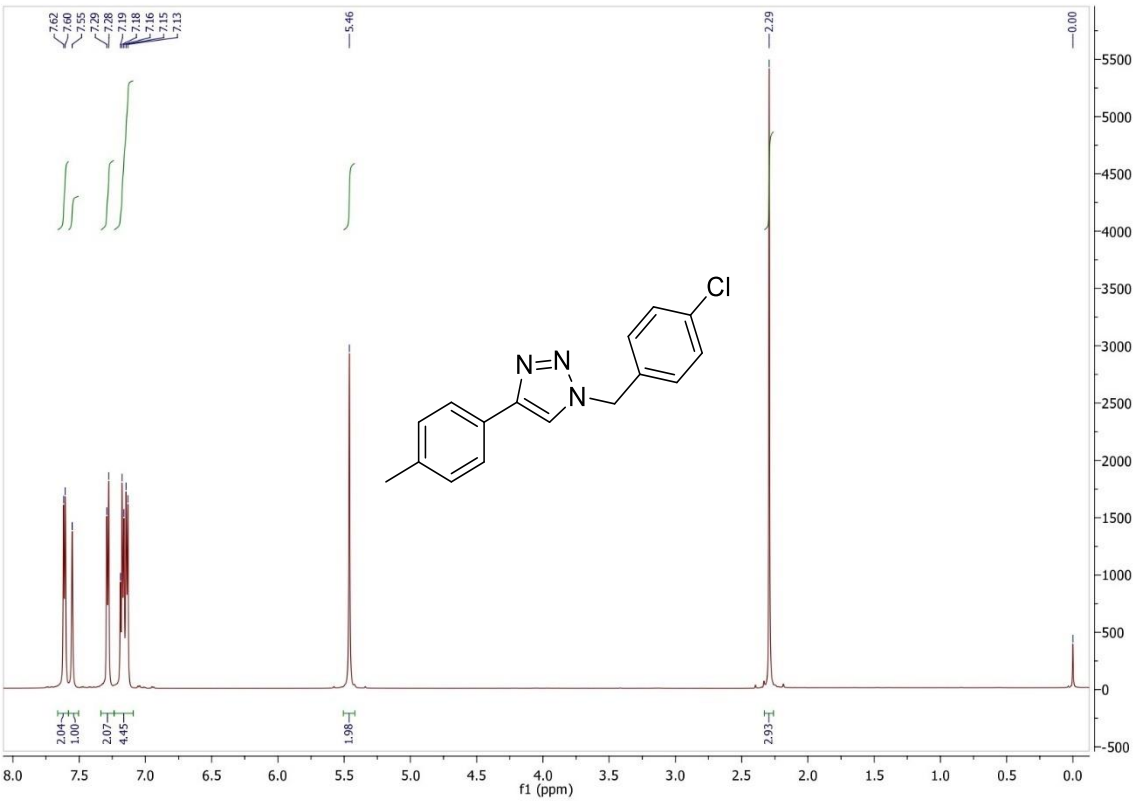
[1]H-NMR spectrum of 1-(4-chlorobenzyl)-4-phenyl-1H-1,2,3-triazole (3i)



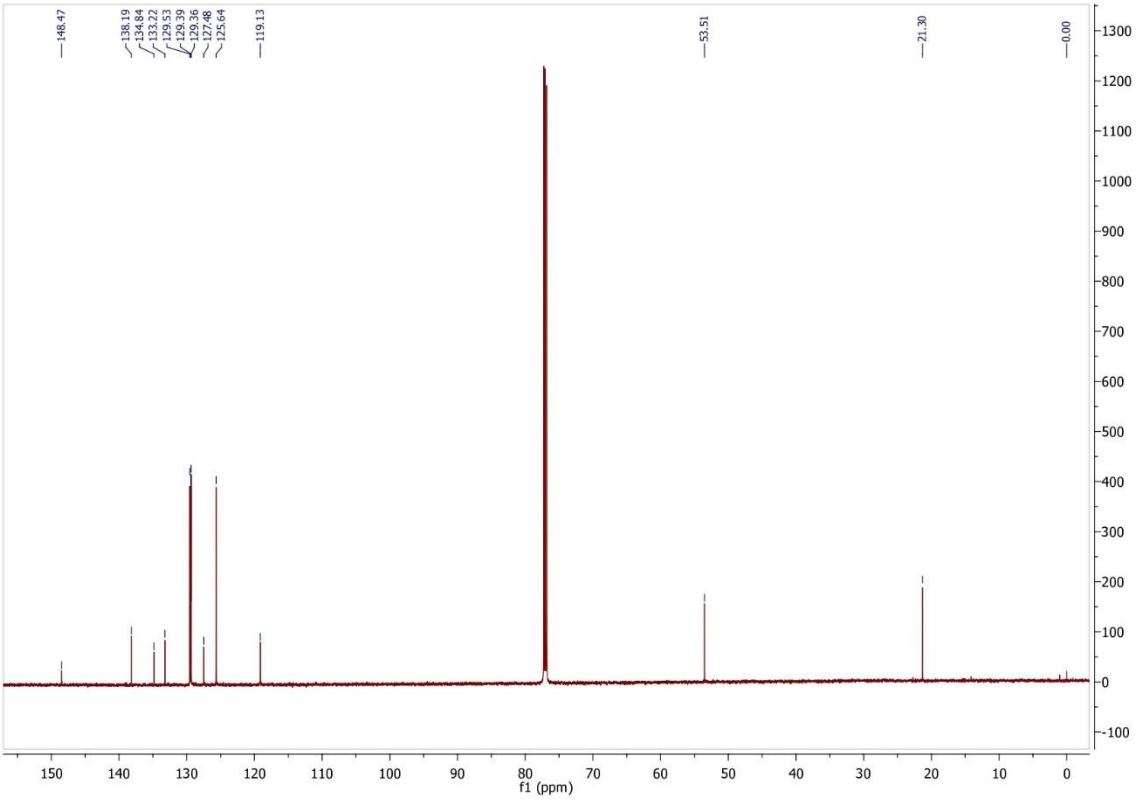
[13]C-NMR spectrum of 1-(4-chlorobenzyl)-4-phenyl-1H-1,2,3-triazole (3i)



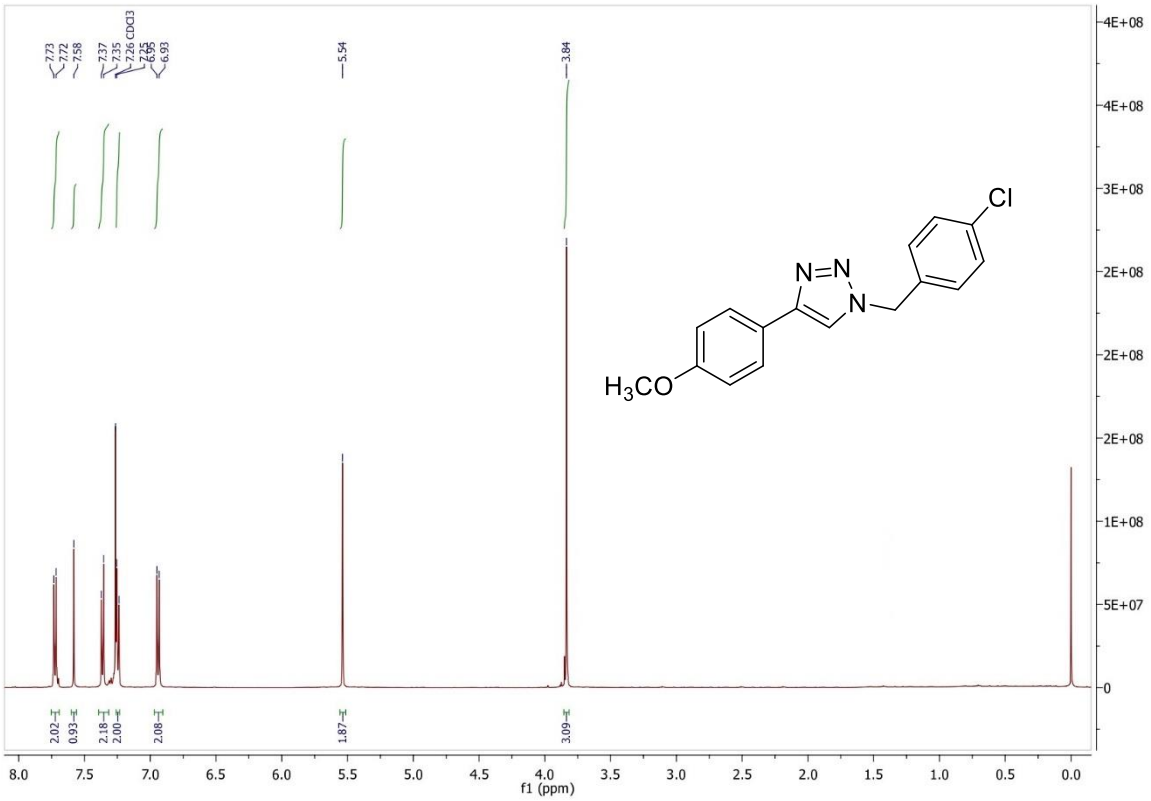
[1]H-NMR spectrum of 1-(4-chlorobenzyl)-4-(p-tolyl)-1H-1,2,3-triazole (3j)



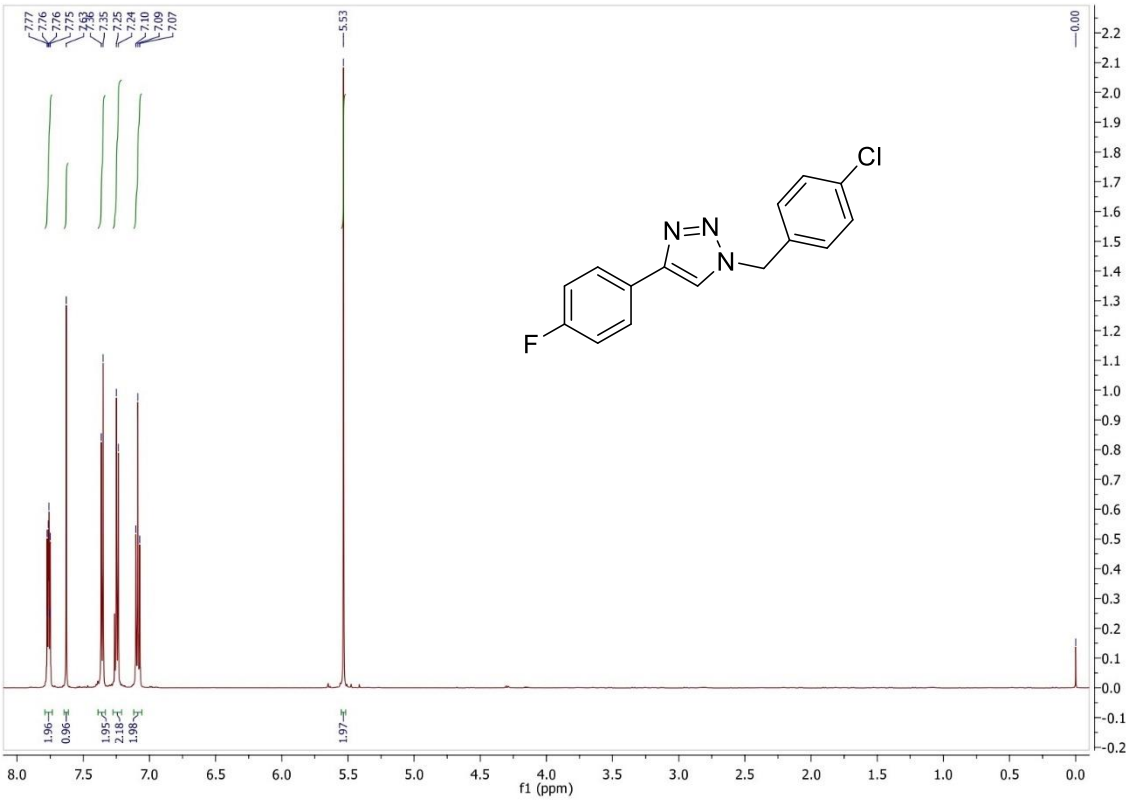
[13]C-NMR spectrum of 1-(4-chlorobenzyl)-4-(p-tolyl)-1H-1,2,3-triazole (3j)



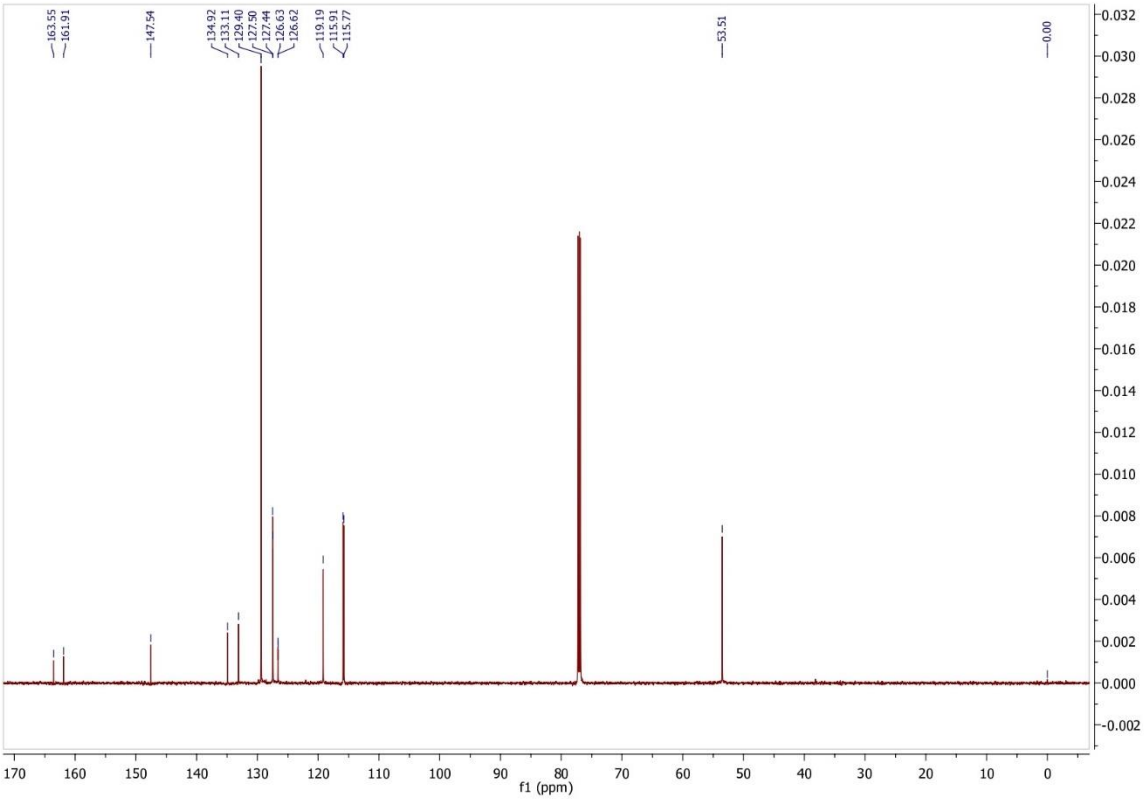
^{1}H-NMR spectrum of 1-(4-chlorobenzyl)-4-(4-methoxyphenyl)-1H-1,2,3-triazole (3k)



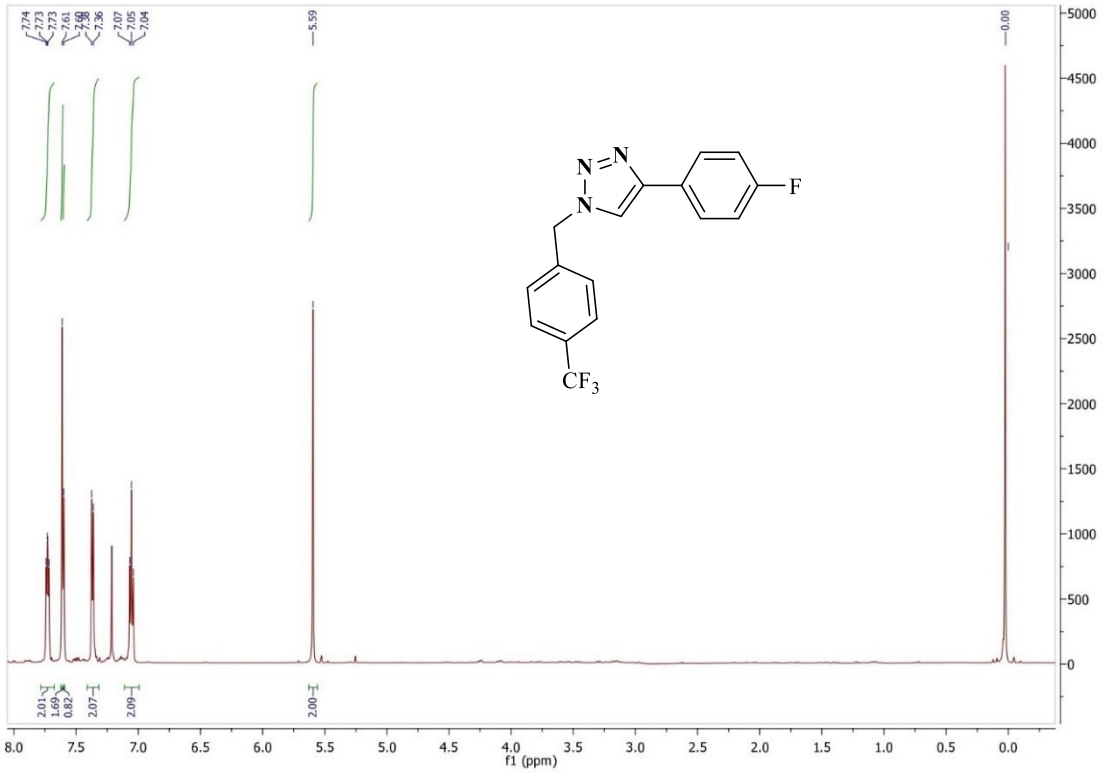
[1]H-NMR spectrum of 1-(4-chlorobenzyl)-4-(4-fluorophenyl)-1H-1,2,3-triazole (3l)



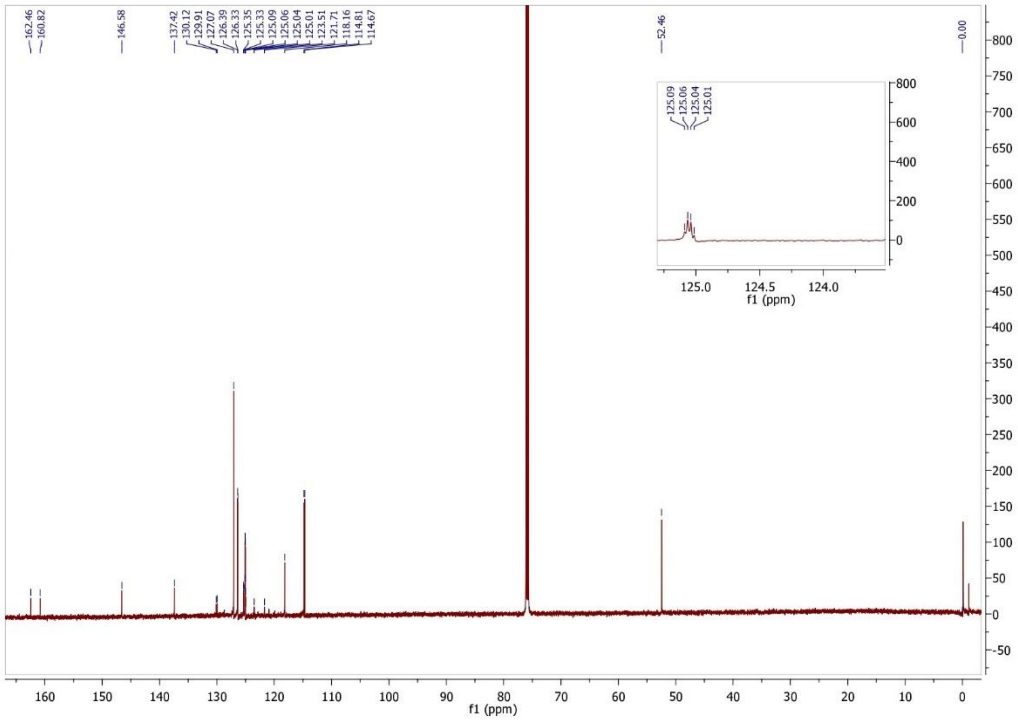
[13]C-NMR spectrum of 1-(4-chlorobenzyl)-4-(4-fluorophenyl)-1H-1,2,3-triazole (3l)



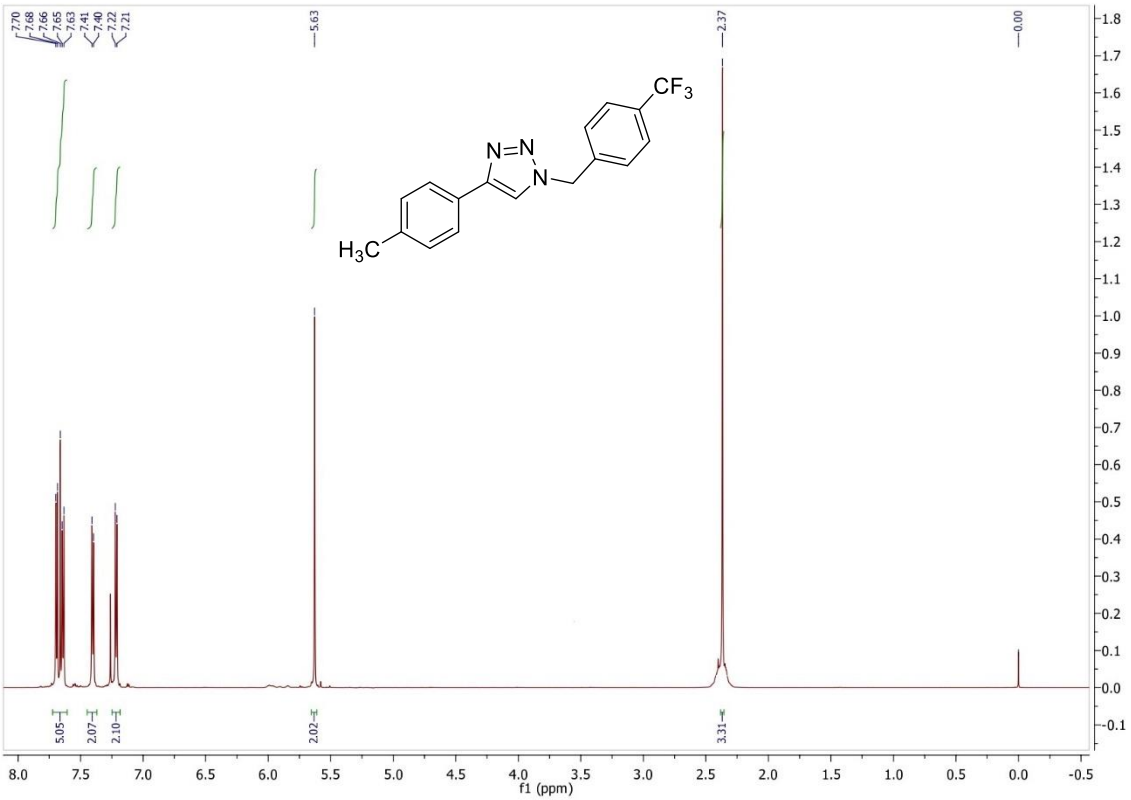
[1]H-NMR spectrum of 4-(4-fluorophenyl)-1-(4-(trifluoromethyl)benzyl)-1H-1,2,3-triazole (3m)



[13]C-NMR spectrum of 4-(4-fluorophenyl)-1-(4-(trifluoromethyl)benzyl)-1H-1,2,3-triazole (3m)



[1]H-NMR spectrum of 4-(p-tolyl)-1-(4-(trifluoromethyl)benzyl)-1H-1,2,3-triazole (3n)



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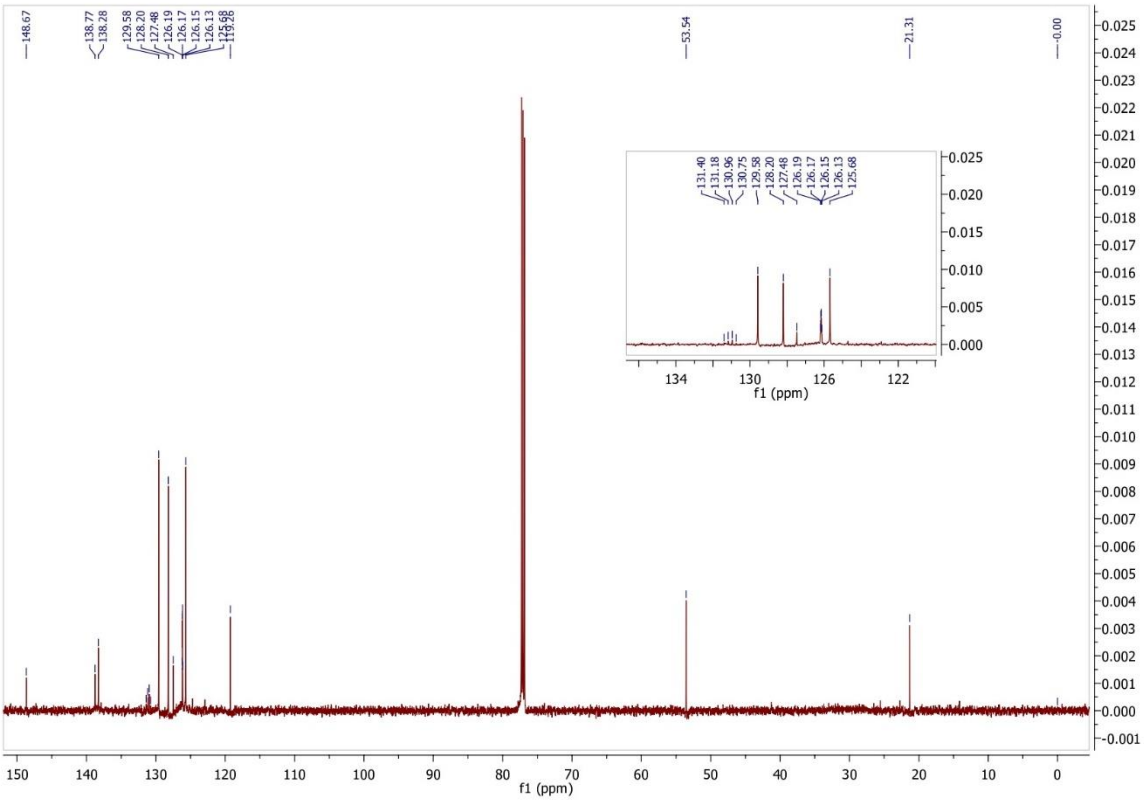

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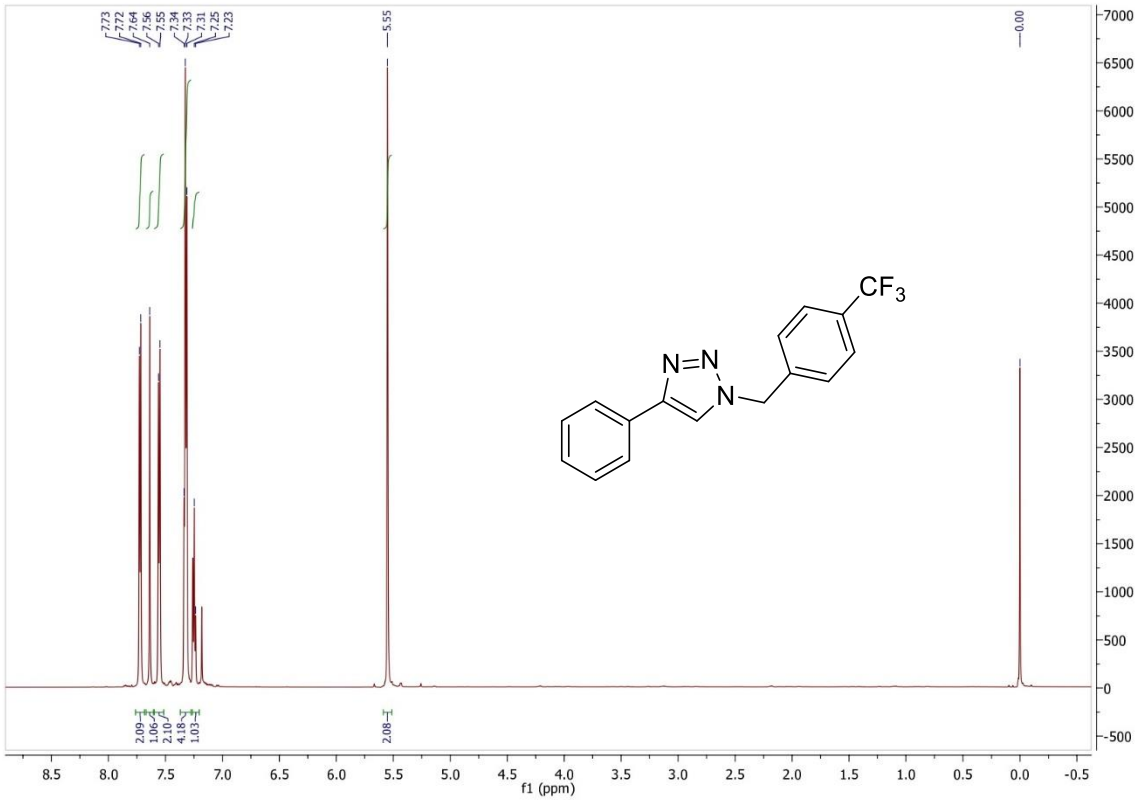
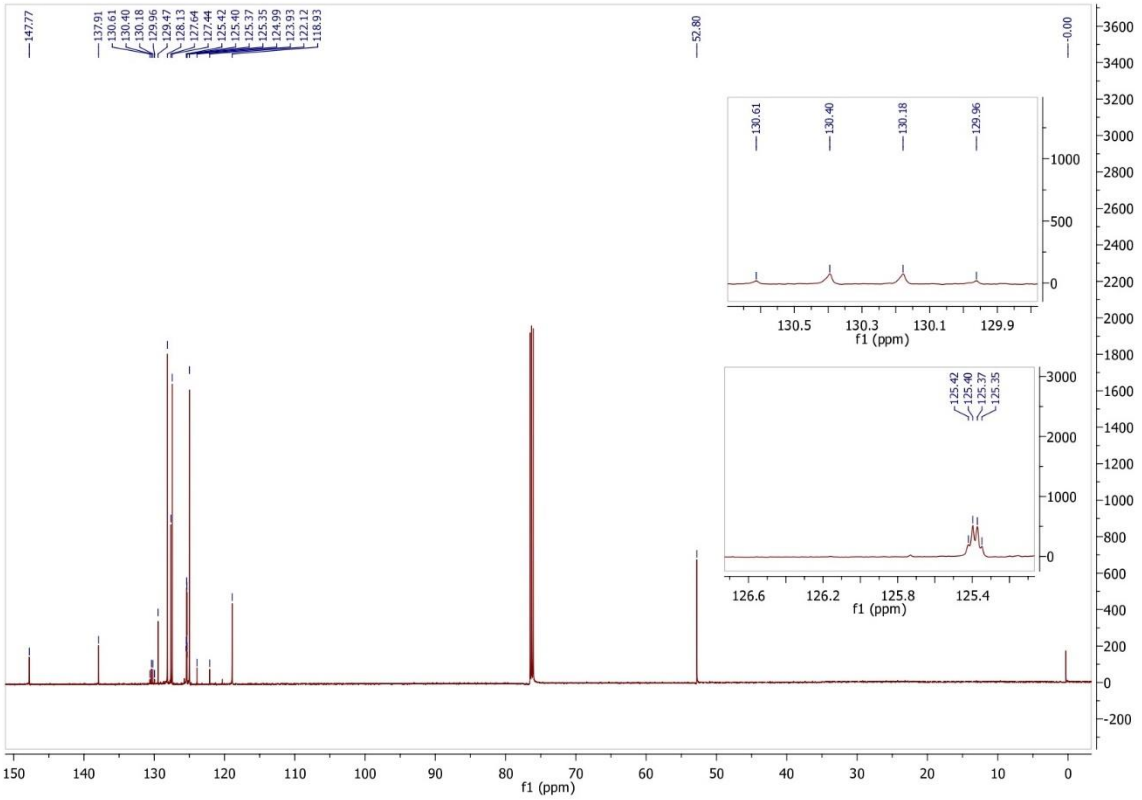
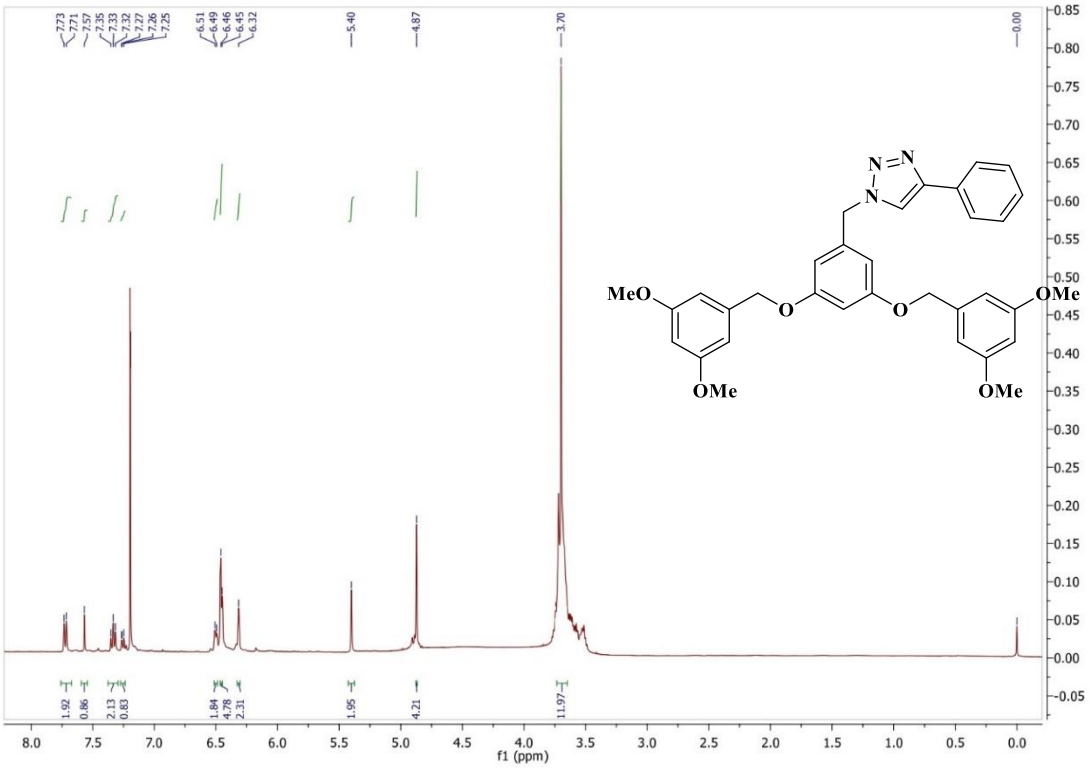


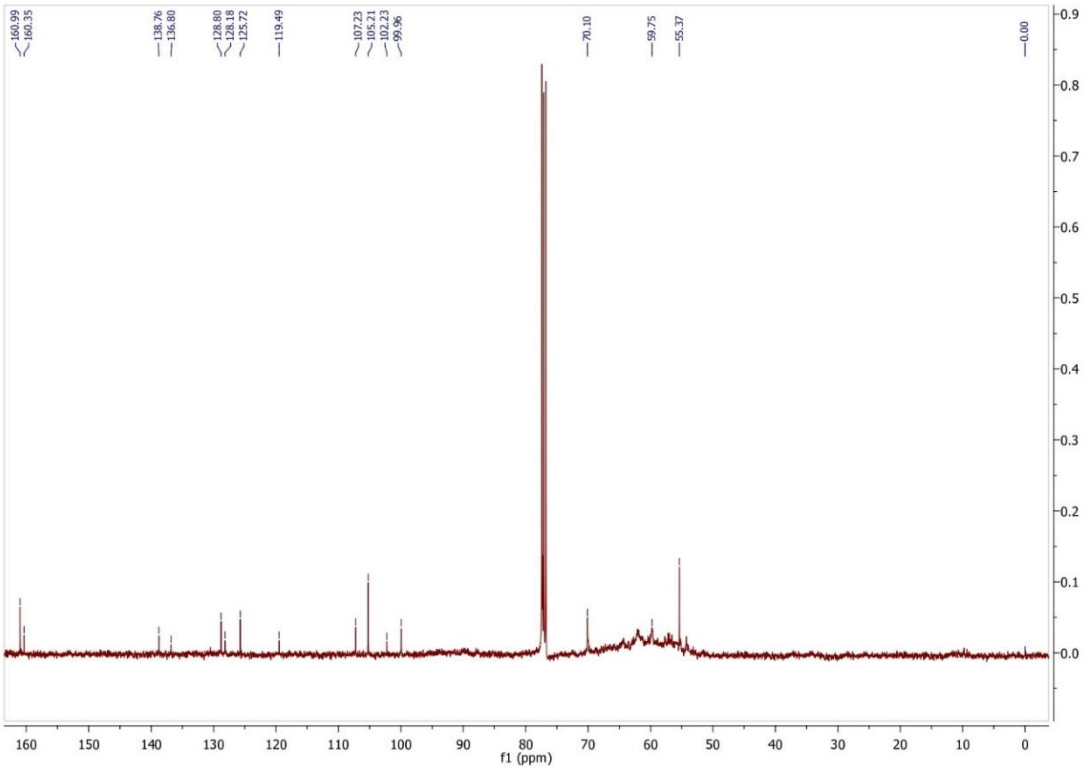
[13]C-NMR spectrum of 4-phenyl-1-(4-(trifluoromethyl)benzyl)-1H-1,2,3-triazole (3o)



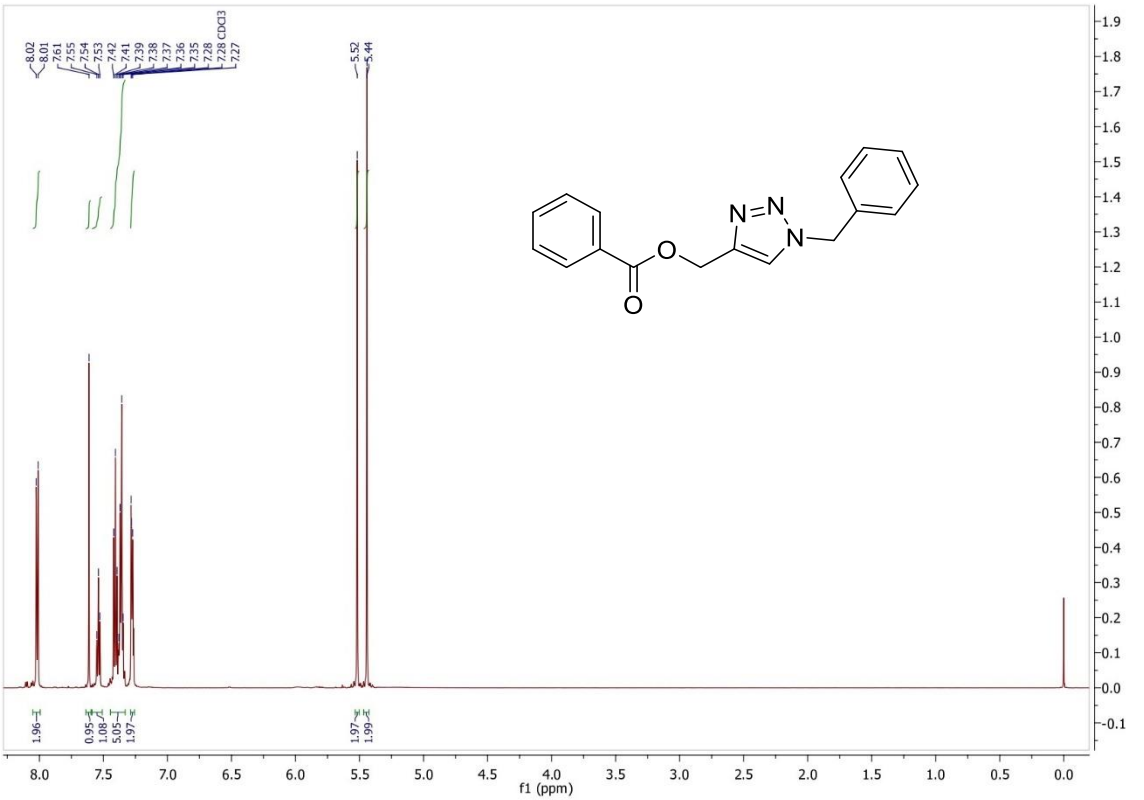
^{1}H-NMR spectrum of 1-(3,5-bis((3,5-dimethoxybenzyl)oxy)benzyl)-4-phenyl-1H-1,2,3-triazole (3p)



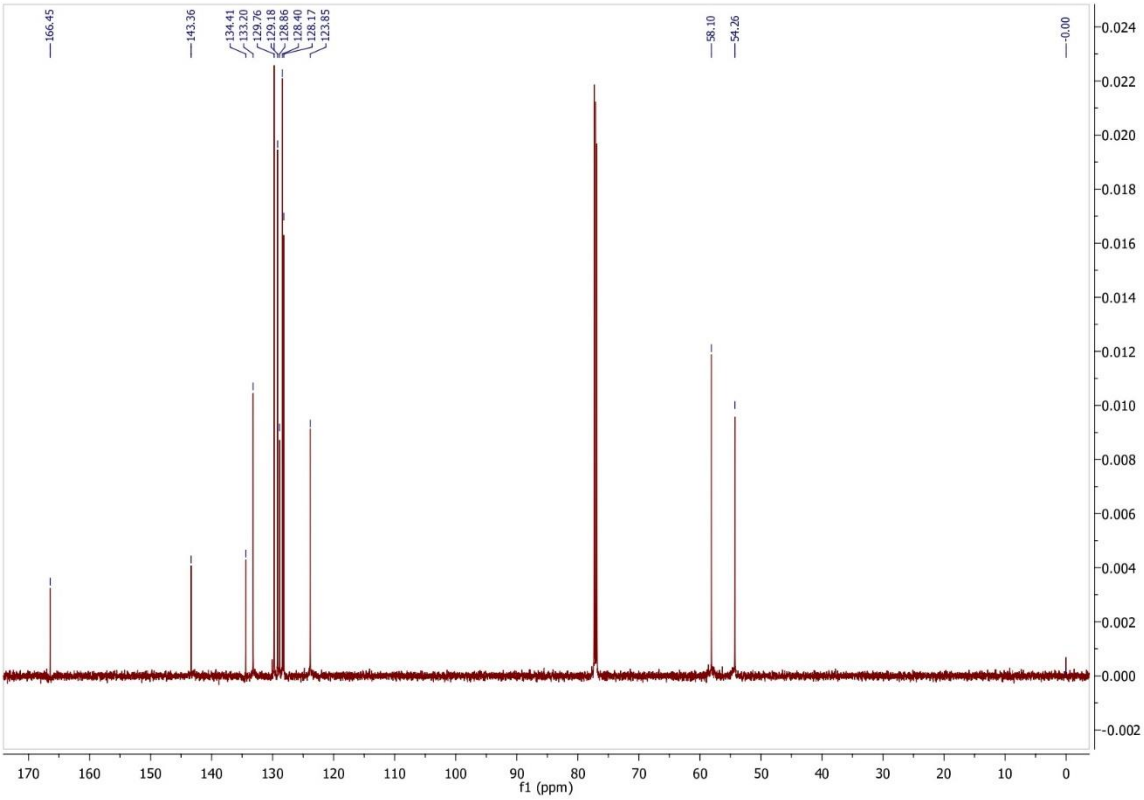
^{13}C-NMR spectrum of 1-(3,5-bis((3,5-dimethoxybenzyl)oxy)benzyl)-4-phenyl-1H-1,2,3-triazole (3p)



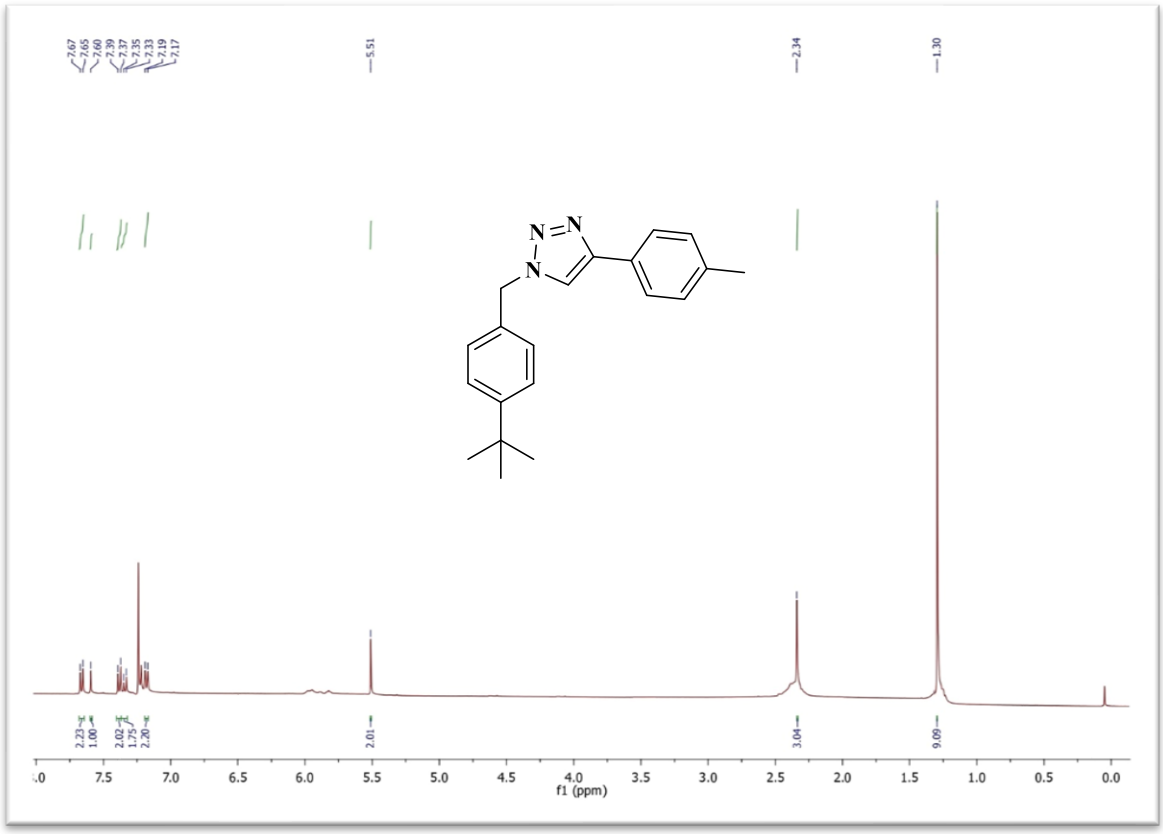
^{1}H-NMR spectrum of (1-benzyl-1H-1,2,3-triazol-4-yl)methyl benzoate (3q)



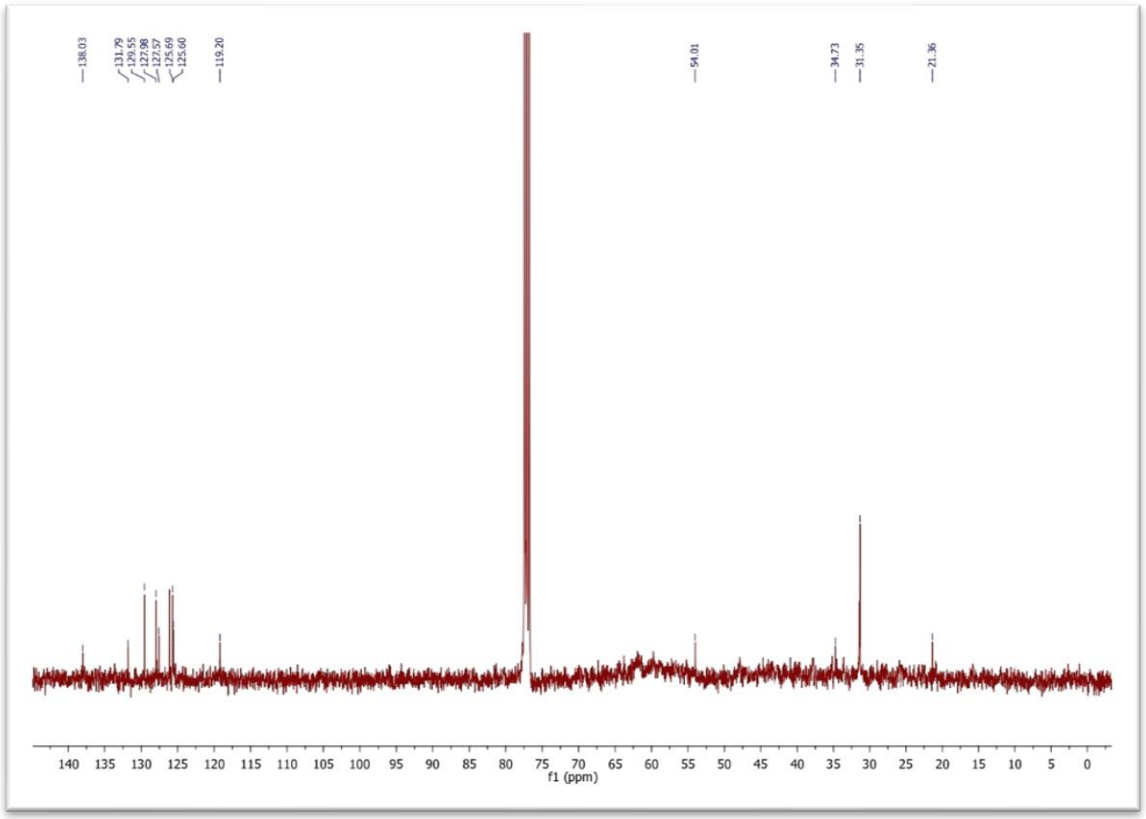
^{13}C-NMR spectrum of (1-benzyl-1H-1,2,3-triazol-4-yl)methyl benzoate (3q)



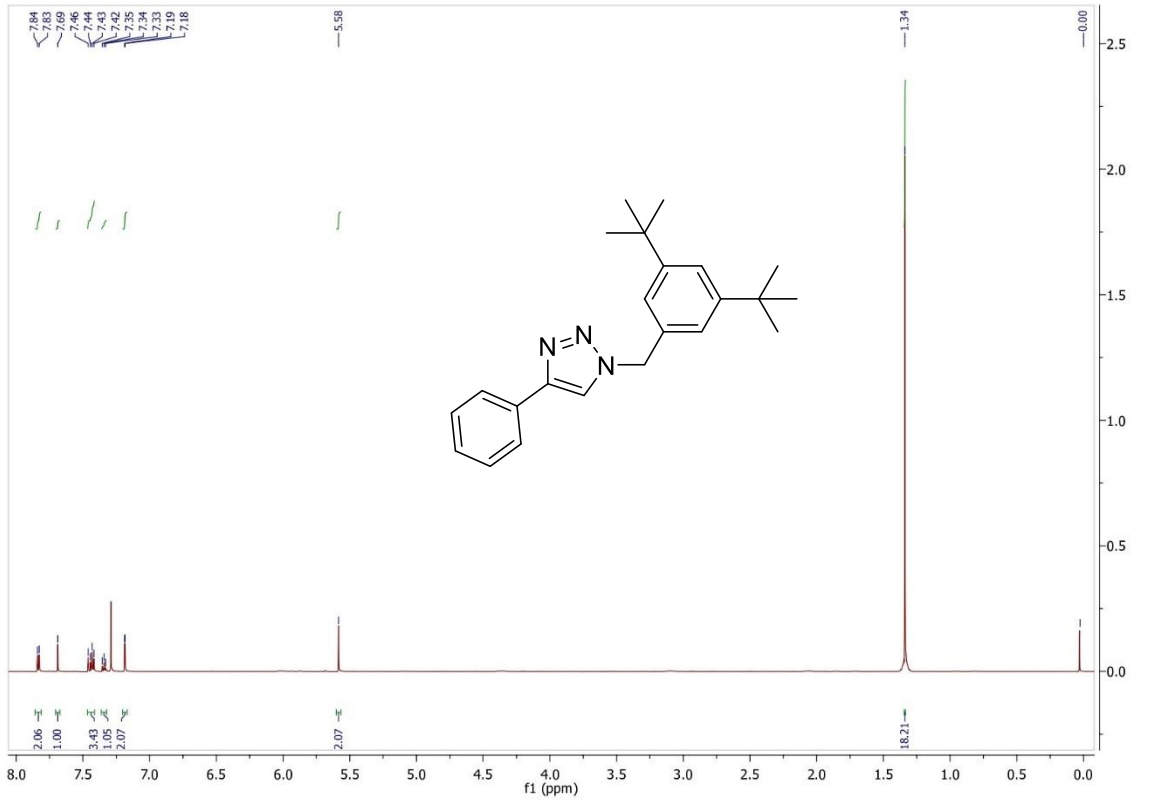
^{1}H-NMR spectrum of 1-(4-(tert-butyl)benzyl)-4-(p-tolyl)-1H-1,2,3-triazole (3r)



^{13}C-NMR spectrum of 1-(4-(tert-butyl)benzyl)-4-(p-tolyl)-1H-1,2,3-triazole (3r)



[1]H-NMR spectrum of 1-(3,5-di-tert-butylbenzyl)-4-phenyl-1H-1,2,3-triazole (3s)



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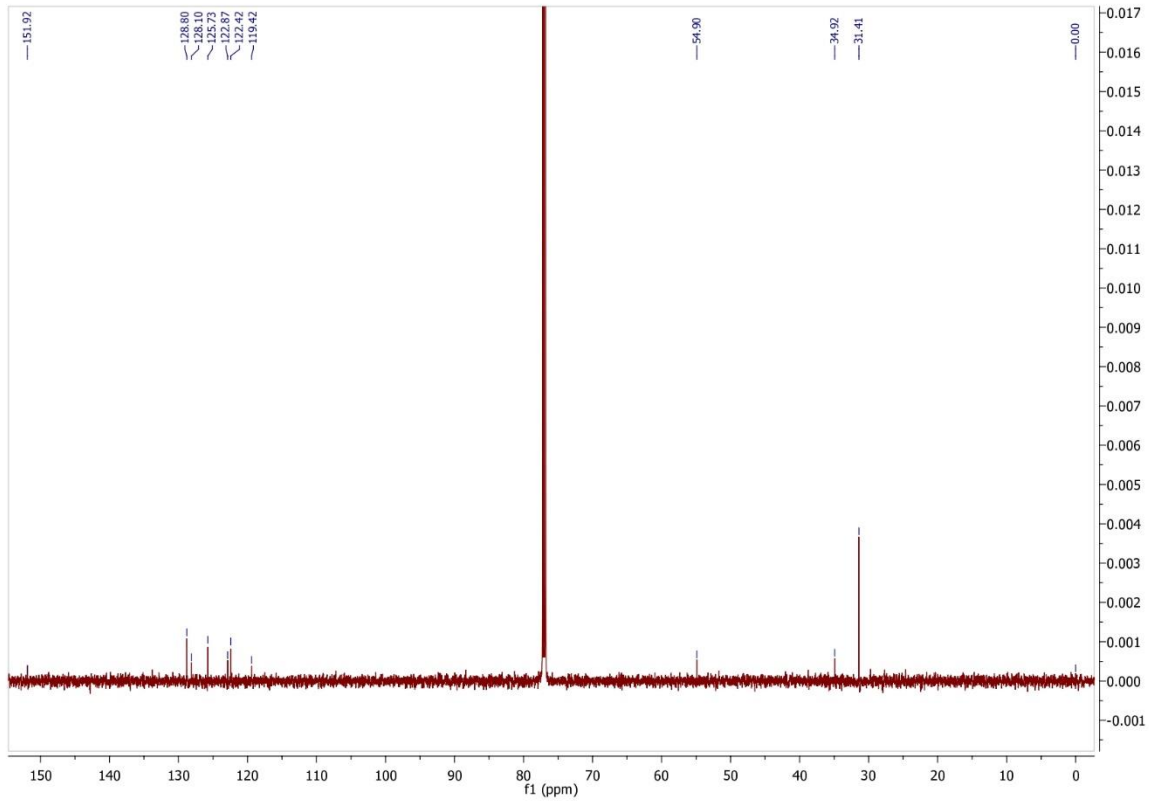

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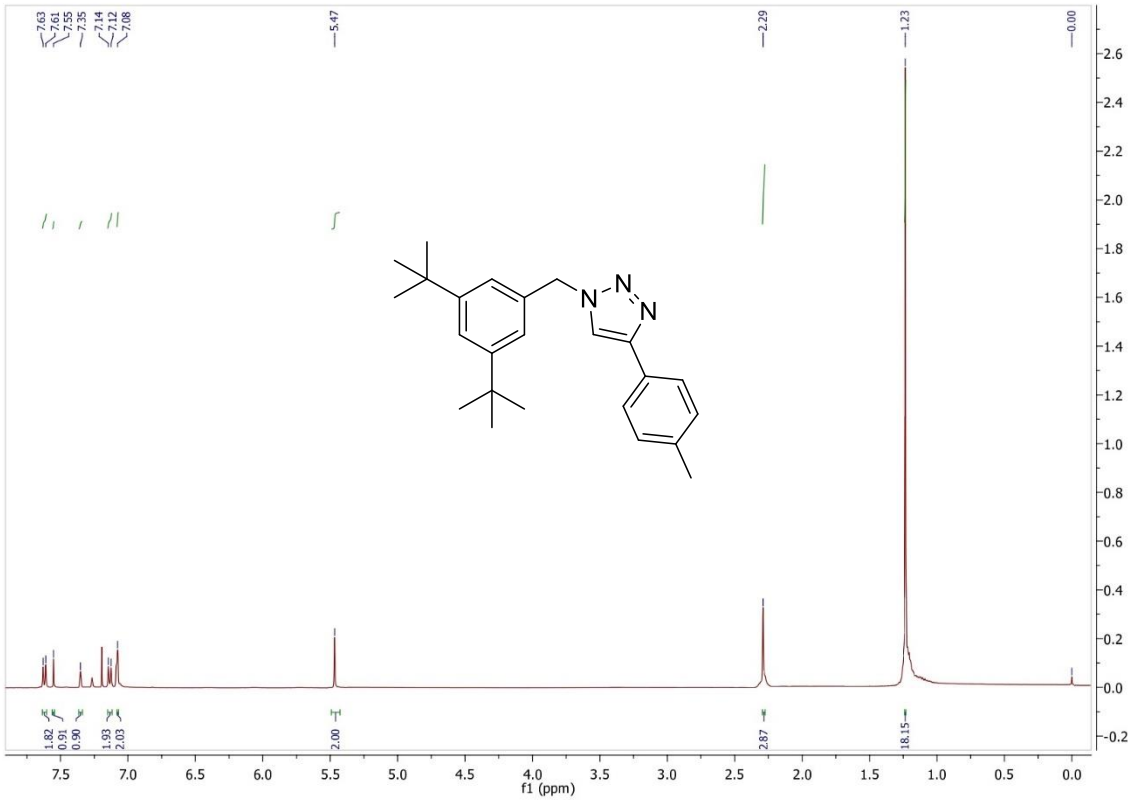
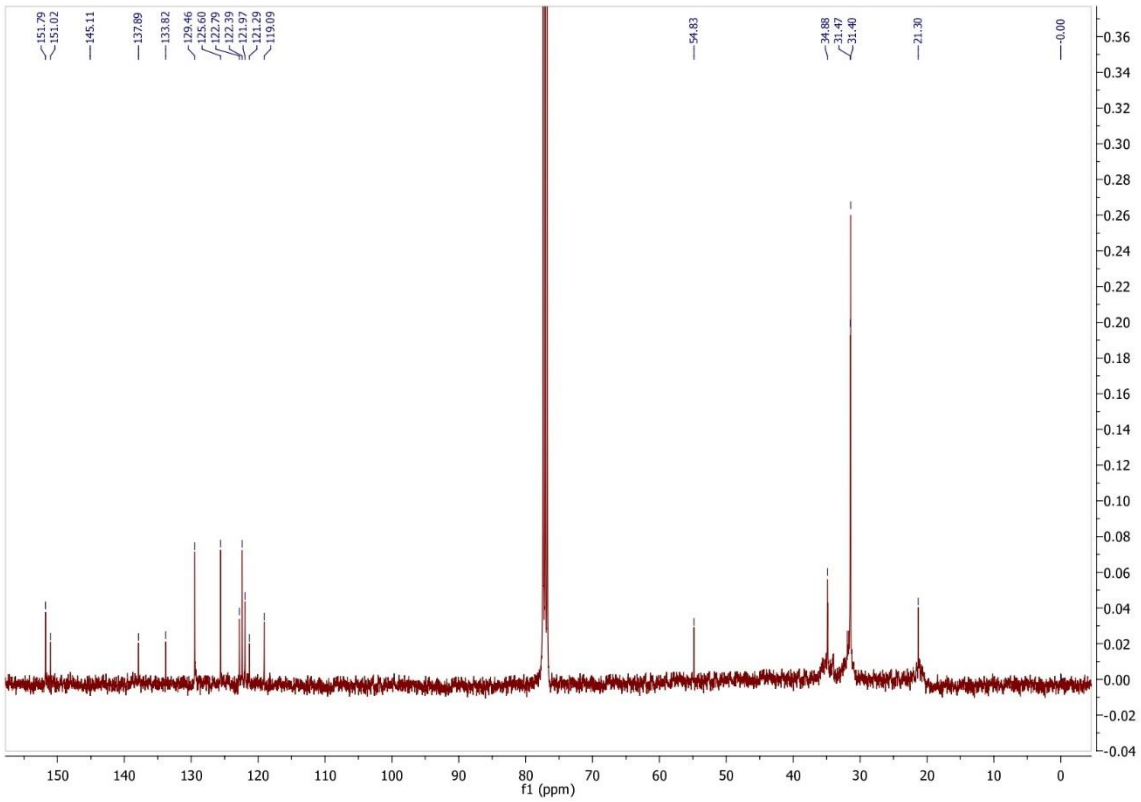
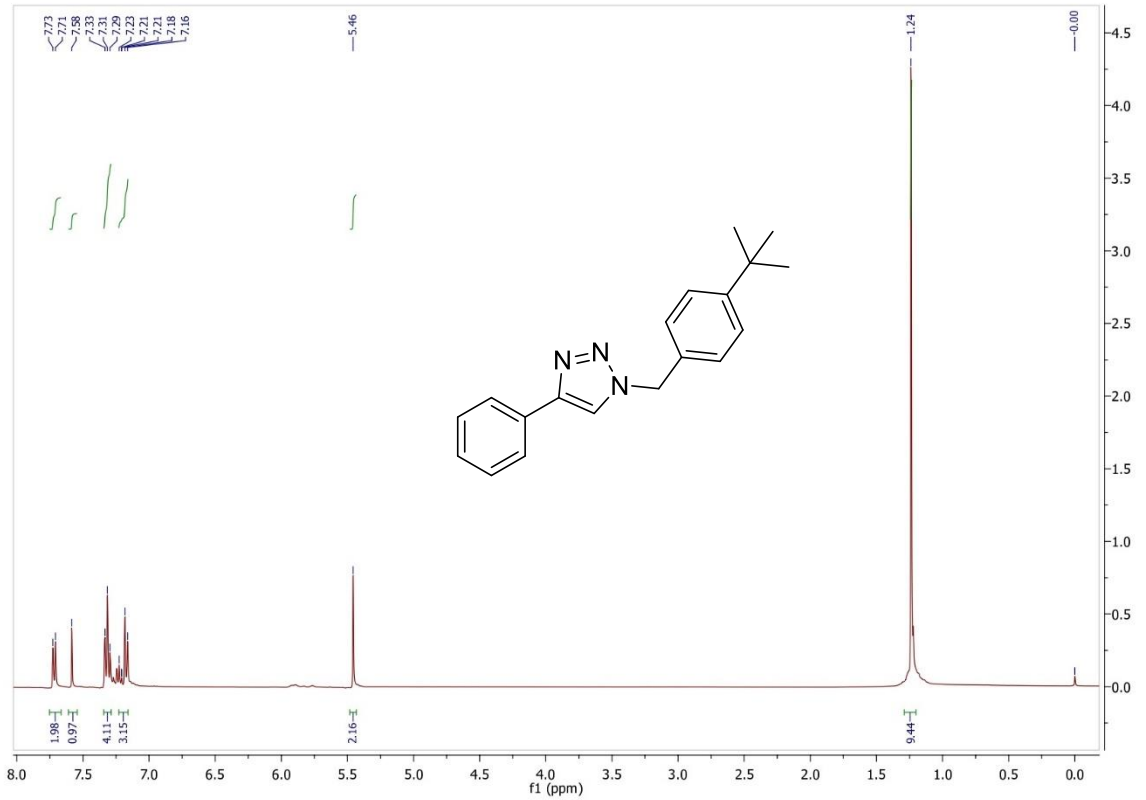


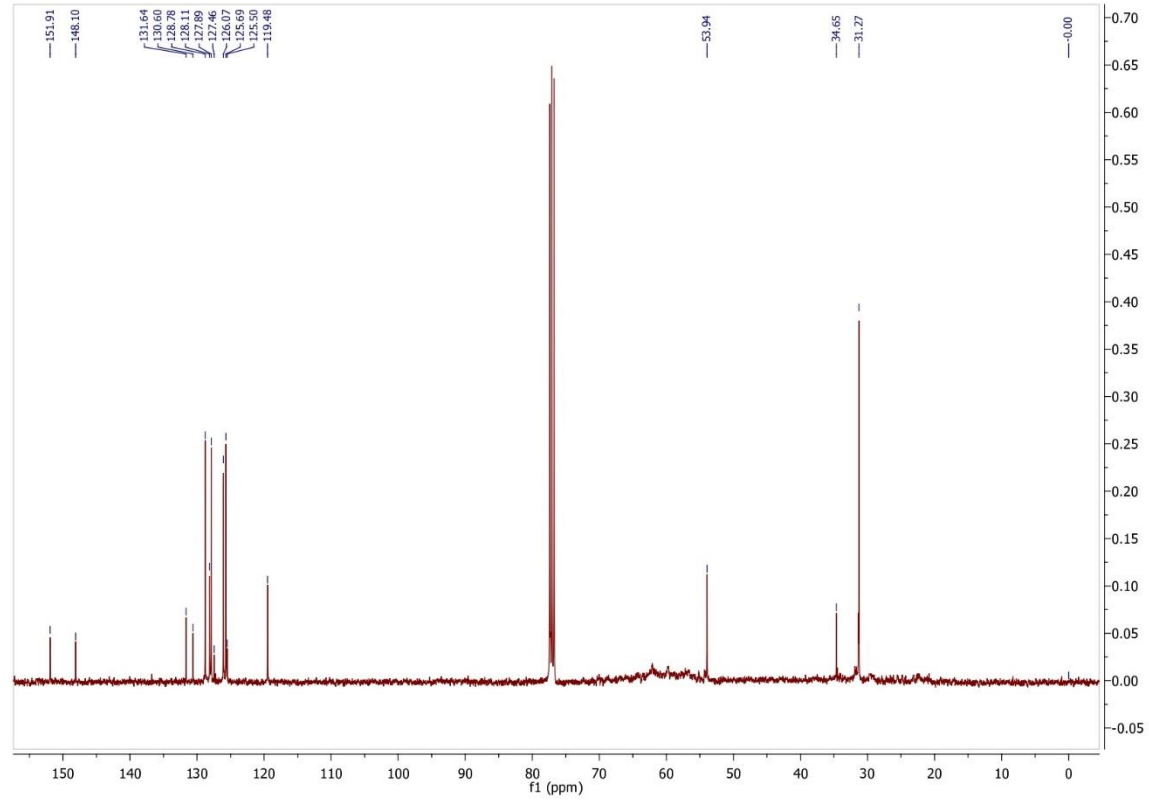
[13]C-NMR spectrum of 1-(3,5-di-tert-butylbenzyl)-4-(p-tolyl)-1H-1,2,3-triazole (3t)



^{1}H-NMR spectrum of 1-(4-(tert-butyl)benzyl)-4-phenyl-1H-1,2,3-triazole (3u)



^{13}C-NMR spectrum of 1-(4-(tert-butyl)benzyl)-4-phenyl-1H-1,2,3-triazole (3u)



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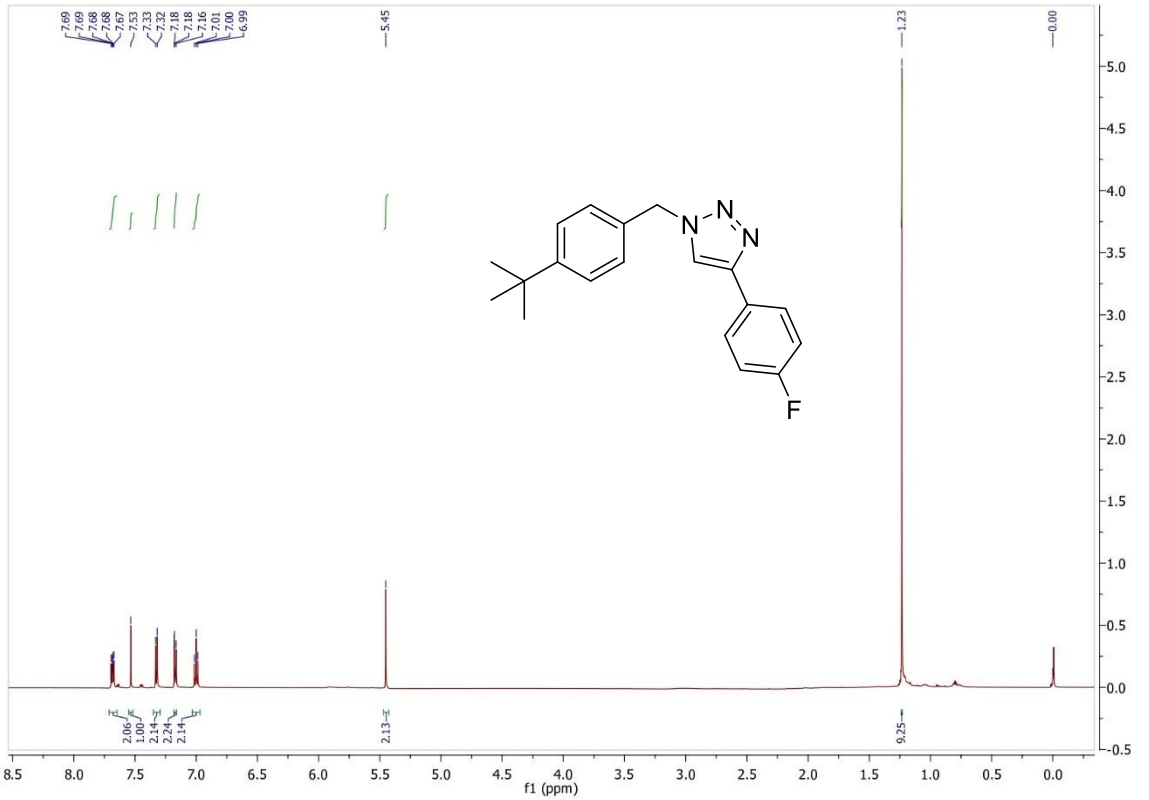
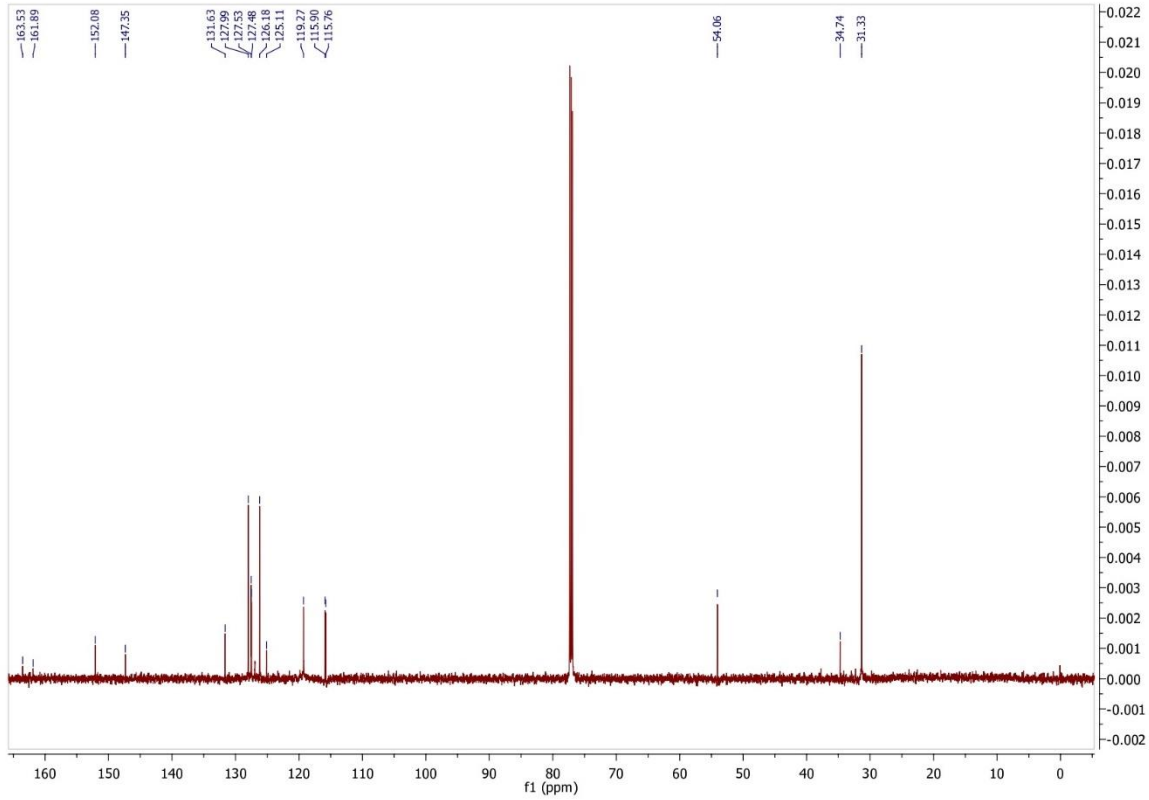
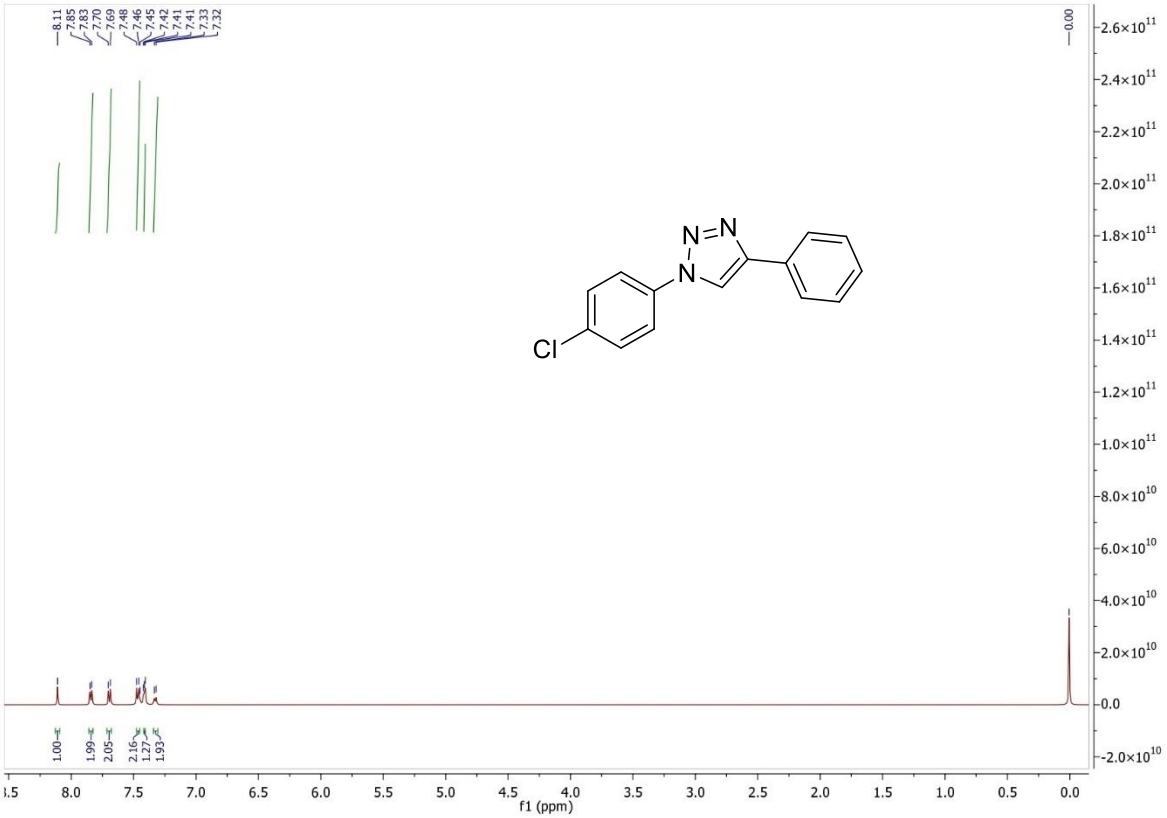


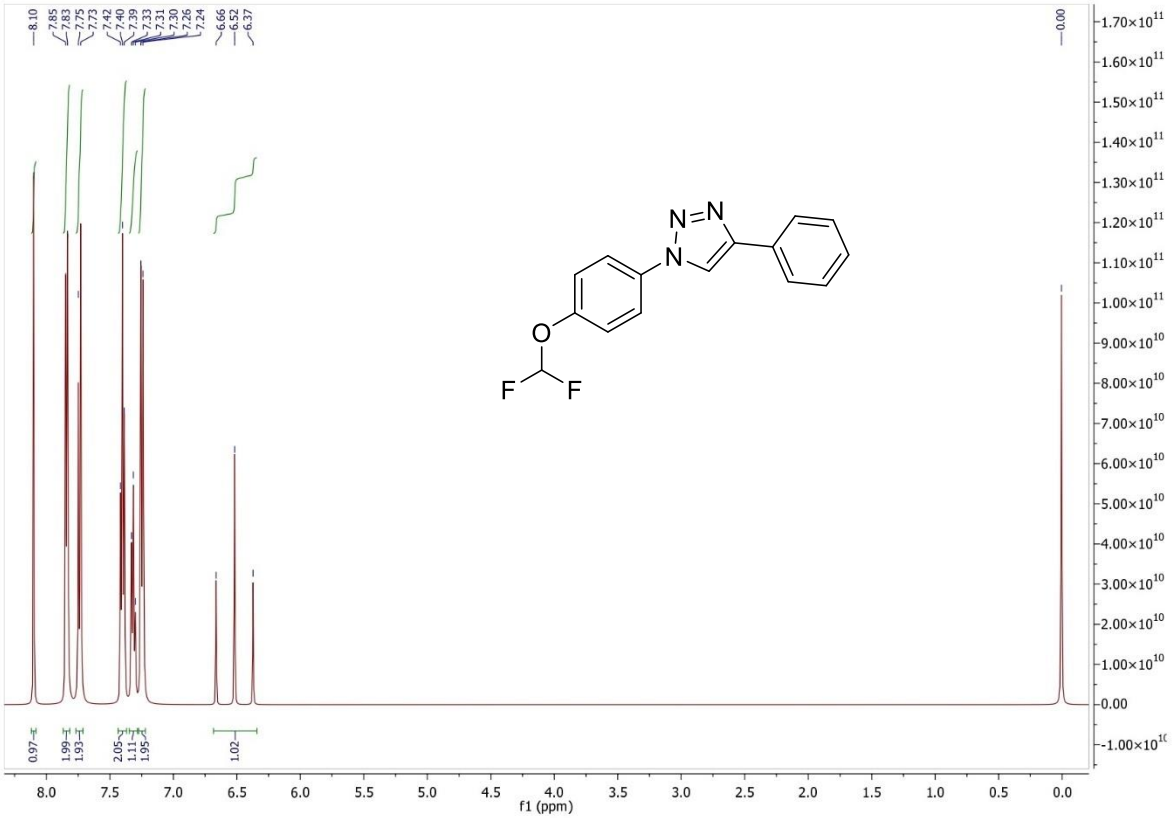
^{13}C-NMR spectrum of 1-(4-(tert-butyl)benzyl)-4-(4-fluorophenyl)-1H-1,2,3-triazole (3v)



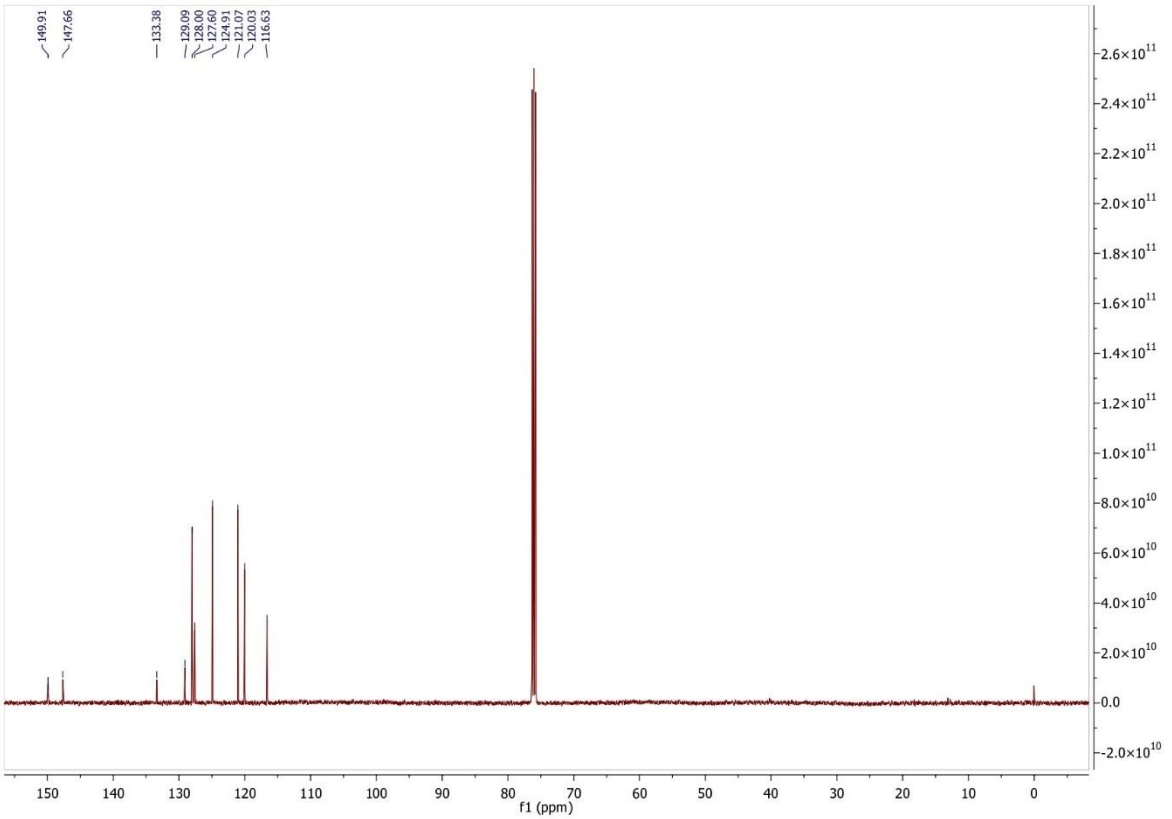
^{1}H-NMR spectrum of 1-(4-chlorophenyl)-4-phenyl-1H-1,2,3-triazole (3w)



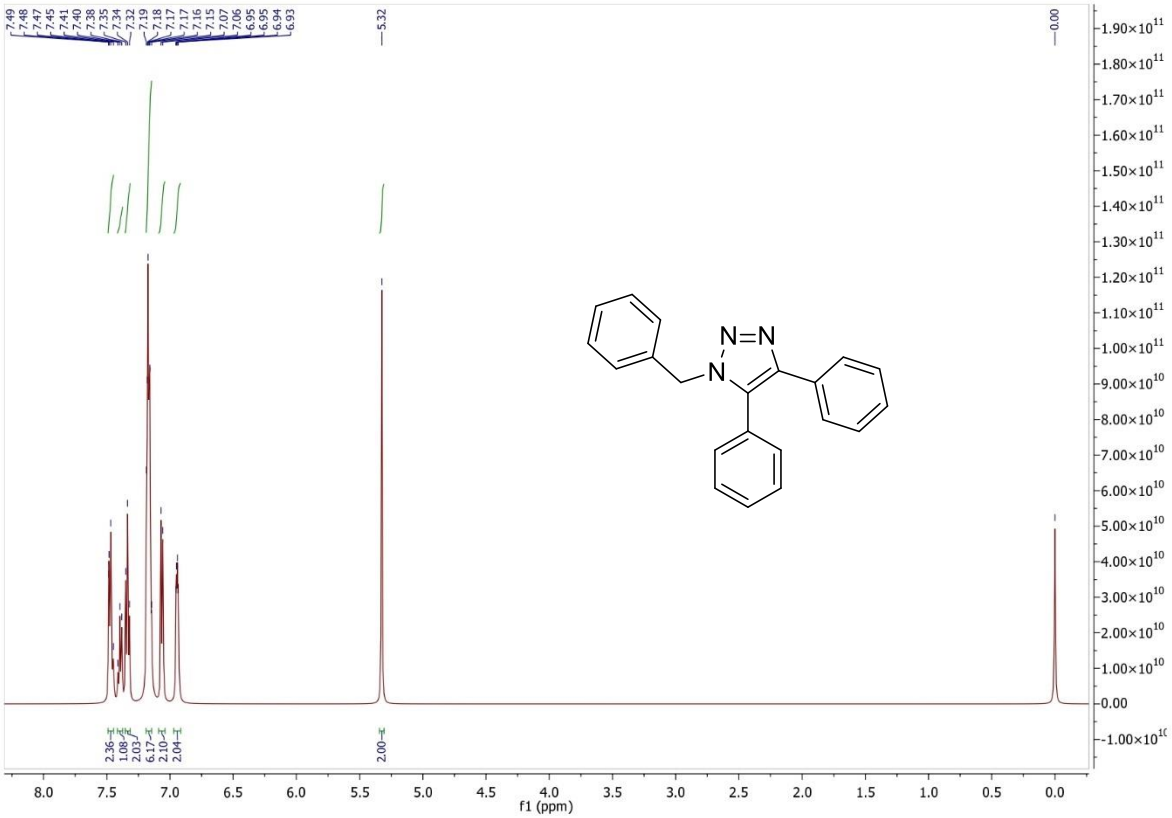
[1]H-NMR spectrum of 1-(4-(difluoromethoxy)phenyl)-4-phenyl-1H-1,2,3-triazole (3x)



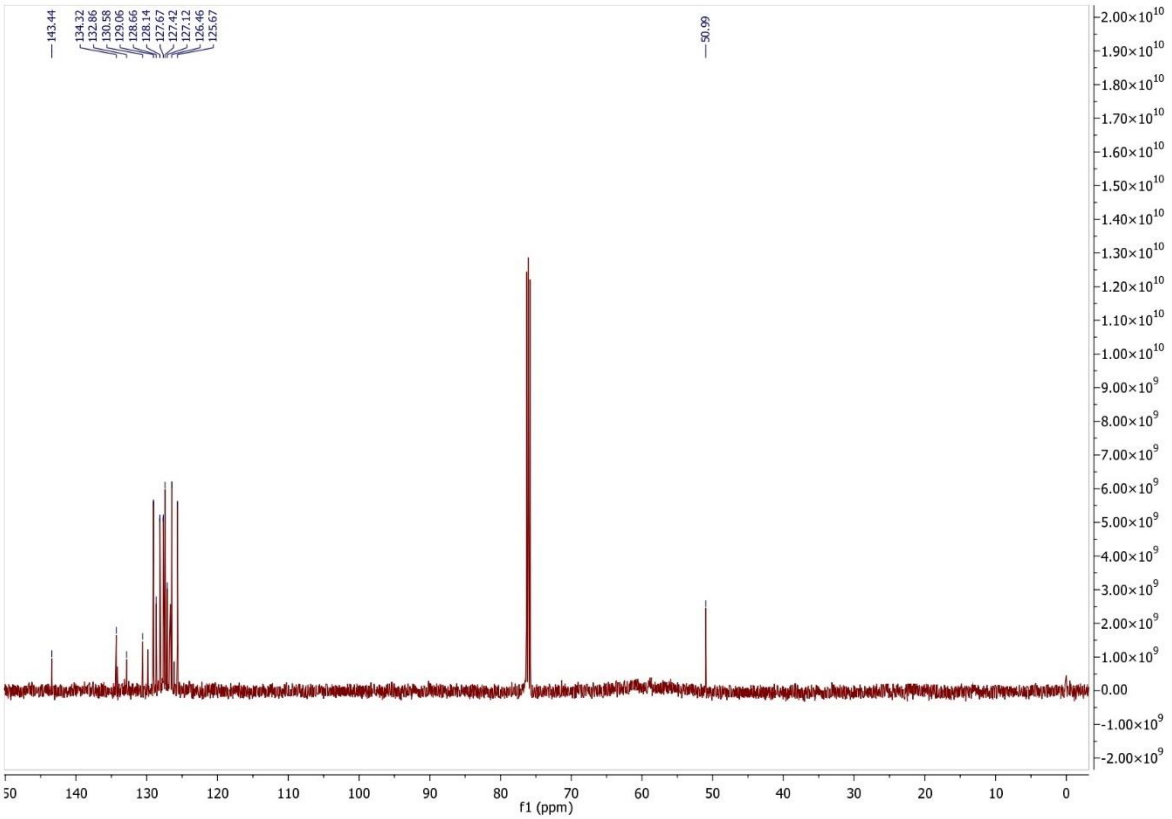
[13]C-NMR spectrum of 1-(4-(difluoromethoxy)phenyl)-4-phenyl-1H-1,2,3-triazole (3x)



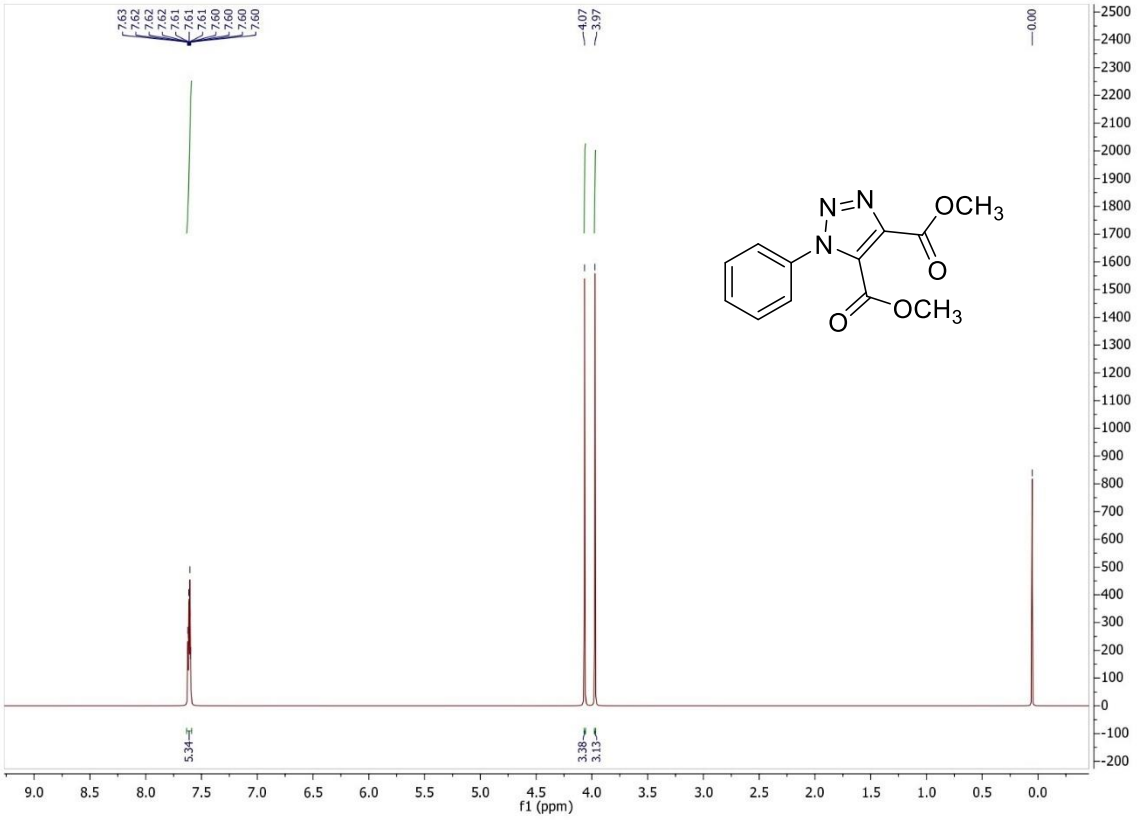
[1]H-NMR spectrum of 1-benzyl-4,5-diphenyl-1H-1,2,3-triazole (3y)



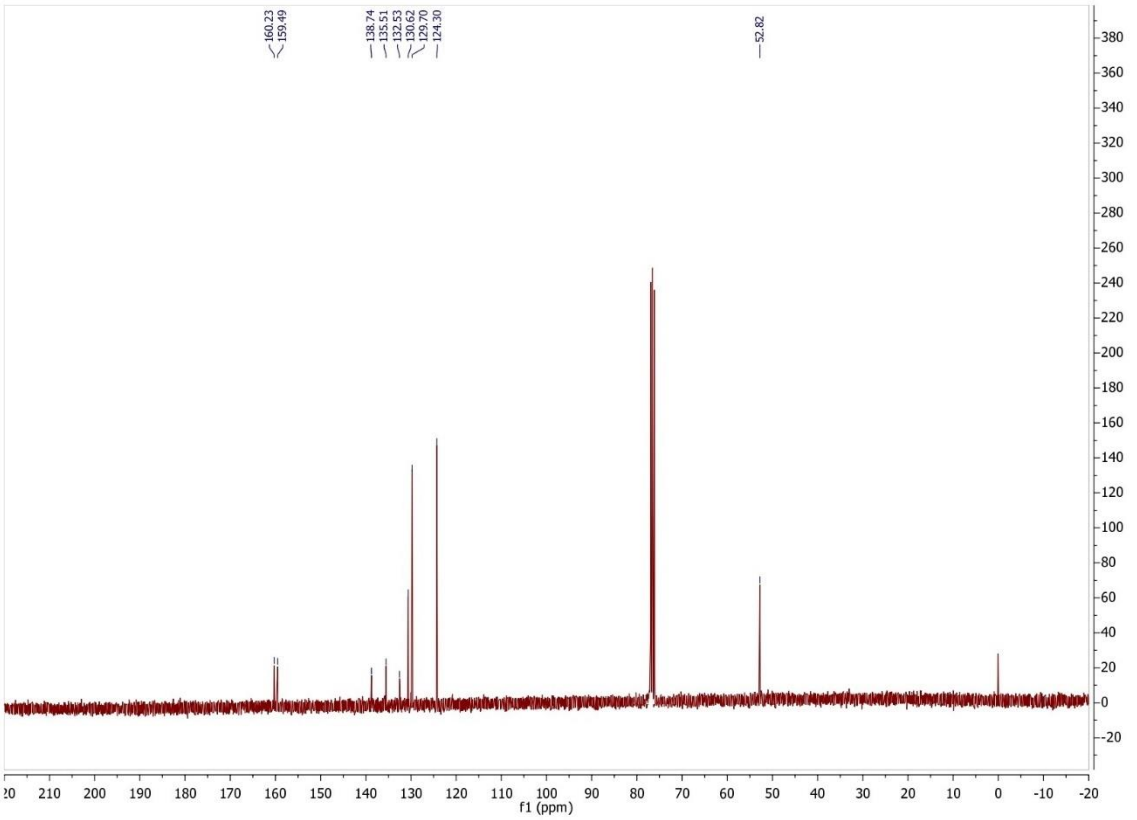
[13]C-NMR spectrum of 1-benzyl-4,5-diphenyl-1H-1,2,3-triazole (3y)



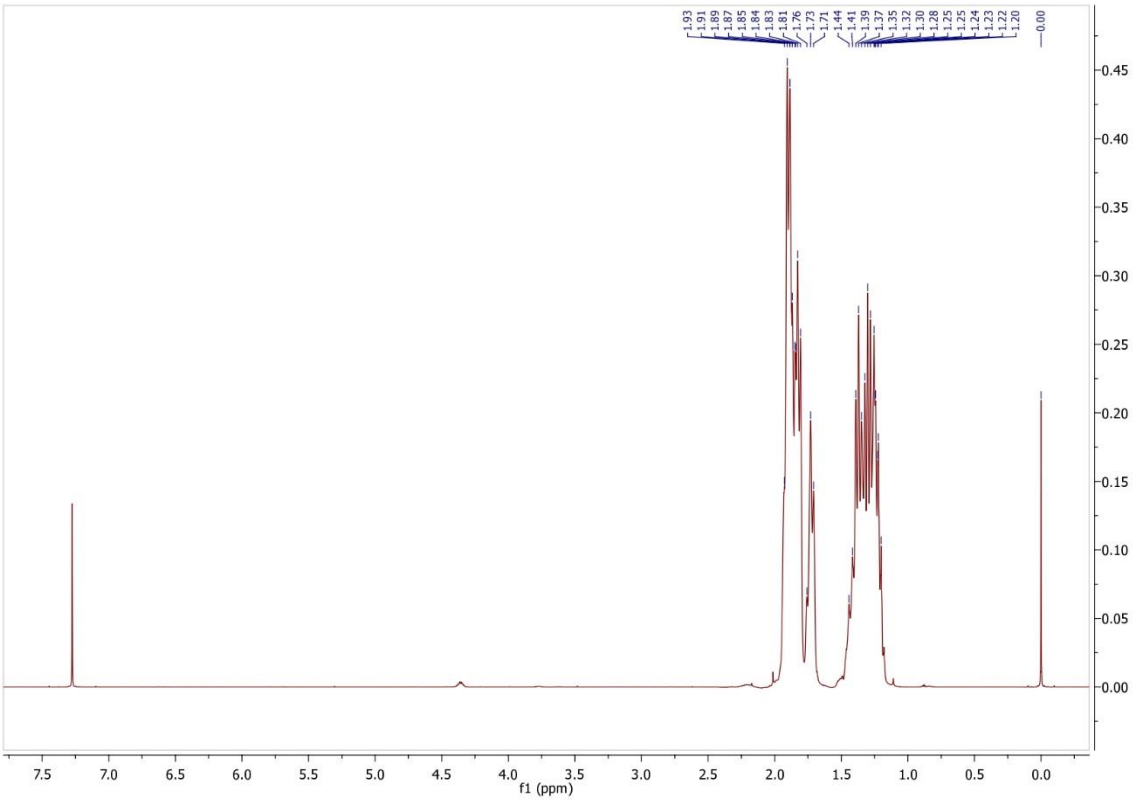
[1]H-NMR spectrum of dimethyl 1-phenyl-1H-1,2,3-triazole-4,5-dicarboxylate (3z)



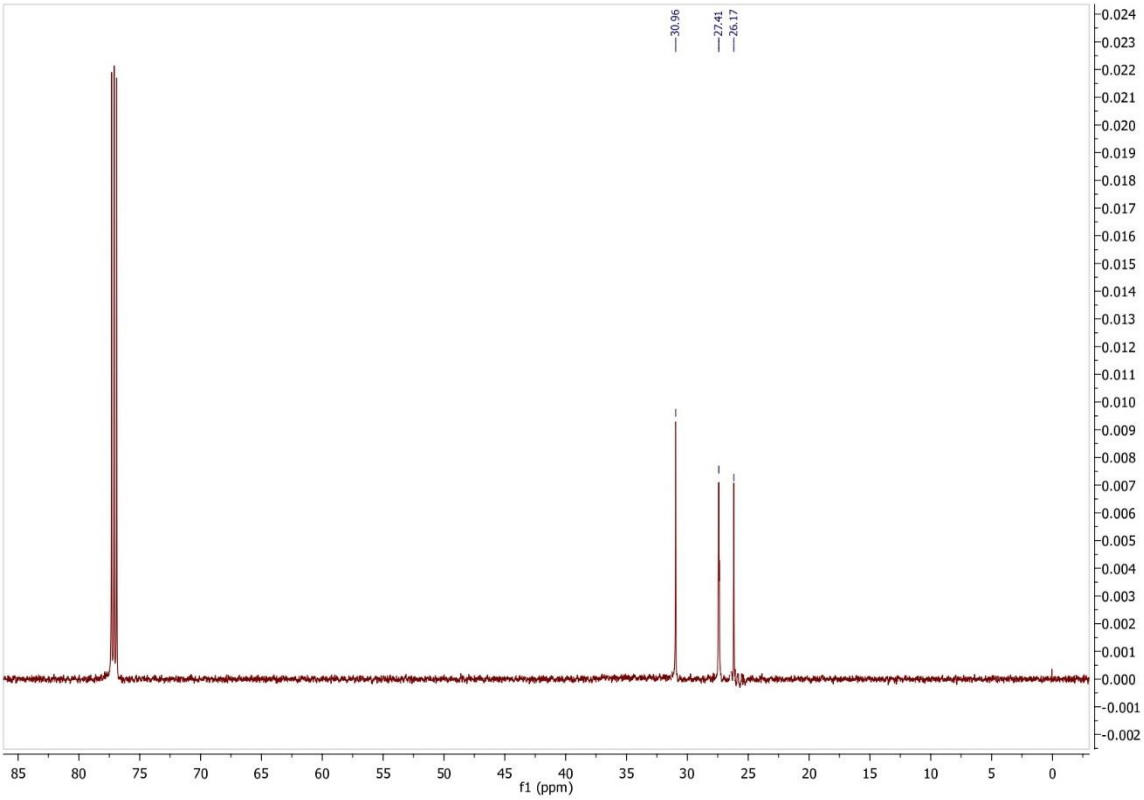
[13]C-NMR spectrum of dimethyl 1-phenyl-1H-1,2,3-triazole-4,5-dicarboxylate (3z)



^{1}H-NMR spectrum of $Ag[(PCy_3)_2]NO_3$



^{13}C-NMR spectrum of $Ag[(PCy_3)_2]NO_3$



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) BS_RN_Ag_1_0m_a

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: BS_RN_Ag_1_0m_a

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Temperature:    100 K

                 Calculated                 Reported
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Hall group       -P 1                       -P 1
Moiety formula   C36 H55 Ag N O3 P2         ?
Sum formula      C36 H55 Ag N O3 P2         C36 H55 Ag N O3 P2
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Dx,g cm-3        1.277                      1.277
Z                2                          2
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F000'            756.85
h,k,lmax         11,12,28                   11,12,28
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Tmin'            0.800

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The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

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PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of        C28 Check
PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of         N1 Check
PLAT919_ALERT_3_B Reflection # Likely Affected by the Beamstop ...          1 Check
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Alert level C

```
PLAT213_ALERT_2_C Atom O3              has ADP max/min Ratio .....        3.2 prolat
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.5 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference O2       --N1       .       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C25      --C26A     .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C28      --C29A     .       0.18 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C16 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Ag1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C14 Check
PLAT329_ALERT_4_C Carbon Atom Hybridisation Unclear for .........       C26A Check
PLAT329_ALERT_4_C Carbon Atom Hybridisation Unclear for .........       C26B Check
PLAT329_ALERT_4_C Carbon Atom Hybridisation Unclear for .........       C29A Check
PLAT329_ALERT_4_C Carbon Atom Hybridisation Unclear for .........       C29B Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00862 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.056 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          2 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          1 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..          1 Check
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.90Ang From C30     .       0.42 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.93Ang From C30     .       0.41 eA-3
```

Alert level G

```
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)       0.006 Degree
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag1      --P2       .        5.2 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag1      --O1       .        5.7 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of C26A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C26B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C29A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C29B       Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )          5% Note
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C25      - C30      .       1.51 Ang.
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C27      - C28      .       1.51 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      28.70 Deg.
             C29A -C30  -C29B    1_555   1_555   1_555 ......     #   64 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      42.50 Deg.
             C26B -C25  -C26A    1_555   1_555   1_555 ......     #   71 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      37.00 Deg.
             C26B -C27  -C26A    1_555   1_555   1_555 ......     #  205 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      32.50 Deg.
             C29B -C28  -C29A    1_555   1_555   1_555 ......     #  215 Check
```

```
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..       52.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   4 ALERT level B = A potentially serious problem, consider carefully
  20 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  19 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  17 ALERT type 2 Indicator that the structure model may be wrong or deficient
   7 ALERT type 3 Indicator that the structure quality may be low
  15 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

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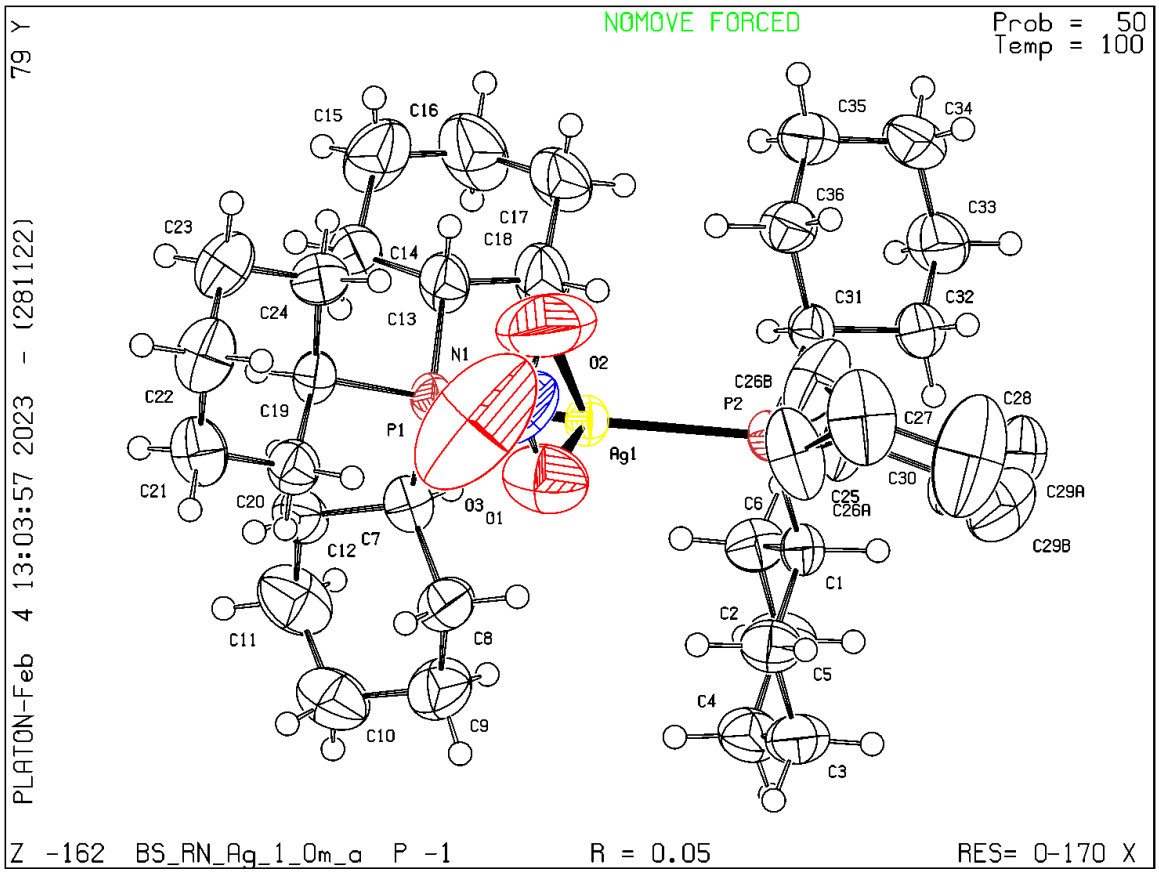
PLATON version of 28/11/2022; check.def file version of 28/11/2022

Datablock BS_RN_Ag_1_0m_a - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) BS_RHP289

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: BS_RHP289

```
Bond precision:   C-C = 0.0034 A          Wavelength=0.71073

Cell:             a=12.664(6)     b=4.767(2)            c=27.831(13)
                  alpha=90        beta=103.124(11)      gamma=90
Temperature:      100 K

                 Calculated                Reported
Volume           1636.3(13)                1636.3(13)
Space group      P 21/n                    P 21/n
Hall group       -P 2yn                    -P 2yn
Moiety formula   C17 H11 F6 N3             ?
Sum formula      C17 H11 F6 N3             C17 H11 F6 N3
Mr               371.29                    371.29
Dx,g cm-3        1.507                     1.507
Z                4                         4
Mu (mm-1)        0.139                     0.139
F000             752.0                     752.0
F000'            752.57
h,k,lmax         15,5,34                   15,5,34
Nref             3216                      3165
Tmin,Tmax        0.972,0.982               0.971,0.981
Tmin'            0.958

Correction method= # Reported T Limits: Tmin=0.971 Tmax=0.981
AbsCorr = MULTI-SCAN

Data completeness= 0.984           Theta(max)= 25.999

R(reflections)= 0.0458( 2082)                wR2(reflections)=
                                             0.1100( 3165)
S = 1.003                Npar= 281
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT213_ALERT_2_B Atom F5B has ADP max/min Ratio ..... 4.2 prolat

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Alert level C

PLAT213_ALERT_2_C Atom F9 has ADP max/min Ratio ..... 3.2 prolat
PLAT234_ALERT_4_C Large Hirshfeld Difference F8 --C8 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F5B --C7 . 0.22 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C18 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C12 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including F1 0.110 Check
PLAT331_ALERT_2_C Small Aver Phenyl C-C Dist C12 --C17 . 1.37 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 3.428 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 52 Report

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Alert level G

PLAT019_ALERT_1_G _diffrn_measured_fraction_theta_full/*_max < 1.0 0.998 Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT230_ALERT_2_G Hirshfeld Test Diff for F1 --C7 . 6.0 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for F6 --F7 . 10.8 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for F6 --F10 . 7.7 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for F7 --F8 . 25.0 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for F8 --F9 . 8.2 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for F9 --F10 . 40.9 s.u.
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C7 Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F1 Constrained at 0.73 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F2 Constrained at 0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F3 Constrained at 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F6 Constrained at 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F7 Constrained at 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F8 Constrained at 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F9 Constrained at 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F10 Constrained at 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F4 Constrained at 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F5 Constrained at 0.27 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F5B Constrained at 0.25 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 23% Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.16 Ratio
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 37.00 Deg.
F1 -C7 -F5 1_555 1_555 1_555 ..... # 40 Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 1 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 50 Note
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 52.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

---

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Datablock BS_RHP289 - ellipsoid plot