Electronic Supplementary Material (ESI) for RSC Sustainability.

Sustainable synthesis of 1,4-disubstituted and N-unsubstituted 1,2,3-triazoles via reusable ZnO-CTAB nanocrystals

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Supporting Information

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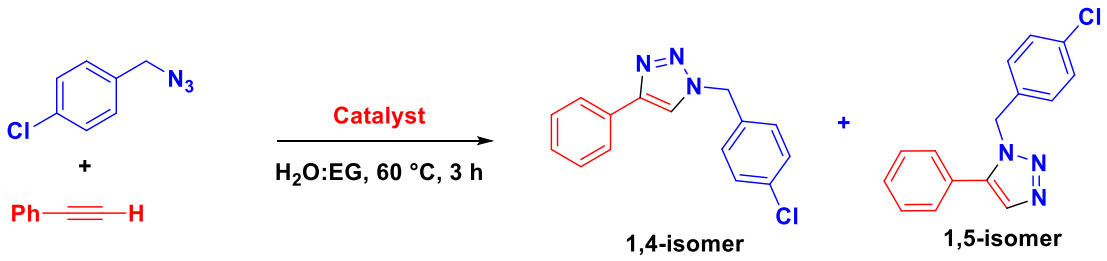
1. General Information

All experiments were done in oven dried glasswares. The reagents and solvents were purchased from commercial suppliers and used without any further purification. All reported products refer to isolated yield of pure products. The NMR were recorded in $CDCl_3$ solvent using TMS as an internal standard The chemical shifts of the analyzed products are informed in parts per million (ppm) and splitting patterns are assigned as: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet). Thermo Scientific Endura LC/MS mass spectrometer has been used for recording mass spectra of the products.

2. Table S1: Controlled Reaction[a]



Serial no.	Catalyst	1,4 and 1,5 isomers ratio	Yield (%)[b]
1	ZnO (without stabilized with CTAB)	80:20	60
2	ZnO-CTAB calcined	100:0	98
3	ZnO-CTAB	100:0	99

[a]*Reaction conditions: 4-chlorobenzylazide (1 mmol), phenylacetylene (1.2 mmol) , H_2O:EG (3 ml), catalyst (5 mg) .*[b]*Isolated Yields*

3. Characterization of ZnO-CTAB nanocrystals

The SEM analysis of the synthesized ZnO-CTAB nanocatalyst features a cloudy hazy like structures as can be seen from **Figure S1**.

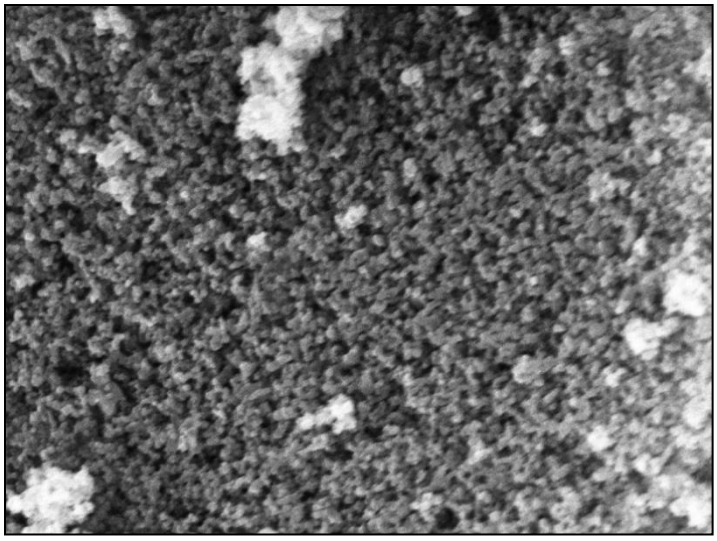
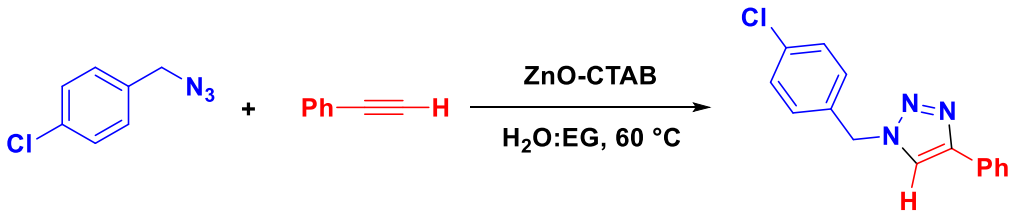


Figure S1*: SEM image of the Synthesized ZnO-CTAB nanoparticles*

4.1. Atom economy calculation:

$$\%\text{Atom Economy} = \frac{\text{Formula weight (FW) of atoms utilized}}{\text{Formula weight (FW) of all reactants used in the reaction}} \text{ x } 100\%$$

In the direct azide-alkyne cycloaddition reaction **(Scheme 2 & 3)**, the 1,4-disubstituted 1,2,3-triazoles are formed without the production of any byproducts. Hence, the atom economy of all the triazoles would be almost 100%. For instance,



	Reactants		Utilized		Unutilized	
	Formula	FW	Formula	FW	Formula	FW
	$C_7H_6ClN_3$	167.03	$C_{15}H_{12}ClN_3$	269.07	-	-

	C_8H_6	102.05			-	-
Total		269.08		269.07		

$$\%\text{Atom Economy} = \frac{\text{Formula weight of atoms utilized}}{\text{Formula weight of all reactants used in the reaction}} \text{ x } 100\%$$

$$= \frac{269.07}{269.08} \times 100\%$$

$$=100\%$$

The % atom economy of the other 1,4-disubstituted 1,2,3- triazoles products of **Scheme 2** are as follows:

Entry	**% Atom economy**	**Entry**	**% Atom economy**
3a	99	3e	100
3b	99	3f	100
3c	99	3g	100
3d	99		

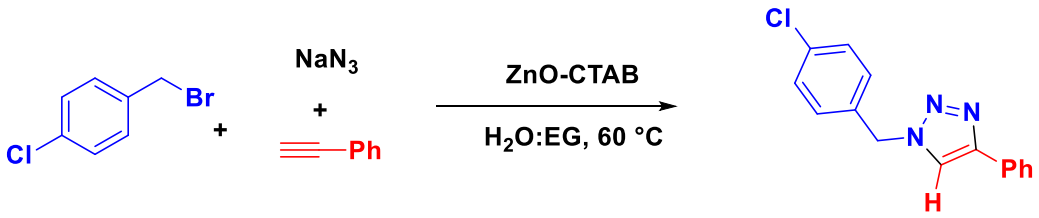
The atom economy of the,2,3- triazoles products of **Scheme 3** are shown below:

Entry	**% Atom economy**	**Entry**	**% Atom economy**
6a	100	6l	100
6b	100	6m	100
6c	100	6n	100
6d	100	6o	100
6e	100	6p	100
6f	100	6q	100
6g	100	6r	100
6h	100	6s	100
6i	100	6t	100
6j	100	6u	100

6k	100	6v	100

Atom econonmy calculation for the One-pot method:

During the one-pot three component reaction, NaBr is released along with the product. Hence, the atom economy of this zinc catalyzed reaction will be as follows:



Reactants		**Utilized**		**Unutilized**	
Formula	**FW**	**Formula**	**FW**	**Formula**	**FW**
C_7H_6ClBr	205.93	$C_{15}H_{12}ClN_3$	269.07	NaBr	101.91
C_8H_6	102.05				
NaN_3	65.00				
Total	372.98		269.07	NaBr	

$$\%\text{Atom Economy} = \frac{\text{Formula weight of atoms utilized}}{\text{Formula weight of all reactants used in the reaction}} \text{ x } 100\%$$

$$= \frac{269.07}{372.98} \times 100\%$$

=72.14%

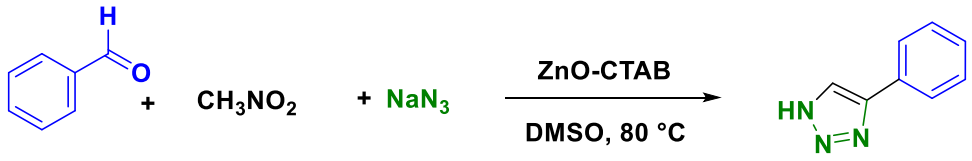
The calculated atom economy of the other triazole derivatives (Scheme 4, Entry 9a-9h) are as follows:

Entry	**% Atom economy**	**Entry**	**% Atom economy**
9a	73.59	9e	76.29
9b	75.43	9f	72.52

9c	69.76	9g	74.58
9d	76.24	9h	73.32

Atom econonmy calculation for N-unsubstituted 1,2,3-triazole:

For the one-pot multicomponent synthesis of N-unsubstituted 1,2,3-triazole, $NaNO_2$ is released during the reaction. Hence, the atom economy of the reaction will be as follows:



Reactants		Utilized		Unutilized	
Formula	**FW**	**Formula**	**FW**	**Formula**	**FW**
C_7H_6O	106.04	$C_7H_6N_3$	145.06	$NaNO_2$	68.98
CH_3NO_2	61.02				
NaN_3	65.00				
Total	232.06		145.06		68.98

$$\%\text{Atom Economy} = \frac{\text{Formula weight of atoms utilized}}{\text{Formula weight of all reactants used in the reaction}} \text{ x } 100\%$$

$$= \frac{145.06}{232.06} \times 100\%$$

=62.52%

Entry	% Atom economy	Entry	% Atom economy
14a	66.30	14f	71.09
14b	65.22	14g	73.85
14c	64.65	14h	63.49

14d	69.42	14i	60.83
14e	72.02	14j	66.30

The calculated atom economy for 1,4,5-trisubstituted 1,2,3-triazole derivatives **(Scheme 6, Entry 17a-17c)** are as follows:

Entry	**% Atom economy**	**Entry**	**% Atom economy**
17a	100	17c	100
17b	100		

(10) Use of reactants and solvents allows to improve sustainability scores. To prove that E-factor and Eco-scale should be given for these ZnAAC reactions.

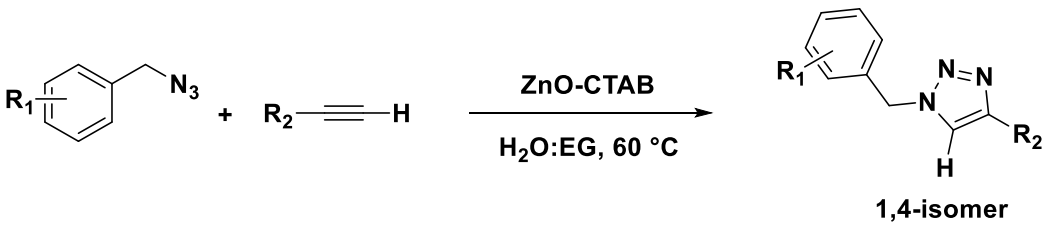
4.2. Environmental factor (E-factor)

The E-factor of a reaction is a simple metric to define how green a reaction is and is defined as the ratio of mass of waste per mass of product.

$$\text{E factor} = \frac{\text{mass of total waste}}{\text{mass of product}}$$

$$\text{Or E factor} = \frac{\text{mass used} - \text{mass recovered}}{\text{mass of product}}$$

<u>Procedure for the synthesis of 1,4-disubstituted 1,2,3-triazoles (Scheme 2)</u>



The as-synthesized catalyst (5 mg) was added to a mixture of substituted benzylazide (1 mmol) and alkyne (1.2 mmol) in H_2O:EG reaction medium (6: 1 ratio, 3 ml) at room temperature. Then, the reaction mixture was heated in an oil bath at constant temperature of 60 °C for 3-4 h. After that, the reaction mixture was allowed to cool and the product was extracted by adding ethyl acetate (1 ml) and water (1 ml). The solvent was evaporated under reduced pressure. The final product was purified by column chromatography over silica gel using hexane/ethyl acetate mixture and the products obtained were characterized by NMR and mass spectroscopy.

E-factor calculation for the synthesis of 1,4-disubstituted 1,2,3-triazoles (Scheme 2, Entry 3a):

Substrate: Benzylazide (1 mmol) = 0.133 g

Phenylacetylene (1.2 mmol) = 0.122 g

Catalyst: ZnO-CTAB = 0.005 g

Solvent: Water + ethylene glycol (3 ml) = 3g

Wash solvent (ethyl acetate + water, 2 ml) = 2 g

Product: 1,4-disubstituted 1,2,3-triazoles = 0.232 g

$$\text{E factor} = \frac{\text{mass used} - \text{mass recovered}}{\text{mass of product}}$$

$$\text{E factor} = \frac{(0.133 + 0.122 + 0.005 + 3 + 2) - (0.232 + 5)}{0.232}$$

$$\text{E factor} = 0.12$$

The calculated E-factor for the other triazoles are as follows (**Scheme 2,** Entry 3a-3g):

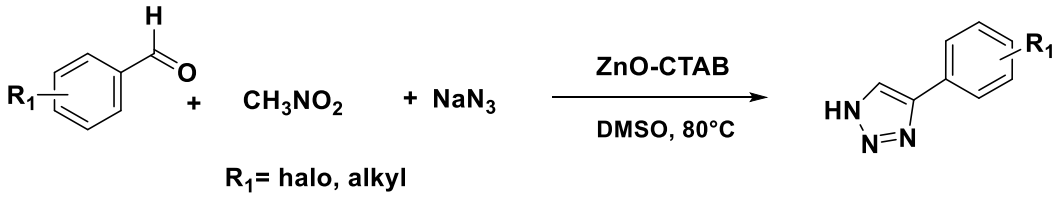
Entry	**E-factor**	**Entry**	**E-factor**
3a	0.12	3e	0.20
3b	0.12	3f	0.11
3c	0.26	3g	0.57

3d	0.11

The calculated E-factor for the triazoles (**Scheme 3,** Entry 6a-6v) are as follows:

Entry	**E-factor**	**Entry**	**E-factor**
6a	0.10	6l	0.28
6b	0.39	6m	0.08
6c	0.14	6n	0.40
6d	0.13	6o	0.20
6e	0.21	6p	0.18
6f	0.13	6q	0.08
6g	0.15	6r	0.11
6h	0.15	6s	0.11
6i	0.11	6t	0.14
6j	0.19	6u	0.09
6k	0.12	6v	0.12

Procedure for the synthesis of N-unsubstituted-1,2,3-triazoles (Scheme 5, entry 14a-14k)



The aromatic aldehyde (1 mmol), nitroalkane (2 mmol), sodium azide (3 mmol) and catalyst (5 mg) were stirred in a round-bottom flask containing 3 ml of DMSO solvent at 80 °C. The progress of the reactions was checked by TLC. After completion of the reaction, the mixture was cooled to room temperature and extracted with ethyl acetate (4 × 10 ml). The filtrate was evaporated to dryness under reduced pressure. The final product was purified by column chromatography over silica gel using hexane/ethyl acetate mixture and the products obtained

were characterized by NMR and mass spectroscopy. The recovered catalyst was washed with hot ethanol, dried and reused.

E-factor calculation for the synthesis of N-unsubstituted 1,2,3-triazoles (Scheme 5, entry 14k):

Substrate: Benzaldehyde (1 mmol) = 0.106 g

Nitromethane (2 mmol) = 0.122 g

Sodium azide (3 mmol) = 0.195 g

Catalyst: ZnO-CTAB = 0.005 g

Solvent: DMSO (3 ml) = 3g

Wash solvent (ethyl acetate + water, 2 ml) = 2 g

Product: N-unsubstituted 1,2,3-triazoles = 0.232 g

$$\text{E factor} = \frac{\text{mass used} - \text{mass recovered}}{\text{mass of product}}$$

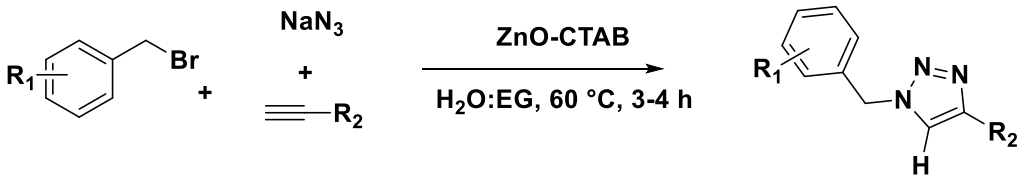
$$\text{E factor} = \frac{(0.106 + 0.122 + 0.195 + 0.005 + 3 + 2) - (0.123 + 5)}{0.123}$$

$$\text{E factor} = 2.40$$

The calculated E-factor for the other N-unsubstituted 1,2,3-triazoles are as follows:

Entry	E-factor	Entry	E-factor
14a	1.75	14f	1.40
14b	2.20	14g	2.84
14c	2.42	14h	2.32
14d	1.61	14i	2.37
14e	1.39	14j	2.40

Procedure for the synthesis of 1,4-disubstituted 1,2,3-triazoles-One-Pot method (Scheme 4, entry 9a-9h)



In this case, benzyl bromide (1 mmol), sodium azide (2 mmol) and phenyl acetylene (1.2 mmol) are added simultaneously to a solution of water-ethylene glycol (6:1. 3 ml) with the catalyst (5 mg) and reacted at 60 °C for 3-4 h. The product obtained was then extracted with ethylacetate and purified using column chromatography. The final products were characterized by NMR and mass spectroscopy.

E-factor calculation (Scheme 4, entry 9b)

Substrate: 4-Bromobenzylbromide (1 mmol) = 0.249 g

Phenylacetylene (1.2 mmol) = 0.121 g

Sodium azide (2 mmol) = 0.130 g

Catalyst: ZnO-CTAB = 0.005 g

Solvent: Water + ethylene glycol (3 ml) = 3g

Wash solvent (ethyl acetate + water, 2 ml) = 2 g

Product: 1,4-disubstituted 1,2,3-triazoles = 0.267 g

$$\text{E factor} = \frac{\text{mass used} - \text{mass recovered}}{\text{mass of product}}$$

$$\text{E factor} = \frac{(0.249 + 0.121 + 0.130 + 0.005 + 3 + 2) - (0.267 + 5)}{0.267}$$

$$\text{E factor} = 0.89$$

The calculated E-factor for the other triazoles are as follows:

Entry	E-factor	Entry	E-factor
9a	0.97	9e	1.27
9b	0.89	9f	0.99
9c	1.13	9g	0.82
9d	0.70	9h	1.24

The calculated E-factor of the other 1,4,5-trisubstituted 1,2,3-triazole derivatives (**Scheme 6, Entry 17a-17c**) are as follows:

Entry	E-factor	Entry	E-factor
17a	0.18	17c	0.21
17b	0.22		

4.3 Eco-Scale

The eco-scale of the above protocol has been calculated using Van-Aken et.al. quantitative tool. On the basis of this analytical score, the greenness of the methodology can be determined. For, eco-score above 75 are considered excellent green methods, above 50 acceptable green methods and below 50 as inadequate greenness. (**Ref: S5**)

Serial no.	Parameter	Values	Penalty points (Scheme 2,3,4,5&6)
1	Yield	(100-99)/2= 0.5	0.5
2	Price of reaction component	Inexpensive	0
3	Safety	Non-toxic	0
4	Technical setup	Common setup	0
5	Temperature	Heating, >1h	3
6	Workup and purification	Extraction with AcOEt Silica gel column chromatography	3 10

Total penalty points	16.5
***Based on the hazard warning symbols**	

Eco-scale = 100- sum of individual penalties

= 100-16.5

= 83.5

As per the above results, it can be concluded that theses ZnAAC reactions have a low E-factor, high atom-economy and high eco-scale value. These values clearly indicate the eco-friendliness of the present work.

5. Single Crystal XRD Studies:

The single crystal data collections were carried out using a Bruker D-8 Quest diffractometer with a photon detector (Mo Kα: 0.71073 Å, monochromator: graphite). Frames were collected at room temperature by ω, φ, and 2θ rotation at 3 s per frame. The SAINT software was used to integrate the measured intensities. Structure solution, refinement and data output were carried out using the inbuilt SHELXTL-2018 program. Non-hydrogen atoms were refined anisotropically. C–H hydrogen atoms were placed in geometrically calculated positions by using a riding model. Images were created by using the ORTEP program.

Crystal data and structure refinements for the crystals are summarized below:

For H1: $C_{15}H_{12}N_3Cl$, Mr = 269.73, monoclinic, space group P21/c, a = 5.6930(6), b = 8.6279(9), c = 26.812(3) Å, α = 90, β = 90.943(3), γ = 90°, V = 1316.8(2) $Å^3$, Z = 4, D_{calc} = 1.361 g cm^{-3}, μ = 0.278 mm^{-1}, T = 297(2) K, total of 29359 collected reflections, 2002 unique reflections (R_{int} = 0.0271), 2305 observed reflections [I > 2r(I)], R_1(obs) = 0.0412, wR_1(obs) = 0.1253, R_2(all) = 0.0486, wR_2(all) = 0.1405. CCDC = 1028453

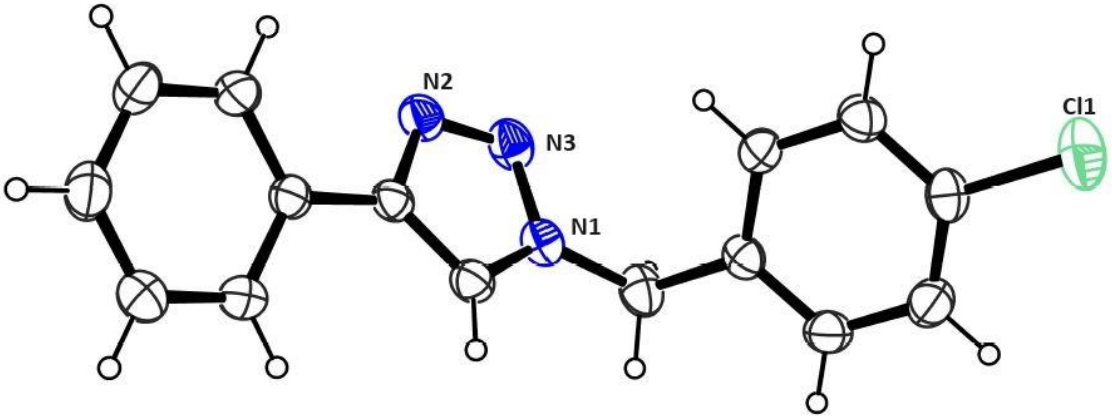
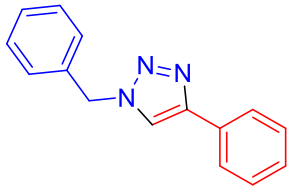


Figure S2*: Ortep diagram of H1 (thermal ellipsoid with 30% probability)*

6. Characterization datas of 1,2,3-triazole derivatives

1-benzyl-4-phenyl-1H-1,2,3-triazole **(Scheme 3, Entry 3a) Ref: S1**

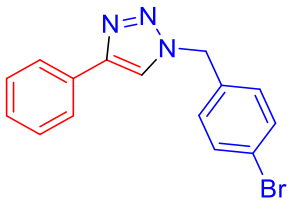


White solid, MS (ESI) m/z: 236.25 $[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.80 (d, *J* = 7.3 Hz, 2H), 7.66 (s, 1H), 7.41 – 7.36 (m, 5H), 7.31 (d, *J* = 7.0 Hz, 3H), 5.57 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ: 54.3, 119.6, 125.8, 128.2, 128.3, 128.9, 129.3, 130.6, 134.8, 148.3.

1-(4-bromobenzyl)-4-phenyl-1H-1,2,3-triazole **(Scheme 2, entry 3b) Ref: S2**

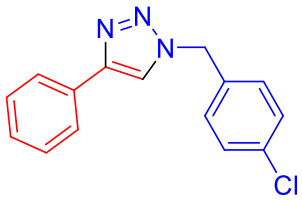


Light yellow Solid; MS (ESI) m/z: 315.21 $[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.81 (d, *J* = 7.1 Hz, 2H), 7.70 (s, 1H), 7.53 (d, *J* = 8.4 Hz, 2H), 7.33 (t, *J* = 6.8 Hz, 1H), 7.20 (d, *J* = 8.5 Hz, 2H), 6.96 (d, *J* = 8.5 Hz, 2H), 5.55 (s, 2H)

^{13}C NMR (125 MHz, $CDCl_3$) δ: 53.4, 119.4, 125.6, 128.2, 128.7, 128.8, 129.0, 129.6, 131.9, 132.2, 133.2, 133.6, 134.3, 148.3.

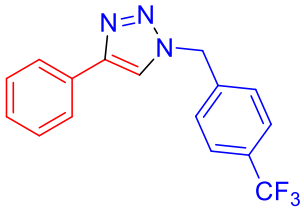
1-(4-chlorobenzyl)-4-phenyl-1H-1,2,3-triazole **(Scheme 2, entry 3d) Ref: S4**



Yellow Solid; MS (ESI) m/z: 271.10 $[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.82 (d, *J* = 7.8 Hz,2H), 7.69 (S, 1H), 7.46 – 7.43 (m, 3H), 7.38 (d, *J* = 8.3 Hz, 2H), 7.02 (d, *J* = 8.3 Hz, 2H), 5.53 (s, 2H).

1-benzyl-4-(4-(trifluoromethyl)phenyl)-1H-1,2,3-triazole **(Scheme 2, entry 3e)**

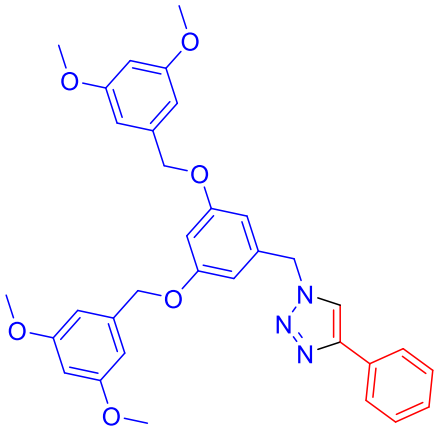


Pale yellow Solid; MS (ESI) m/z: 304.15 $[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.83 (d, *J* = 7.7 Hz, 2H), 7.72 (s, 1H), 7.67 (d, *J* = 7.9 Hz, 2H), 7.46 – 7.41 (m, 4H), 7.35 (d, *J* = 7.4 Hz, 1H), 5.67 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ: 53.6, 119.5, 122.7, 124.9, 125.8, 126.1, 126.2, 126.2, 126.2, 128.2, 128.4, 128.9, 130.3, 131.0, 138.7, 148.6.

1-(3,5-bis((3,5-dimethoxybenzyl)oxy)benzyl)-4-phenyl-1H-1,2,3-triazole **(Scheme 2, entry 3g)**

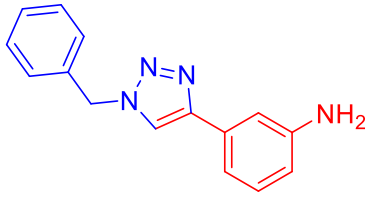


White solid; MS (ESI) m/z: 568.20 $[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.82 (d, *J* = 7.3 Hz, 2H), 7.76 – 7.72 (m, 1H), 7.69 (s, 1H), 7.56 – 7.54 (m, 1H), 7.39 (dt, *J* = 16.4, 7.9 Hz, 5H), 7.28 (d, *J* = 2.6 Hz, 2H), 6.59 (s, 2H), 6.44 (s, 1H), 5.57 (s, 2H), 5.02 (d, *J* = 31.5 Hz, 4H), 3.82 (s, 12H).

^{13}C NMR (125 MHz, $CDCl_3$) δ: 55.4, 61.7, 70.1, 102.2, 105.2, 107.3, 125.8, 127.6, 128.9, 131.0, 136.8, 138.8, 160.4, 161.0.

3-(1-benzyl-1H-1,2,3-triazol-4-yl)aniline **(Scheme 3, entry 6b)**

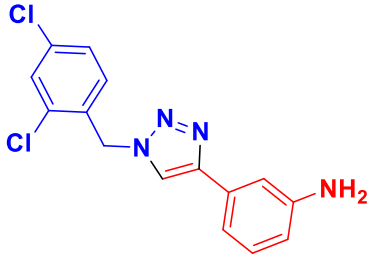


Yellow Solid, MS (ESI) m/z: 251.19 $[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.63 (s, 1H), 7.34 (s, 5H), 7.19 (s, 1H), 7.12 (s, 1H), 7.09 (d, *J* = 7.6 Hz, 1H), 6.61 (d, *J* = 7.1 Hz, 1H), 5.50 (s, 2H), 4.49 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ: 54.1, 112.2, 115.8, 119.9, 127.6, 128.1, 128.2, 129.8, 129.9, 130.6, 131.3, 131.4, 134.8, 147.1, 148.3.

3-(1-(2,4-dichlorobenzyl)-1H-1,2,3-triazol-4-yl)aniline **(Scheme 3, entry 6c)**

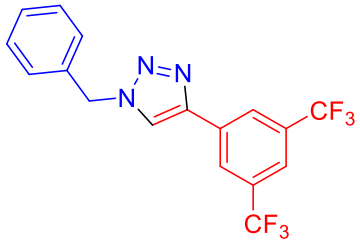


Yellow solid; MS (ESI) m/z: 320.12 $[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.72 (s, 1H), 7.40 (s, 1H), 7.18 (d, *J* = 10.6 Hz, 2H), 7.08 (dd, *J* = 22.6, 10.1 Hz, 3H), 6.62 (d, *J* = 6.1 Hz, 1H), 5.56 (s, 2H), 4.88 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ: 50.8, 112.4, 115.4, 116.1, 120.3, 128.0, 129.7, 129.9, 131.1, 131.3, 134.1, 135.4, 146.7, 148.1.

1-benzyl-4-(3,5-bis(trifluoromethyl)phenyl)-1H-1,2,3-triazole **(Scheme 3, Entry 6d)**

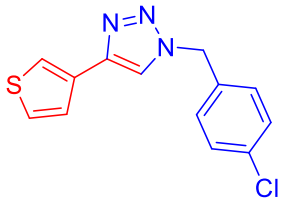


White solid, MS (ESI) m/z: 372.23 $[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.83 (d, *J* = 7.7 Hz, 2H), 7.72 (s, 1H), 7.67 (d, *J* = 7.9 Hz, 2H), 7.46 – 7.41 (m, 4H), 7.35 (d, *J* = 7.4 Hz, 1H), 5.67 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ: 53.6, 119.5, 122.7, 124.9, 125.8, 126.1, 126.2, 126.2, 126.2, 128.2, 128.4, 128.9, 130.3, 131.0, 138.7, 148.6.

1-(4-chlorobenzyl)-4-(thiophen-3-yl)-1H-1,2,3-triazole **(Scheme 3, entry 6e)**

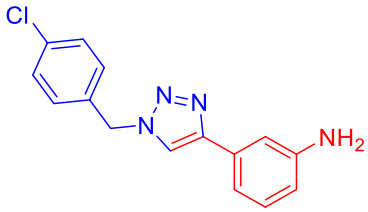


Yellow Solid; MS (ESI) m/z: 277.05 $[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.67 (d, *J* = 1.7 Hz, 1H), 7.60 (s, 1H), 7.43 (dd, *J* = 5.0, 1.3 Hz, 1H), 7.38 – 7.37 (m, 1H), 7.35 (d, *J* = 8.5 Hz, 2H), 7.23 (d, *J* = 8.5 Hz, 2H), 5.53 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ: 53.4, 119.4, 121.3, 125.8, 125.8, 126.5, 129.4, 131.6, 133.2, 134.8, 144.6.

3-(1-(4-chlorobenzyl)-1H-1,2,3-triazol-4-yl)aniline **(Scheme 3, entry 6g)**

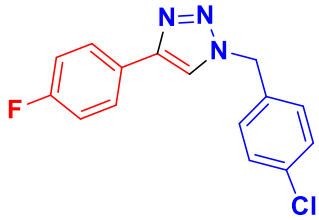


White Solid; MS (ESI) m/z: 286.12 $[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.62 (s, 1H), 7.36 (d, *J* = 6.8 Hz, 3H), 7.21 (s, 1H), 7.17 – 7.13 (m, 2H), 7.10 (d, *J* = 7.6 Hz, 1H), 6.63 (d, *J* = 7.5 Hz, 1H), 5.53 (s, 2H), 3.83 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ: 54.3, 112.4, 115.2, 116.1, 119.9, 128.2, 128.2, 128.9, 129.3, 129.9, 131.5, 134.9, 147.1, 148.4.

1-(4-chlorobenzyl)-4-(4-fluorophenyl)-1H-1,2,3-triazole (**Scheme 3, entry 6h**)



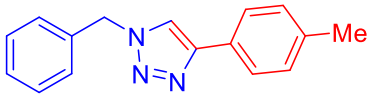
White solid, MS (ESI) m/z: 288.07 $[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.76 (dd, *J* = 8.6, 5.4 Hz, 2H), 7.63 (s, 1H), 7.35 (d, *J* = 8.4 Hz, 2H), 7.24 (d, *J* = 8.4 Hz, 2H), 7.08 (t, *J* = 8.6 Hz, 2H), 5.53 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 162.8 (d, *J* = 247.8 Hz), 161.9, 147.6, 135.0, 133.2, 129.4, 127.5 (d, *J* = 7.9 Hz), 126.7, 126.7, 119.2, 115.9 (d, *J* = 21.7 Hz), 53.5.

^{19}F NMR (470 MHz, $CDCl_3$) δ: -106.57.

1-benzyl-4-(p-tolyl)-1H-1,2,3-triazole **(Scheme 3, entry 6i) Ref: S4**

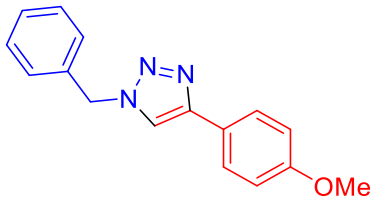


Pale yellow solid; MS (ESI) m/z: 329.19 $[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.70 (d, *J* = 9.5 Hz, 1H), 7.68 (s, 1H), 7.48 (d, *J* = 8.1 Hz, 1H), 7.18 (dd, *J* = 226.1, 8.2 Hz, 7H), 5.49 (s, 2H), 2.36 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ: 21.3, 53.4, 119.3, 122.9, 125.6, 127.6, 128.7, 128.9, 129.6, 129.7, 132.0, 132.2, 133.9, 134.61, 138.1, 139.9, 148.4.

1-benzyl-4-(4-methoxyphenyl)-1H-1,2,3-triazole **(Scheme 3, Entry 6j) Ref: S4**

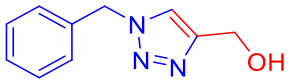


White solid, MS (ESI) m/z: 266.09 $[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.75 (d, 2H), 7.61 (s, 1H), 7.37-7.40 (m, 3H), 7.31-7.33 (d, 2H), 6.95 (d, 2H), 7.31 (s, 2H), 3.84 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ: 54.1, 55.2, 114.1, 118.7, 123.2, 126.9, 128.0, 128.3, 129.1, 134.7, 148.1.

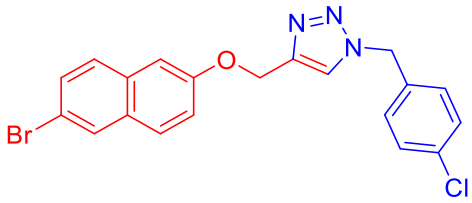
(1-benzyl-1H-1,2,3-triazol-4-yl)methanol **(Scheme 3, entry 6l)**



MS (ESI) m/z: 190.10 $[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.43(s, 1H), 7.37 (dd, *J* = 5.1, 1.8 Hz, 4H), 7.26(t, 1H), 5.30 (s, 2H), 4.77(s, 2H), 5.16 (s, 1H).

4-(((6-bromonaphthalen-2-yl)oxy)methyl)-1-(4-chlorobenzyl)-1H-1,2,3-triazole **(Scheme 3, entry 6m)**

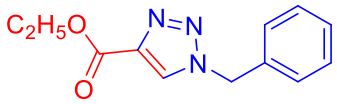


Light yellow Solid; MS (ESI) m/z: 427.12 $[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.92 (s, 1H), 7.67–7.56 (m, 3H), 7.53–7.49 (m, 1H), 7.35 (d, *J* = 8.3 Hz, 2H), 7.25–7.16 (m, 4H), 5.51 (s, 2H), 5.30 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ: 53.5, 62.1, 107.3, 117.5, 119.8, 122.7, 128.6, 128.7, 129.4, 129.5, 129.6, 129.8, 130.2, 132.9, 132.9, 134.9, 144.5, 156.4.

Ethyl 1-benzyl-1H-1,2,3-triazole-4-carboxylate **(Scheme 3, entry 6o)**



MS (ESI) m/z: 232.16 $[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.91 (s, 1H), 7.32 (dd, *J* = 5.2, 2.0 Hz, 3H), 7.23 – 7.20 (m,2H), 5.51 (s, 2H), 4.32 (q, *J* = 7.2 Hz, 2H), 1.31 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ: 14.2, 54.4, 61.2, 76.7, 76.9, 77.2, 127.3, 128.2, 129.1, 129.2, 133.6, 140.5, 160.6.

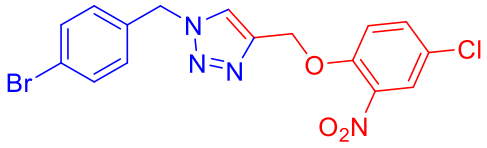
1-(4-bromobenzyl)-4-((4-iodophenoxy)methyl)-1H-1,2,3-triazole **(Scheme 3, entry 6p)**

Yellow solid, MS (ESI) m/z: 470.80 $[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.62 – 7.48 (m, 5H), 7.16 (d, *J* = 8.2 Hz, 2H), 6.76 (d, *J* = 8.7 Hz, 2H), 5.50 (s, 2H), 5.17 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ: 53.6, 62.1, 83.6, 117.2, 122.7, 123.1, 129.7, 132.4, 133.4, 138.3, 144.4, 158.0.

1-(4-bromobenzyl)-4-((4-chloro-2-nitrophenoxy)methyl)-1H-1,2,3-triazole **(Scheme 3, entry 6s)**



Yellow Solid; MS (ESI) m/z: 421.83$[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.82 (d, *J* = 2.6 Hz, 1H), 7.68 (s, 1H), 7.53 – 7.47 (m, 3H), 7.31 (s, 1H), 7.16 (d, *J* = 8.3 Hz, 2H), 5.50 (s, 2H), 5.34 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ: 53.7, 64.0, 116.9, 123.3, 125.6, 126.2, 129.7, 132.4, 133.4, 134.1, 143.3, 150.2.

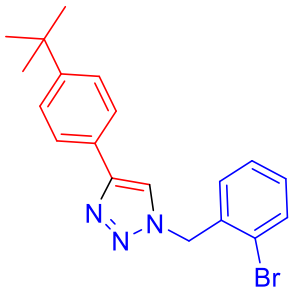
1-benzyl-4-((4-iodophenoxy)methyl)-1H-1,2,3-triazole **(Scheme 3, entry 6t)**

White Solid, MS (ESI) m/z: 392.14 $[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.47 (d, *J* = 8.5 Hz, 2H), 7.44 (s, 1H), 7.30 (s, 2H), 7.20 (d, *J* = 8.1 Hz, 2H), 6.67 (d, *J* = 8.5 Hz, 2H), 5.46 (s, 2H), 5.08 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ: 54.3, 62.1, 83.5, 117.2, 122.6, 127.1, 128.1, 128.9, 129.2, 134.4, 138.3, 144.2, 158.1.

1-(2-bromobenzyl)-4-(4-(tert-butyl)phenyl)-1H-1,2,3-triazole **(Scheme 3, entry 6u)**

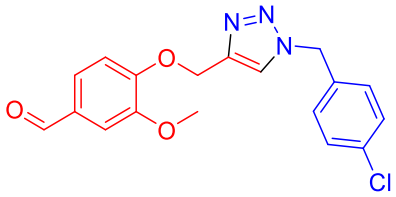


White solid; MS (ESI) m/z: 371.12 $[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.78 (d, *J* = 7.2 Hz, 3H), 7.64 (d, *J* = 7.9 Hz, 1H), 7.46 (d, *J* = 8.3 Hz, 2H), 7.32 (t, *J* = 7.3 Hz, 1H), 7.24 (t, *J* = 7.0 Hz, 1H), 7.16 (d, *J* = 7.6 Hz, 1H), 5.71 (s, 2H), 1.36 (s, 9H).

^{13}C NMR (125 MHz, $CDCl_3$) δ: 31.3, 34.7, 53.9, 119.7, 123.4, 125.5, 125.8, 127.6, 128.3, 130.2, 130.4, 133.2, 134.4, 148.2, 151.4.

4-((1-(4-chlorobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)-3-methoxybenzaldehyde **(Scheme 3, entry 6v)**

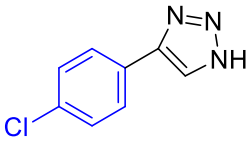


Yellow Semi-liquid; MS (ESI) m/z: 359.19 $[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ: 9.80 (s, 1H), 7.63 (s, 1H), 7.41 – 7.31 (m, 3H), 7.18 (q, *J* = 8.7, 8.2 Hz, 4H), 5.47 (s, 2H), 5.31 (s, 2H), 3.85 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ: 53.5, 56.0, 62.7, 109.3, 112.5, 123.3, 129.1, 129.3, 129.5, 130.6, 132.8, 134.9, 143.7, 149.9, 153.0, 191.1.

4-(4-chlorophenyl)-1H-1,2,3-triazole **(Scheme 5, entry 14a)** (**Ref: 29**)

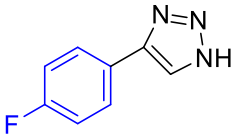


Yellow solid, MS (ESI) m/z: 180.03 $[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.45 (s, 1H), 7.94 (s, 1H), 7.76 (d, *J* = 8.2 Hz, 2H), 7.42 (d, *J* = 8.4 Hz, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ: 127.3, 129.0, 129.2, 129.8, 130.0, 155.9

4-(4-fluorophenyl)-1H-1,2,3-triazole **(Scheme 5, entry 14b)**



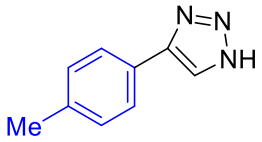
White solid, MS (ESI) m/z: 164.03 $[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.43 (s, 1H), 7.95 (s, 1H), 7.72 (s, 2H), 7.27 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ: 117.0 (d , *J* = 21.7 Hz), 126.0, 129.7, 129.8 (d, *J* = 8.4 Hz), 142.81, 163.9, 164.9 (d, *J* = 250.0 Hz).

^{19}F NMR (470 MHz, $CDCl_3$) δ: -109.88.

4-(p-tolyl)-1H-1,2,3-triazole **(Scheme 5, entry 14c)**

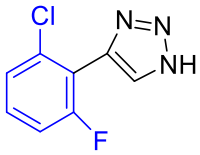


Dark Red, MS (ESI) m/z: 160.11 $[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.43 (s, 1H), 7.95 (s, 1H), 7.72 (d, *J* = 7.9 Hz, 2H), 7.25 (d, *J* = 18.1 Hz, 2H), 1.28 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ: 21.3, 126.1, 126.9, 128.6, 129.7, 138.7, 146.7

4-(2-chloro-6-fluorophenyl)-1H-1,2,3-triazole **(Scheme 5, entry 14d)**



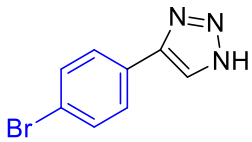
Pale yellow solid, MS (ESI) m/z: 198.02 $[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ: 12.56 (s, 1H), 8.05 (s, 1H), 7.33 – 6.99 (m, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ: 160.6 (d, *J* = 252.0 Hz), 159.6, 136.7, 134.5, 134.4, 130.5 (d, *J* = 9.7 Hz), 130.5, 126.0, 125.9 (d, *J* = 3.4 Hz), 117.8 (d, *J* = 16.9 Hz), 114.6 (d, *J* = 22.8 Hz).

^{19}F NMR (470 MHz, $CDCl_3$) δ: -109.76.

4-(4-bromophenyl)-1H-1,2,3-triazole **(Scheme 5, entry 14e)** (**Ref: 29**)

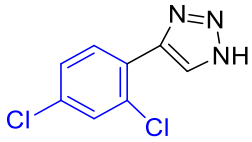


Yellow solid, MS (ESI) m/z: 223.90 $[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.45 (s, 1H), 7.93 (s, 1H), 7.69 (d, *J* = 8.4 Hz, 2H), 7.56 (d, *J* = 8.4 Hz, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ: 76.8, 77.1, 77.3, 127.6, 128.8, 129.2, 132.1, 175.3, 175.8.

4-(2,4-dichlorophenyl)-1H-1,2,3-triazole **(Scheme 5, entry 14f)**

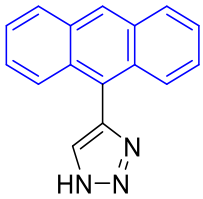


Yellow solid, MS (ESI) m/z: 213.91 $[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ: 10.29 (s, 1H) 8.24 (s, 1H), 7.89 (d, *J* = 8.4 Hz, 1H), 7.34 (d, *J* = 8.2 Hz, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ: 127.4, 129.1, 129.5, 130.0, 130.7, 130.9.

4-(anthracen-9-yl)-1H-1,2,3-triazole **(Scheme 5, entry 14g)**



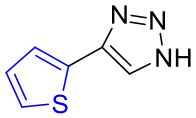
Light yellow, MS (ESI) m/z: 256.05 $[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ: 9.7 (s, 1H), 8.57 (s, 1H), 8.37 (d, *J* = 8.8 Hz, 1H), 8.07 (s, 1H), 7.95 (d, *J* = 16.7 Hz, 1H), 7.71 (s, 1H), 7.67 (d, *J* = 8.8 Hz, 1H), 7.43 (s, 4H).

^{13}C NMR (125 MHz, $CDCl_3$) δ: 111.3, 112.1, 118.7, 118.9, 126.6, 127.1, 132.4, 132.9, 134.6, 146.2.

4-(thiophen-2-yl)-1H-1,2,3-triazole **(Scheme 5, entry 14h)**

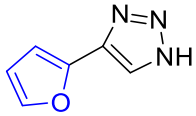
Brown solid, MS (ESI) m/z: 152.23 $[M+H]^+$



^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.90 (s, 1H), 7.43 (d, *J* = 3.4 Hz, 1H), 7.34 (d, *J* = 5.0 Hz, 1H), 7.12 – 7.07 (m, 1H), 8.51(s, 1H)

^{13}C NMR (125 MHz, $CDCl_3$) 125.2, 125.9, 127.8, 132.0, 142.2, 155.9

4-(furan-2-yl)-1H-1,2,3-triazole **(Scheme 5, entry 14i)**

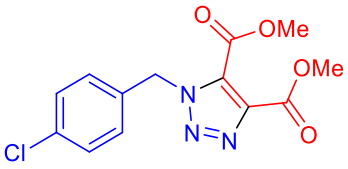


Pale yellow, MS (ESI) m/z: 138.18 $[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.66 (s, 1H), 7.91 (s, 1H), 7.51 (d, *J* = 1.8 Hz, 1H), 7.43 – 7.35 (t, 1H), 6.81 (d, *J* = 3.4 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ: 108.0, 111.6, 113.1, 139.5, 142.6, 155.3.

Dimethyl 1-(4-chlorobenzyl)-1H-1,2,3-triazole-4,5-dicarboxylate **(Scheme 6, entry 17a)**

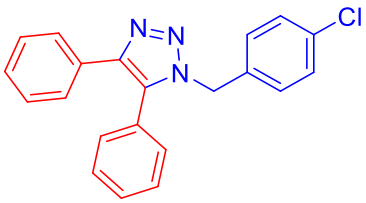


White solid; MS (ESI) m/z: 311.19 $[M+H]^+$

^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.27 (d, *J* = 8.5 Hz, 2H), 7.19 (d, *J* = 8.5 Hz, 2H), 5.74 (s, 2H), 3.92 (s, 3H), 3.87 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ: 52.8, 53.2, 53.2, 53.4, 123.0, 128.8, 129.1, 129.4, 129.5, 129.8, 131.0, 133.0, 132.5, 133.0, 134.8, 140.4, 158.7, 160.4.

1-(4-chlorobenzyl)-4,5-diphenyl-1H-1,2,3-triazole **(Scheme 6, entry 17c)**



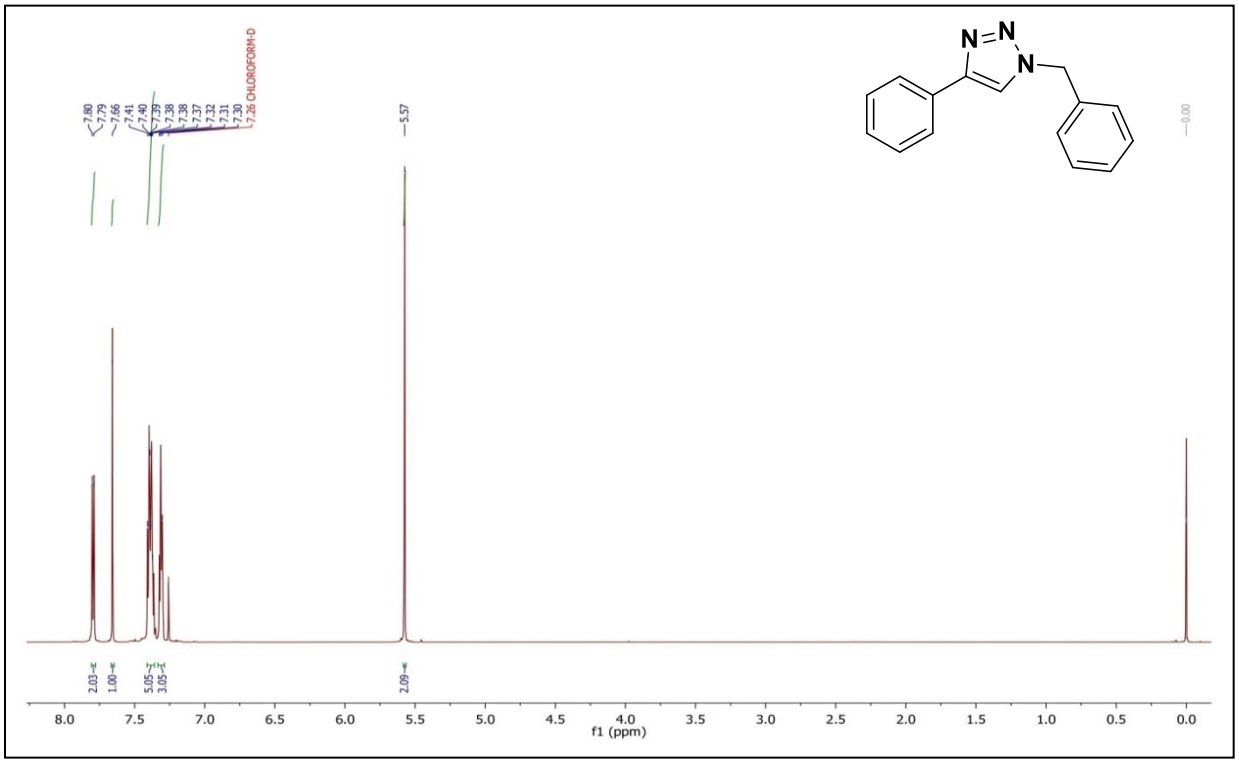
White Solid; MS (ESI) m/z: 347.16 $[M+H]^+$

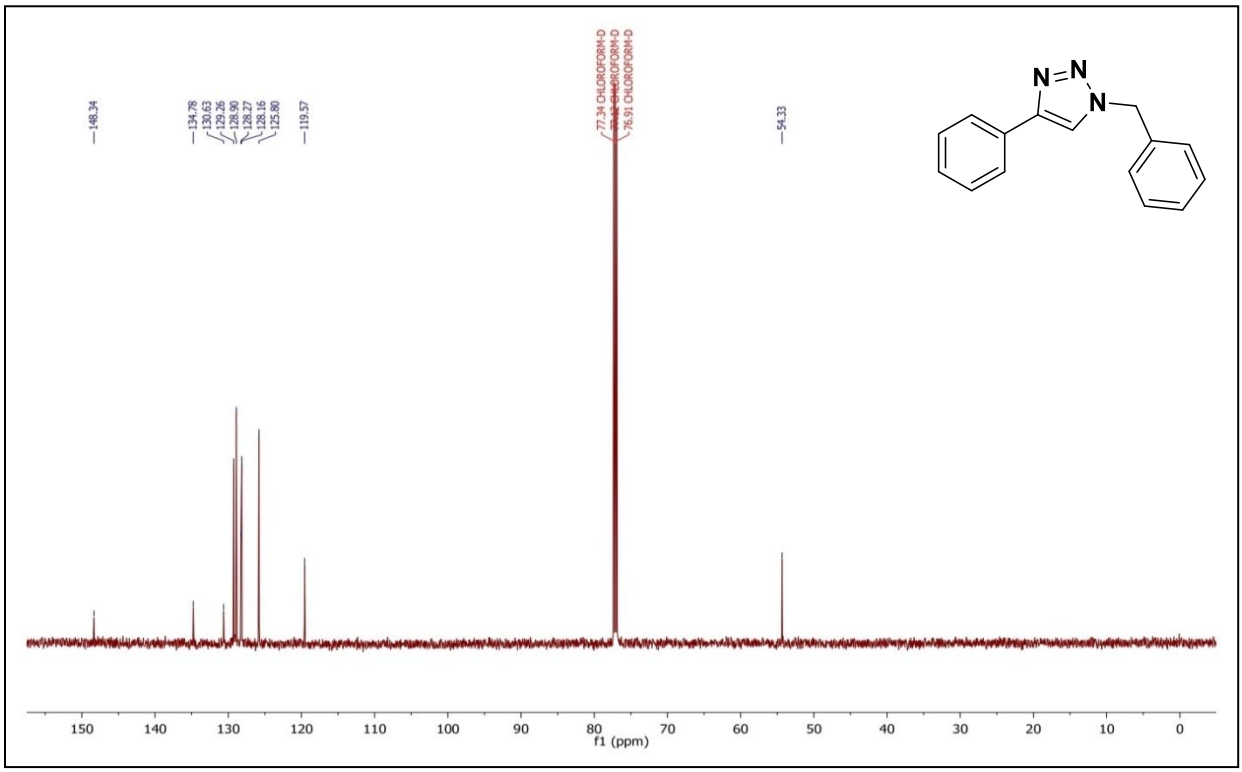
^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.61 – 7.54 (m, 2H), 7.51 (d, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.4 Hz, 2H), 7.40 (d, *J* = 8.4 Hz, 2H), 7.26 (d, *J* = 5.1 Hz, 3H), 7.16 (d, *J* = 7.1 Hz, 2H), 6.92 (d, *J* = 8.3 Hz, 2H), 5.38 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ: 51.4, 126.7, 127.8, 128.5, 129.3, 129.3, 129.9, 130.1, 130.7, 131.9, 134.3.

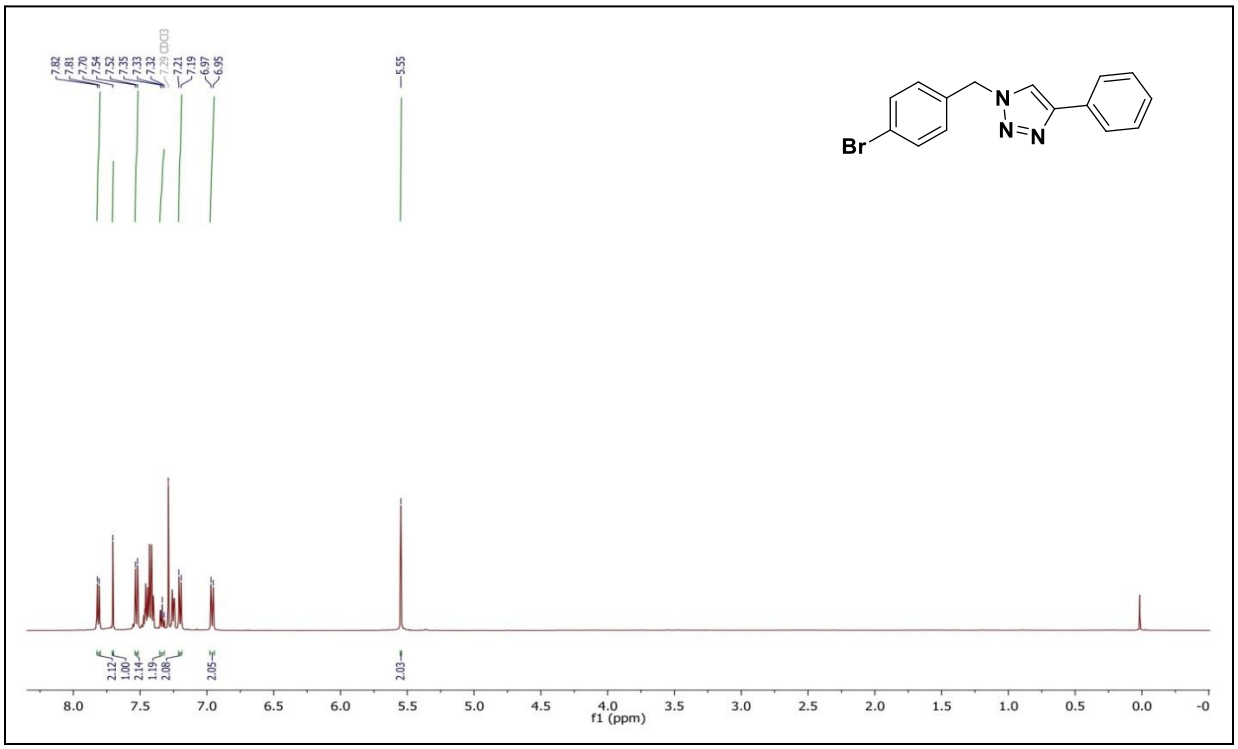
7. ^{1}H NMR and ^{13}C NMR spectra of triazoles derivatives:

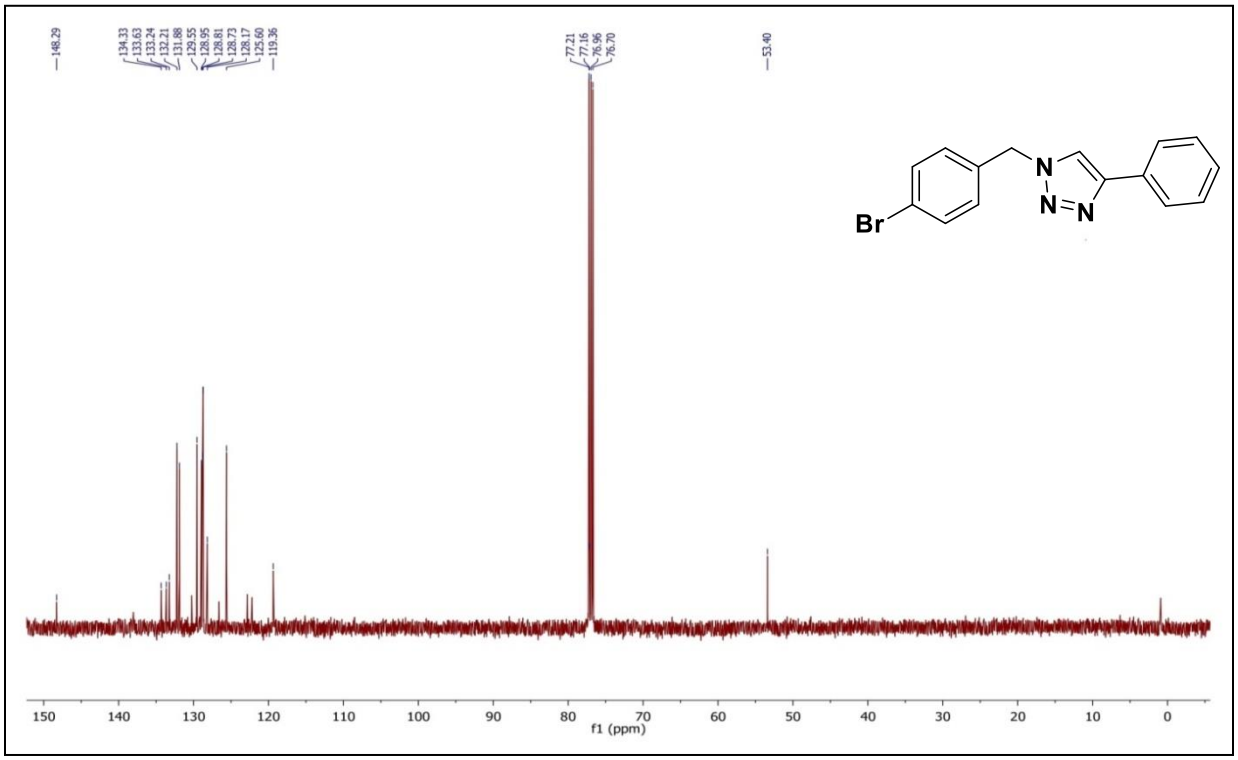
^{1}H NMR and ^{13}C NMR spectra of 1-benzyl-4-phenyl-1H-1,2,3-triazole **(Scheme 3, Entry 3a)** respectively. **Ref: S1**



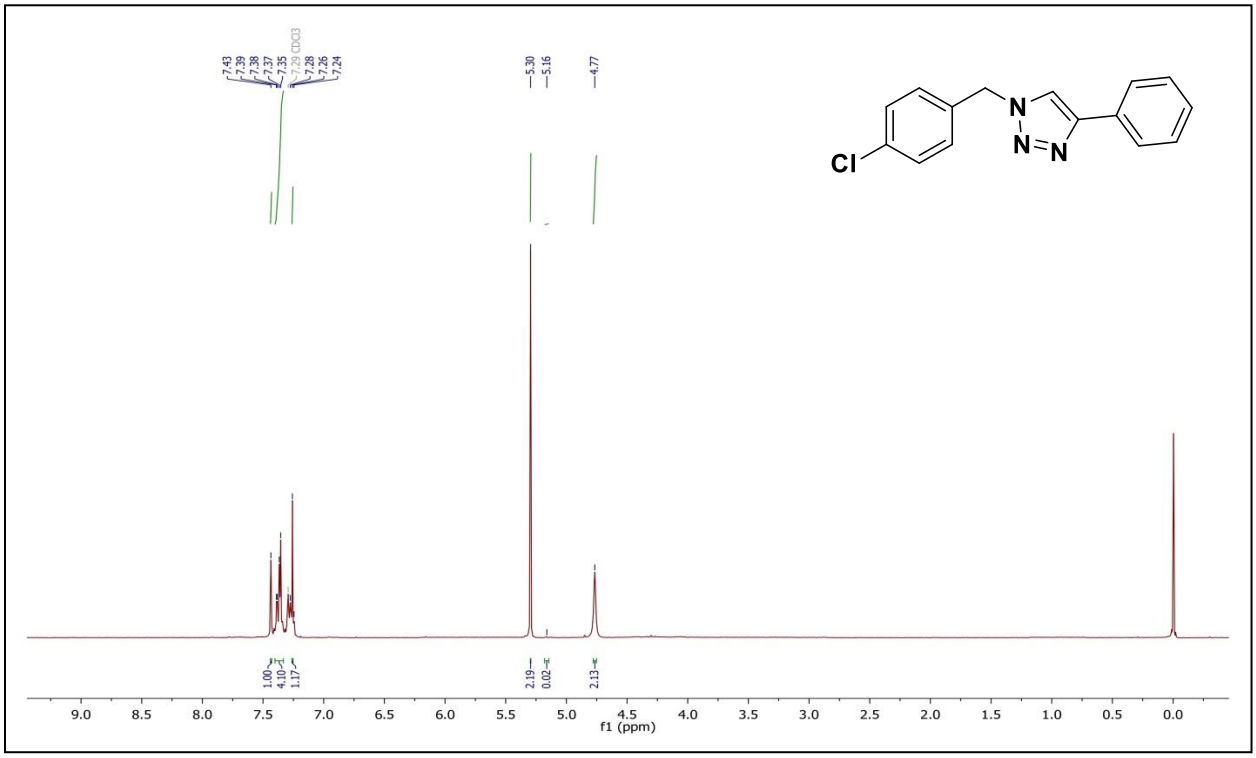


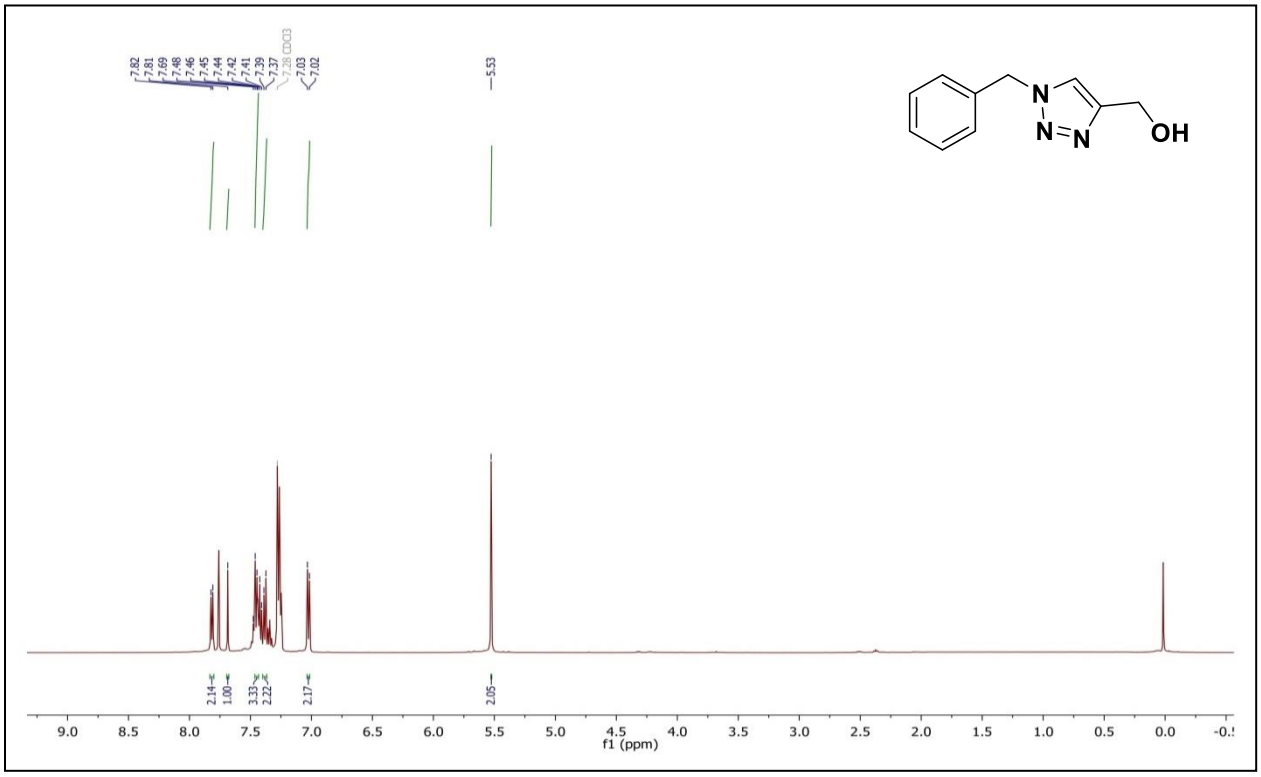
^{1}H NMR and ^{13}C NMR spectra of 1-(4-bromobenzyl)-4-phenyl-1H-1,2,3-triazole (**Scheme 2, Entry 3b**) respectively. **Ref: S2**



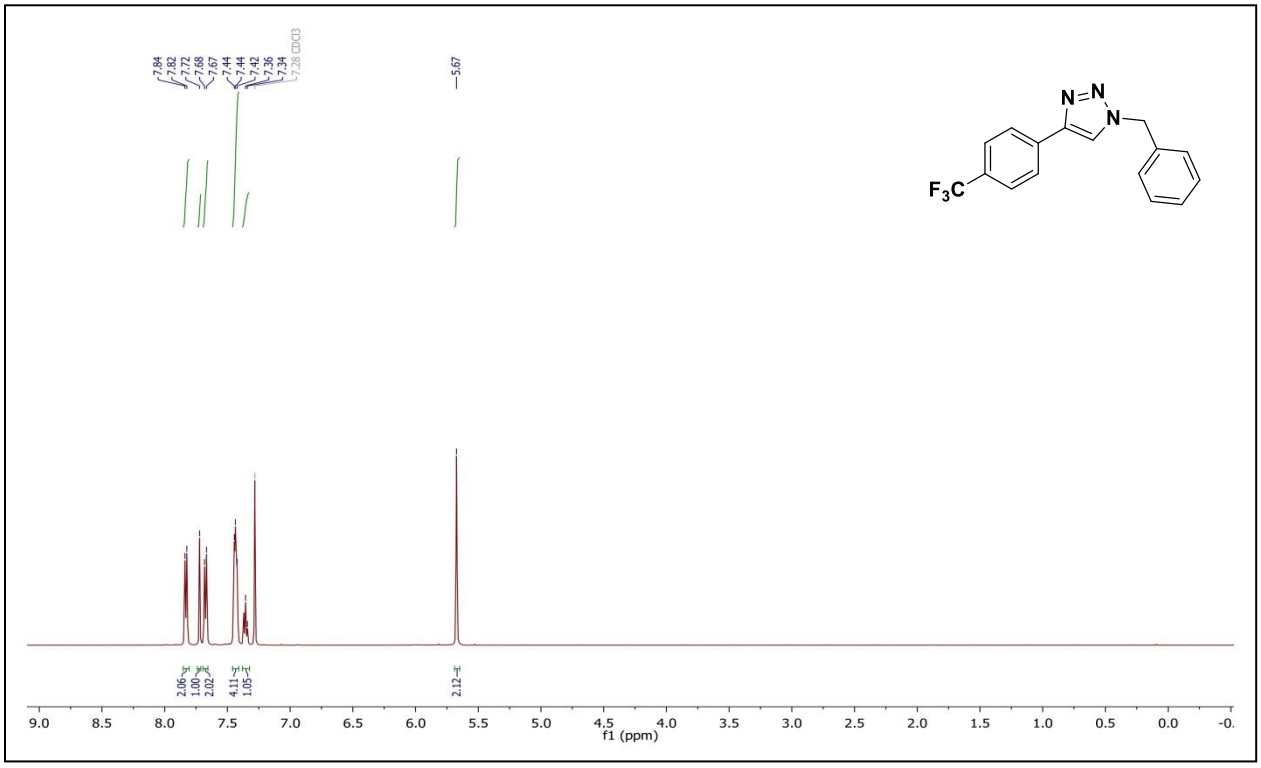


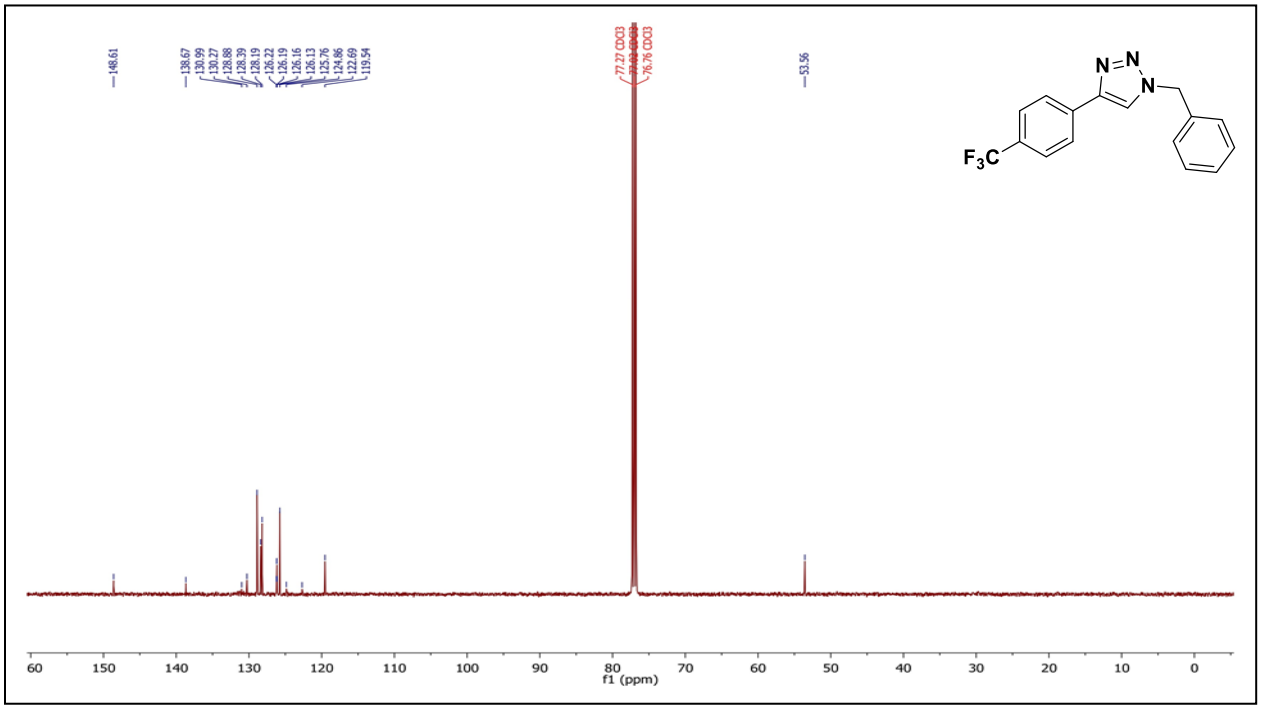
^{1}H NMR spectra of 1-(4-chlorobenzyl)-4-phenyl-1H-1,2,3-triazole **(Scheme 2, Entry 3d) Ref: S4** and (1-benzyl-1H-1,2,3-triazol-4-yl)methanol **(Scheme 3, entry 6l)** respectively.



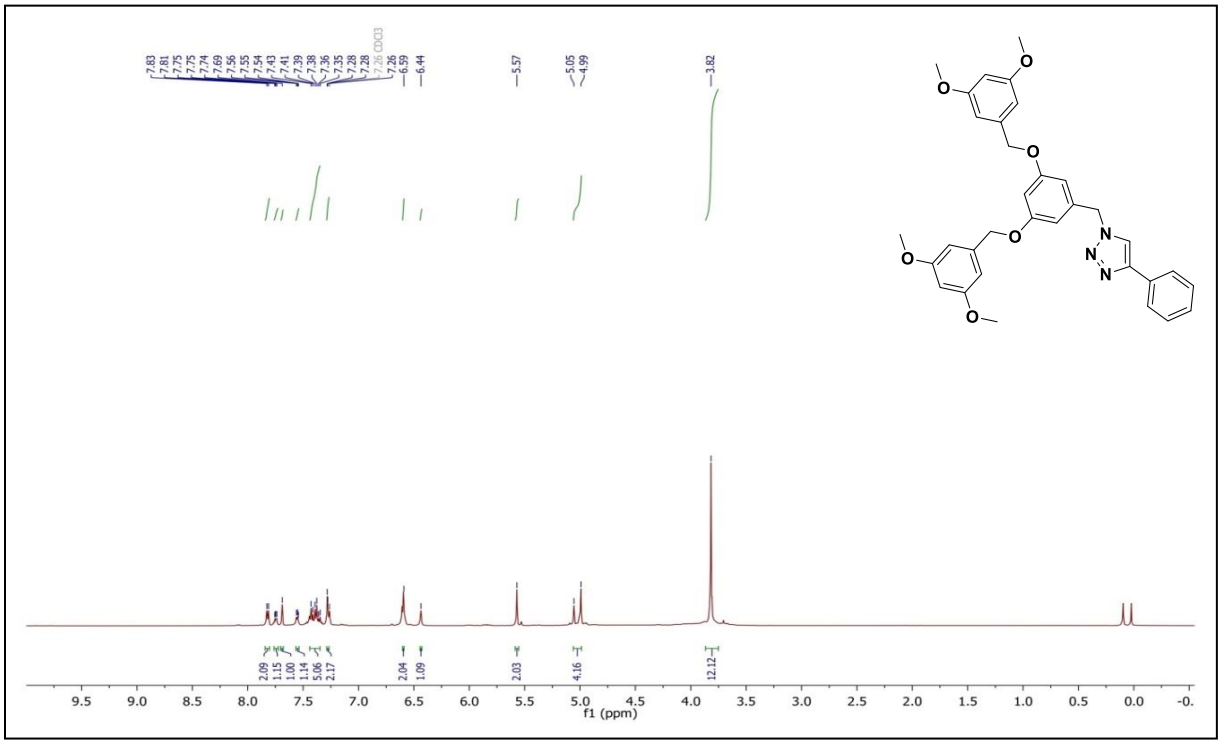


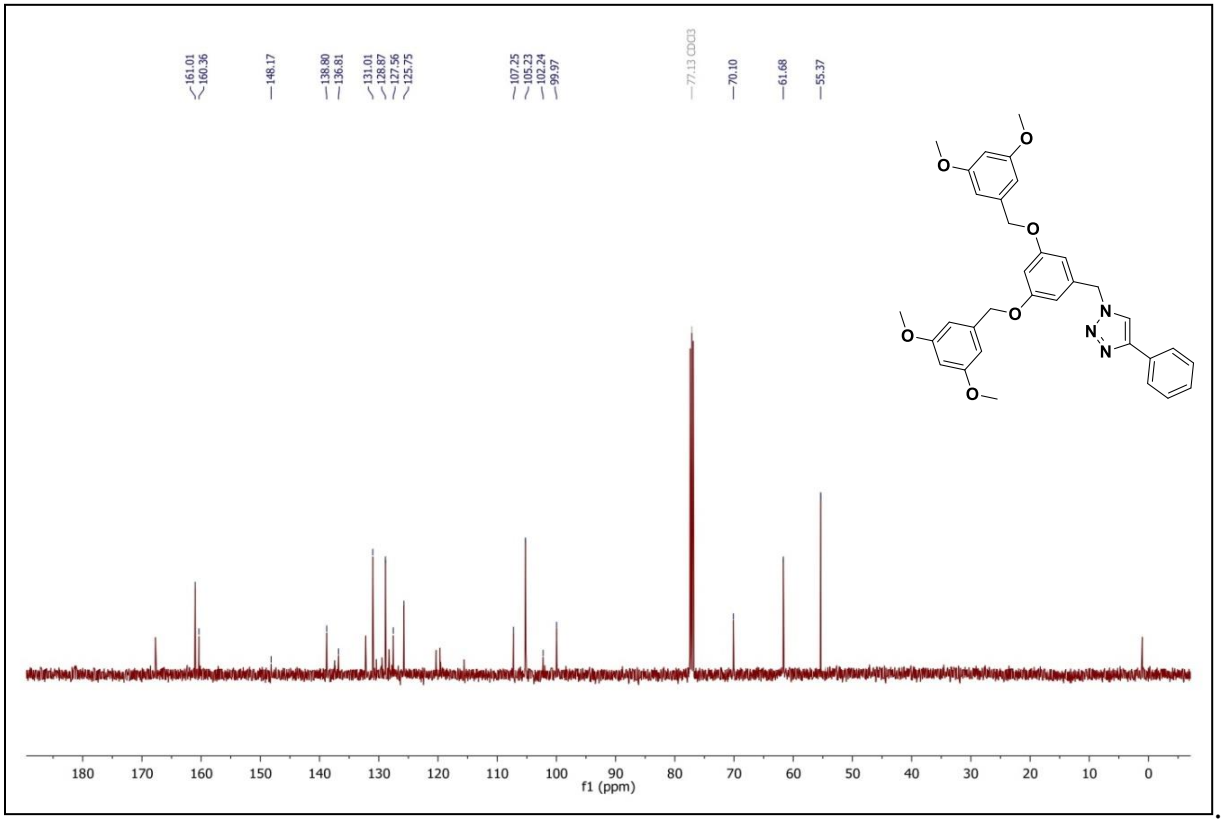
^{1}H NMR and ^{13}C NMR spectra of 1-benzyl-4-(4-(trifluoromethyl)phenyl)-1H-1,2,3-triazole **(Scheme 2, entry 3e)** respectively.



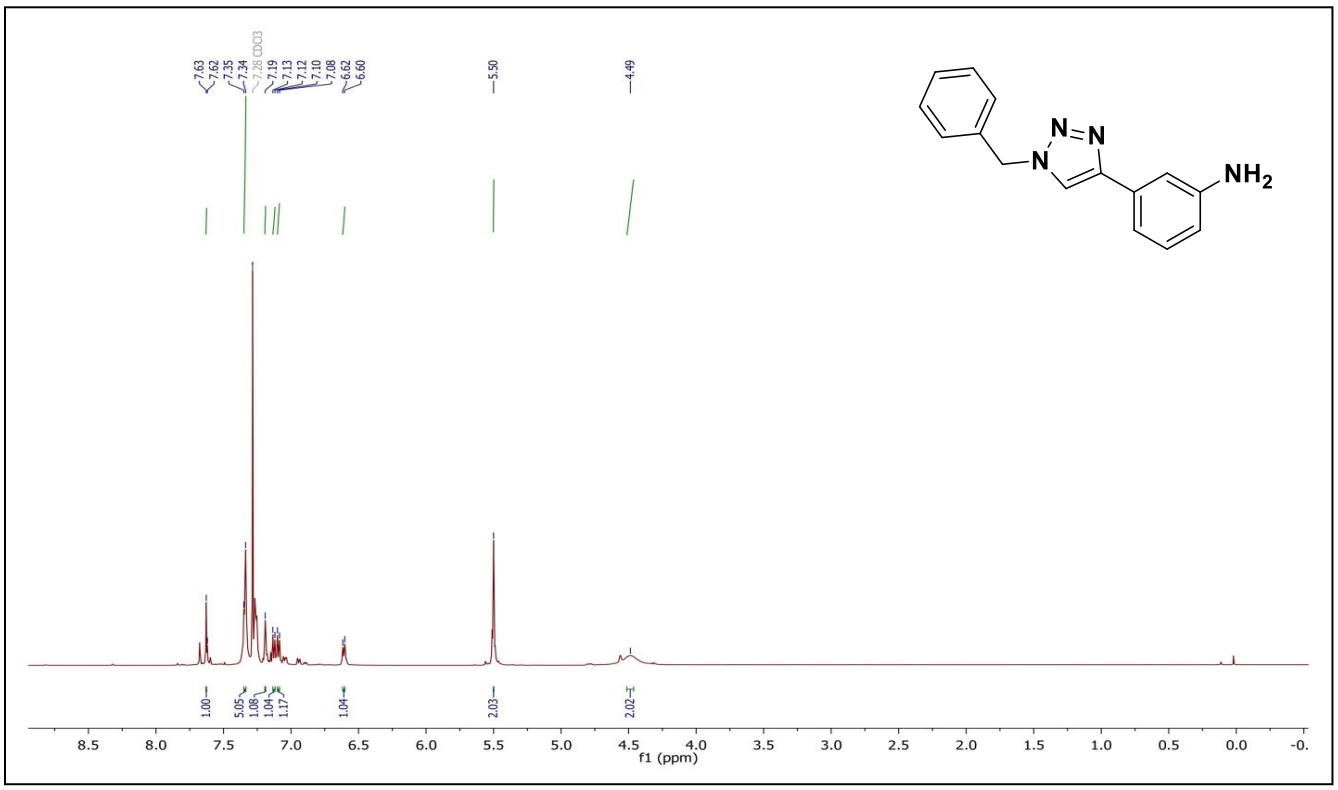


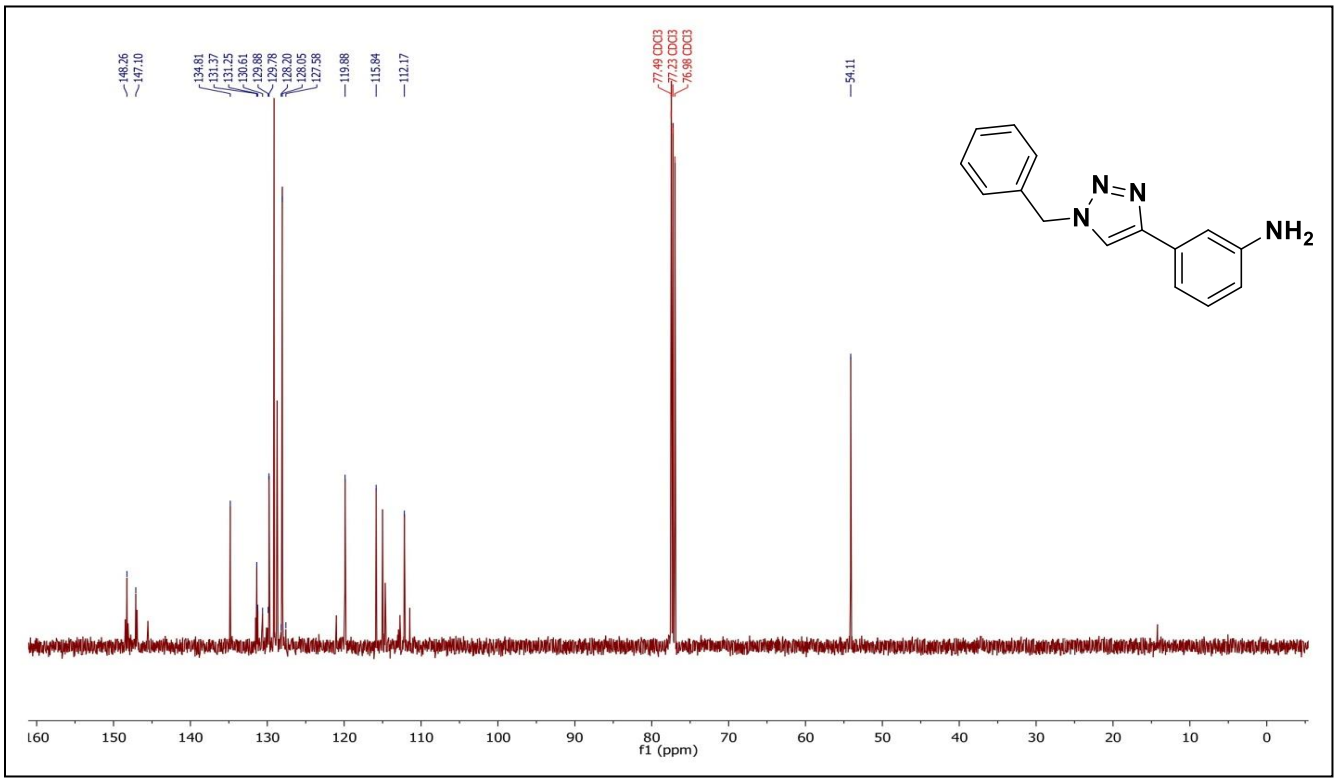
^{1}H NMR and ^{13}C NMR spectra of 1-(3,5-bis((3,5-dimethoxybenzyl)oxy)benzyl)-4-phenyl-1H-1,2,3-triazole **(Scheme 2, Entry 3g)** respectively



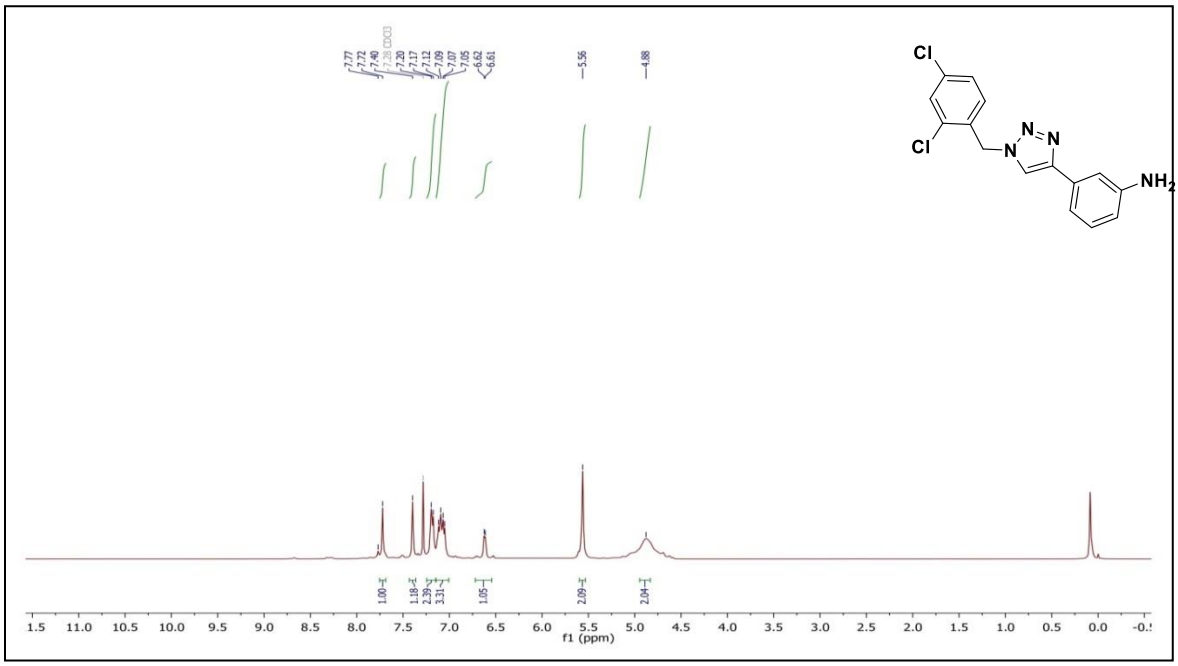


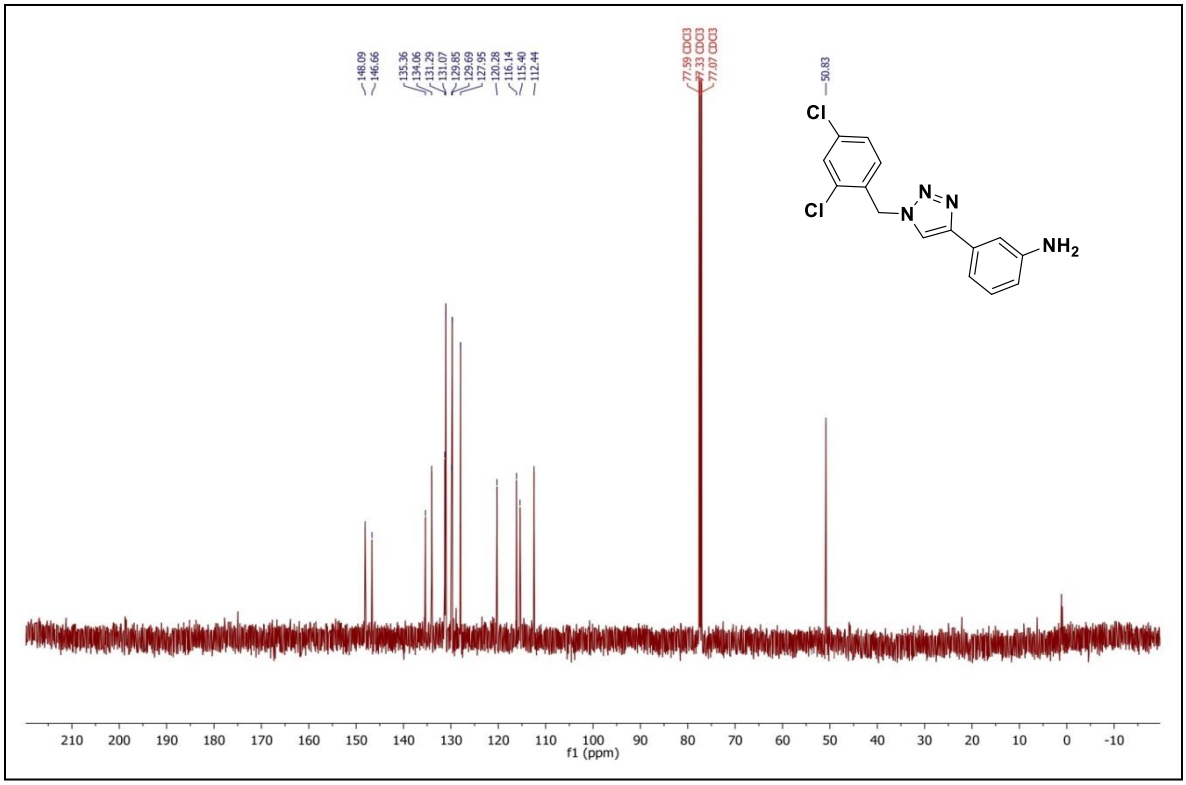
^{1}H NMR and ^{13}C NMR spectra of 3-(1-benzyl-1H-1,2,3-triazol-4-yl)aniline **(Scheme 3, Entry 6b)** respectively.



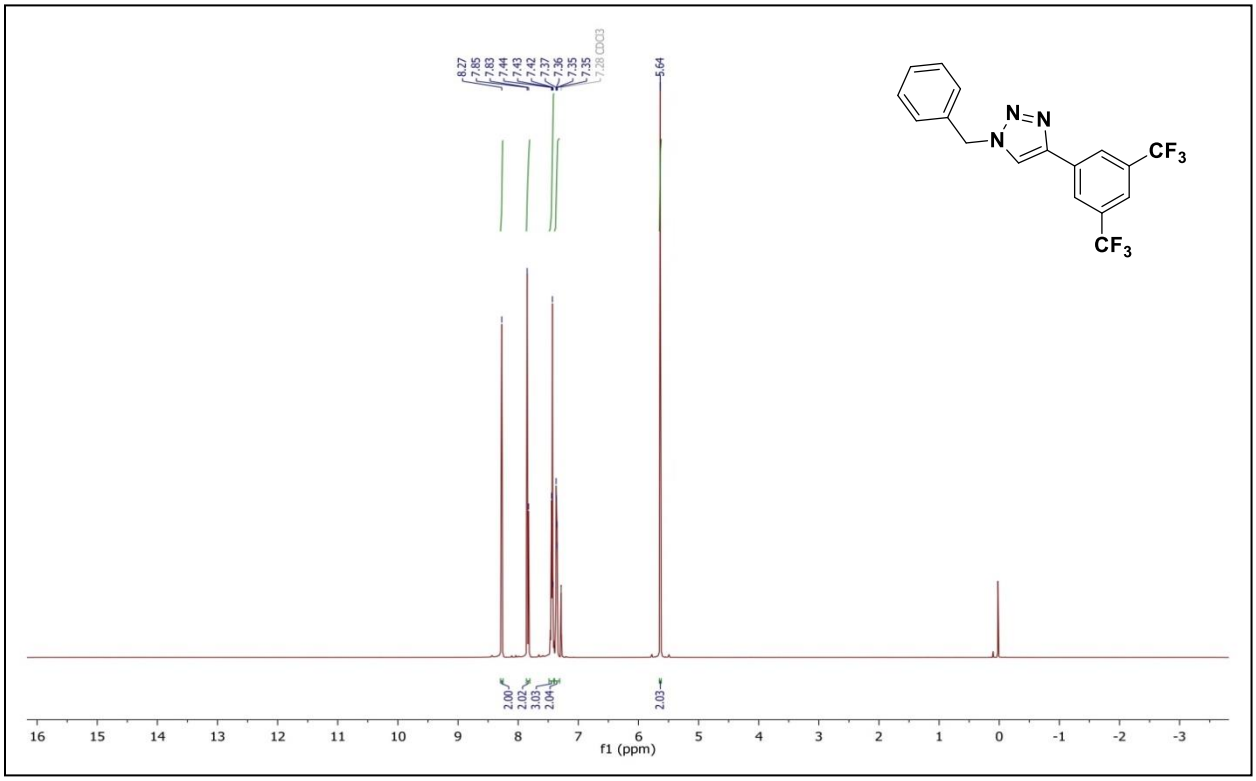


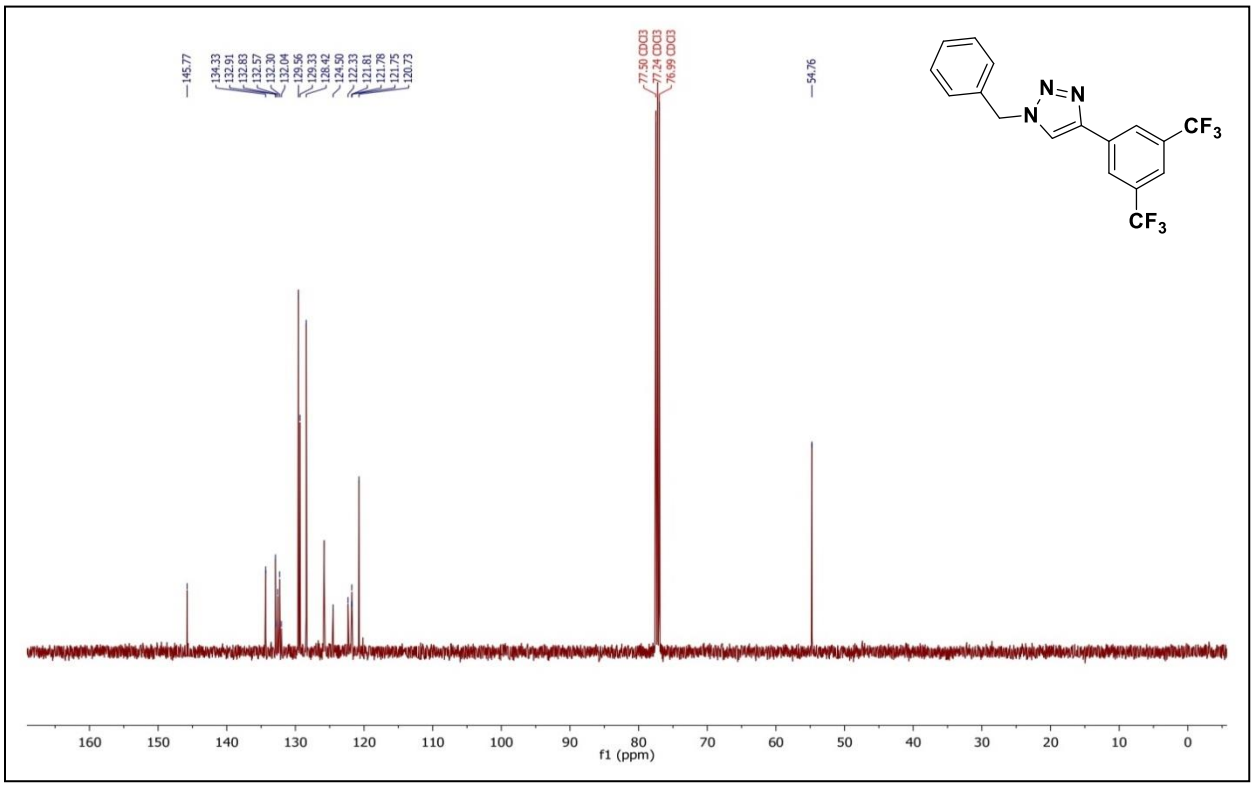
^{1}H NMR and ^{13}C NMR spectra of 3-(1-(2,4-dichlorobenzyl)-1H-1,2,3-triazol-4-yl)aniline **(Scheme 3, Entry 6c)** respectively.



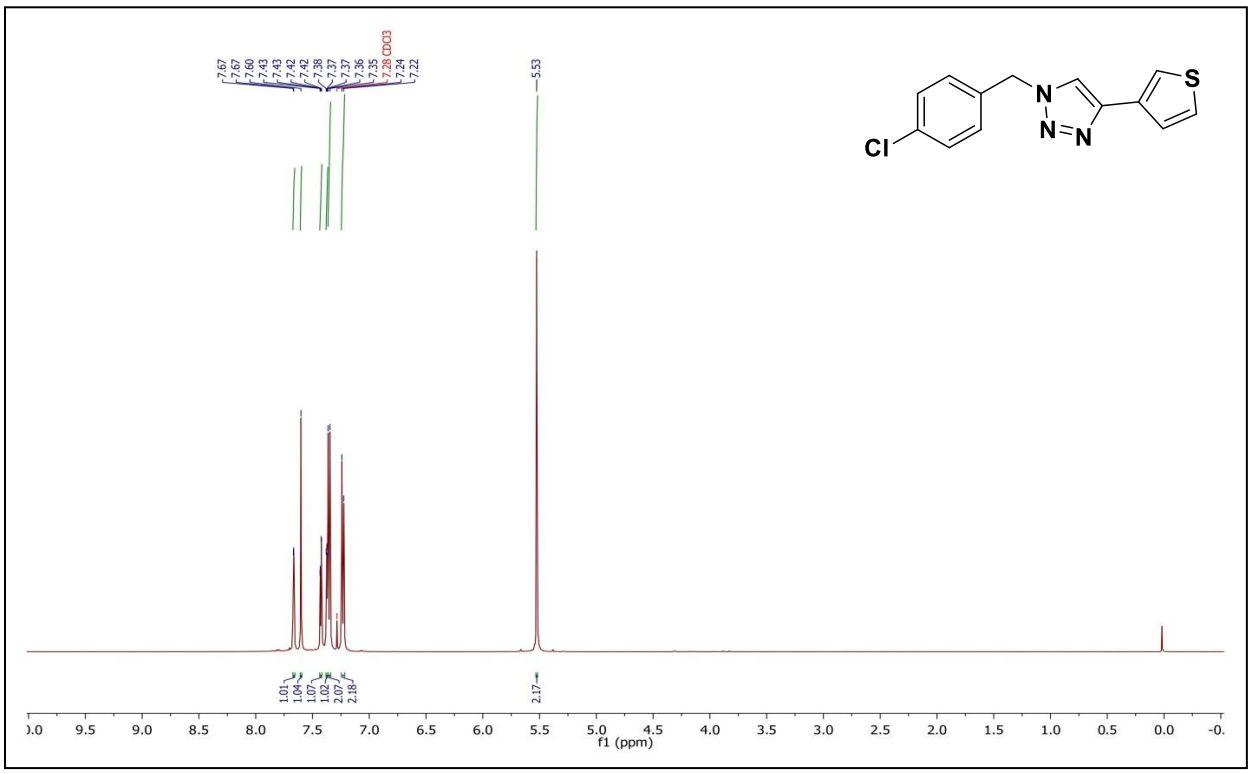


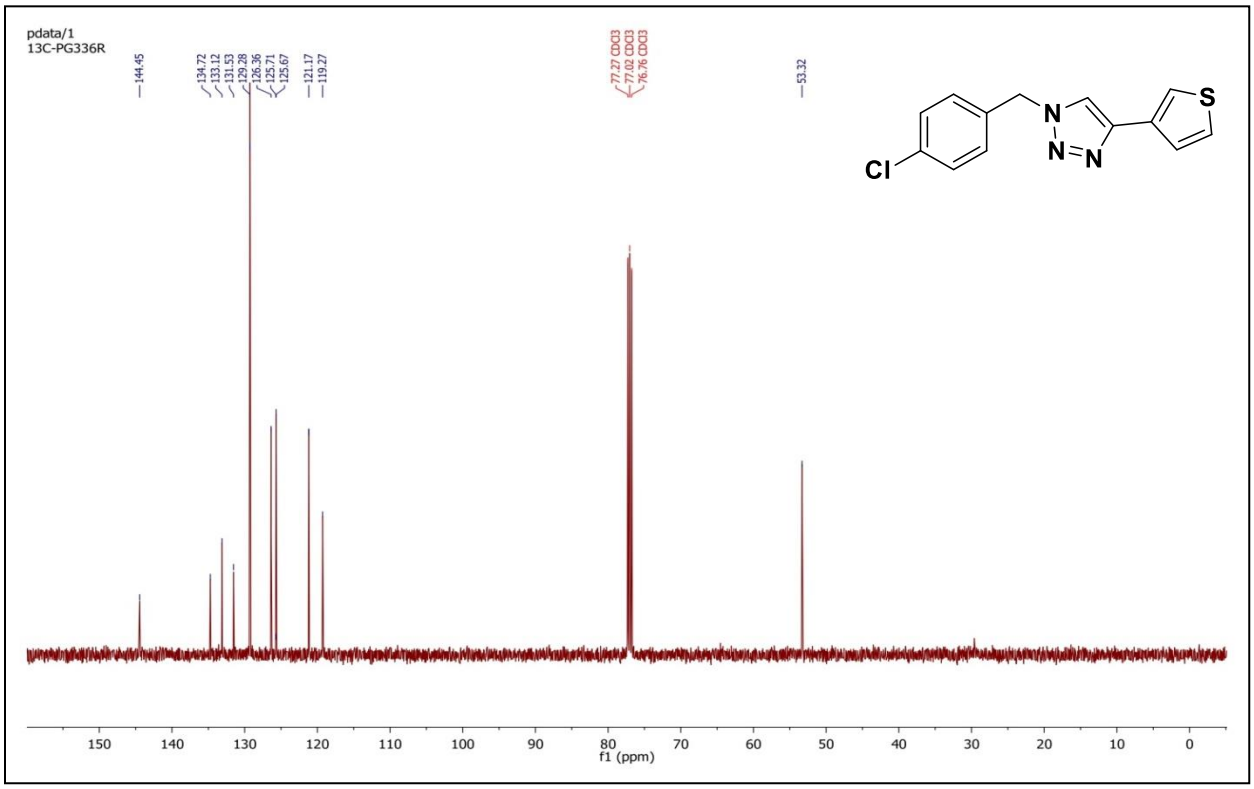
^{1}H NMR and ^{13}C NMR spectra of 1-benzyl-4-(3,5-bis(trifluoromethyl)phenyl)-1H-1,2,3-triazole **(Scheme 3, Entry 6d)** respectively.



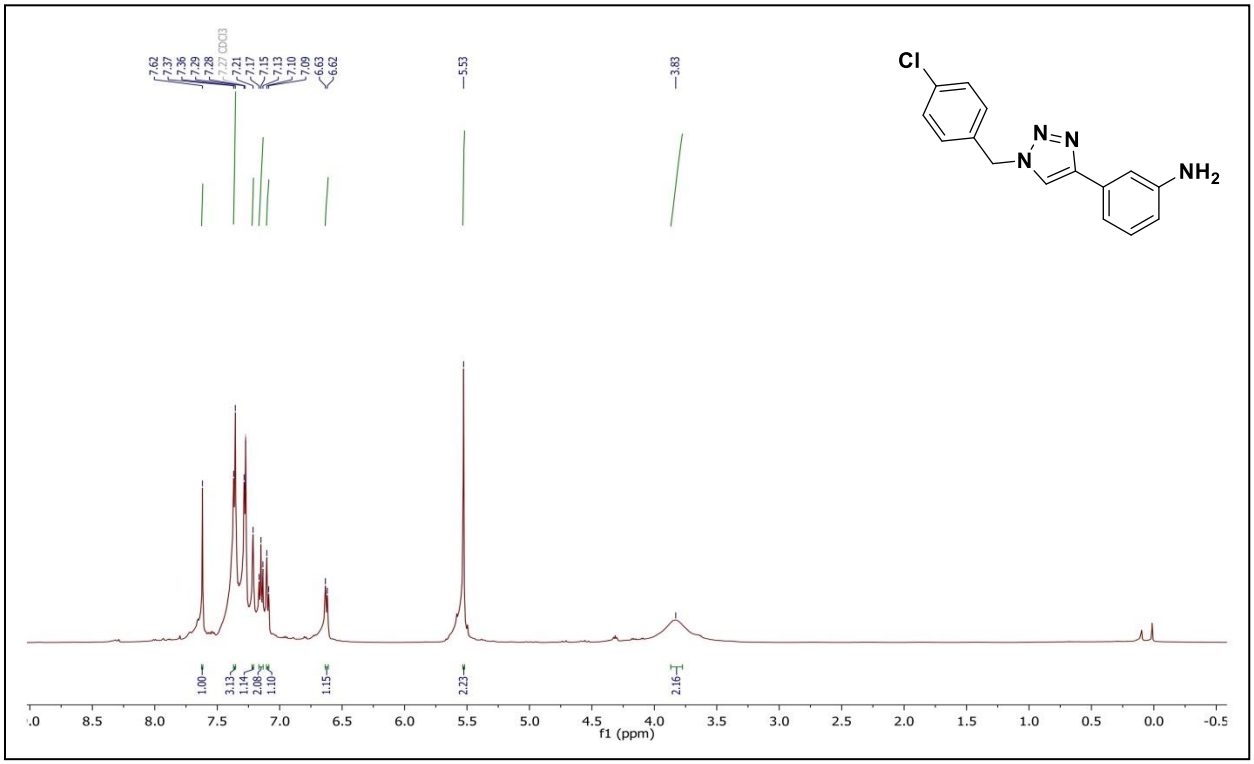


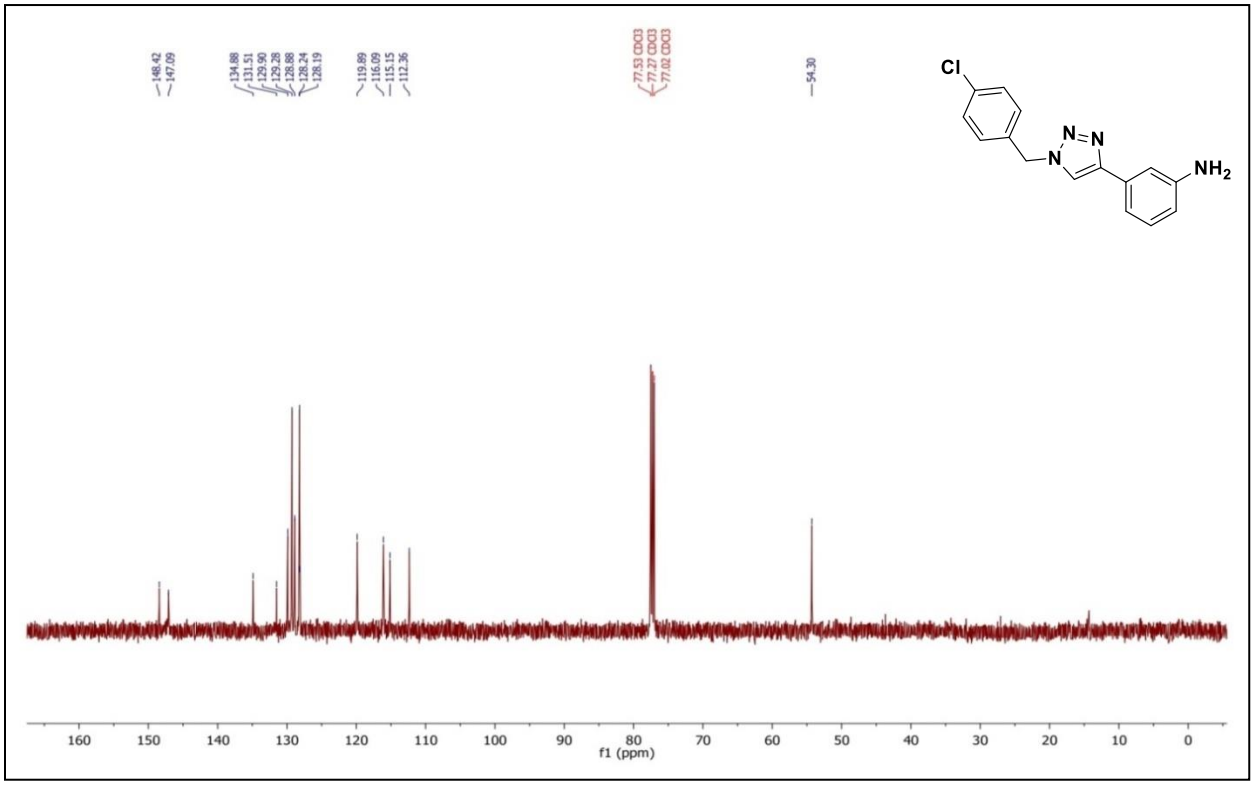
^{1}H NMR and ^{13}C NMR spectra of 1-(4-chlorobenzyl)-4-(thiophen-3-yl)-1H-1,2,3-triazole **(Scheme 3, Entry 6e)** respectively.



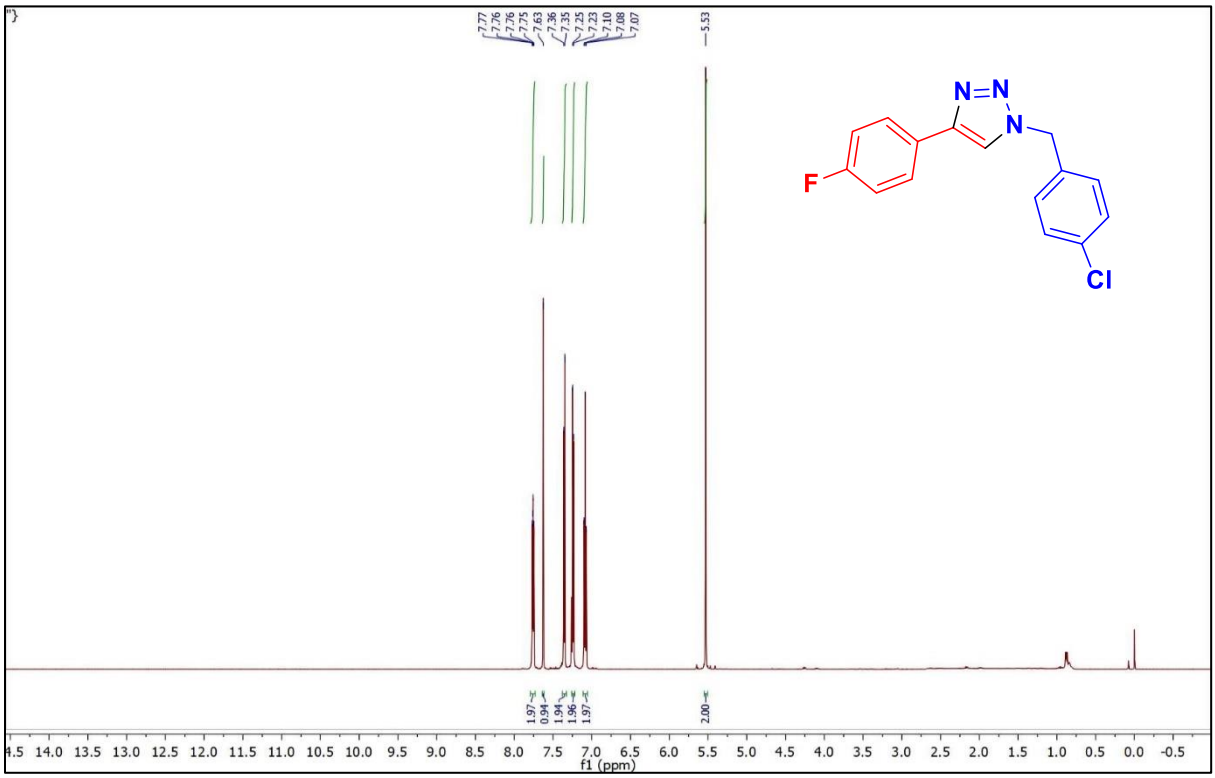


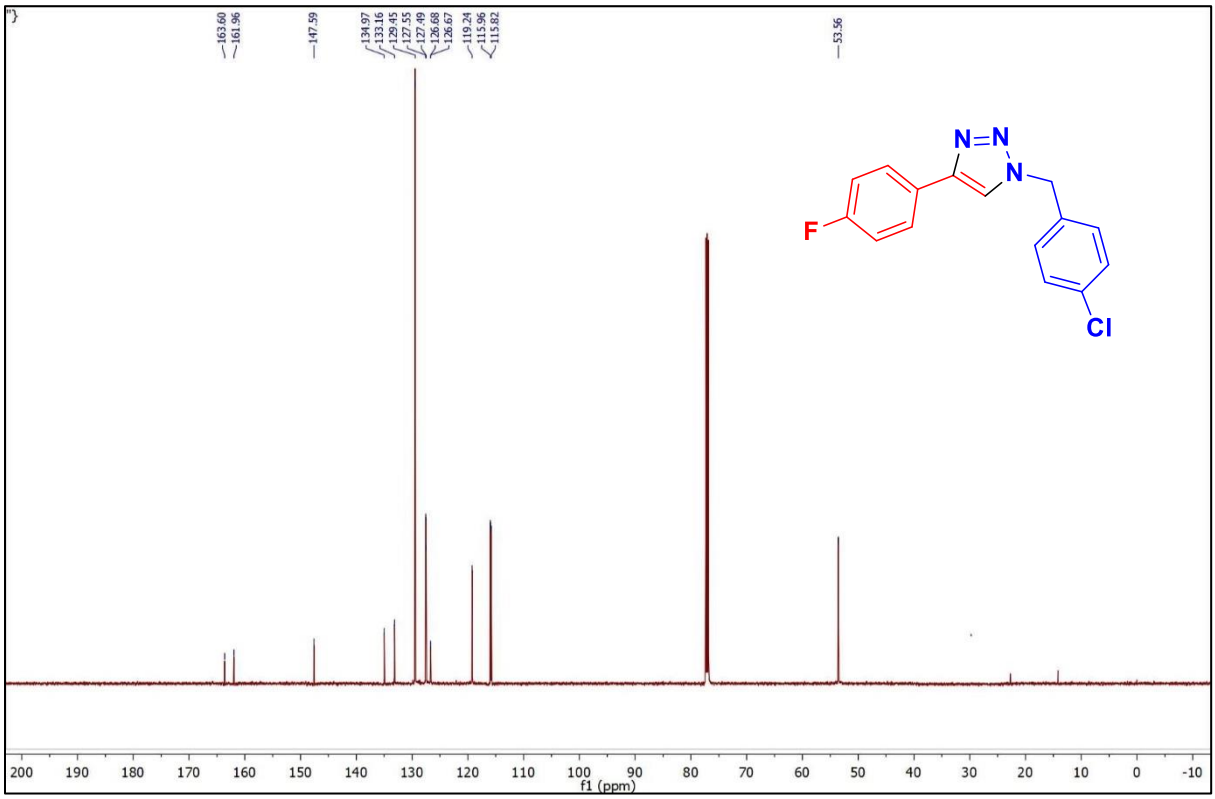
^{1}H NMR and ^{13}C NMR of 3-(1-(4-chlorobenzyl)-1H-1,2,3-triazol-4-yl)aniline **(Scheme 3, Entry 6g)** respectively.



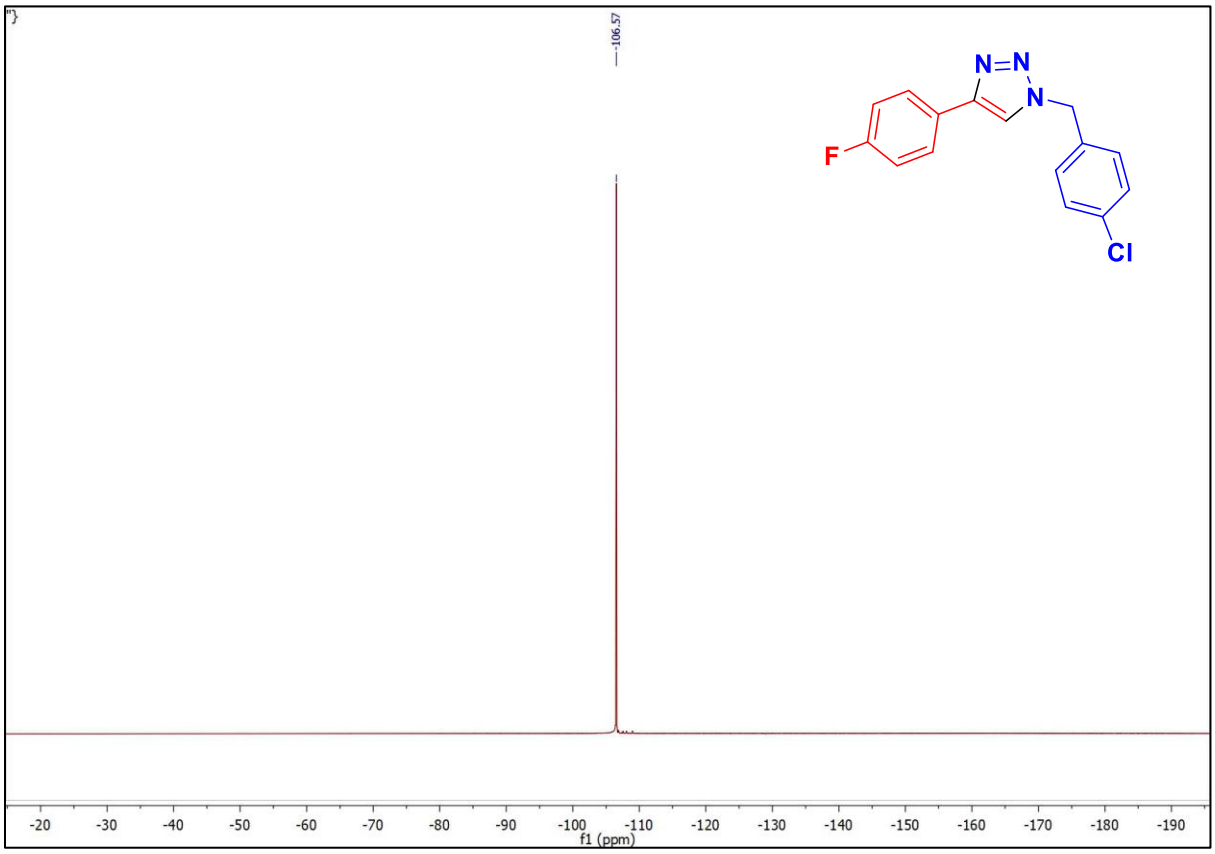


^{1}H NMR and ^{13}C NMR of 1-(4-chlorobenzyl)-4-(4-fluorophenyl)-1H-1,2,3-triazole (**Scheme 3, entry 6h**) respectively.

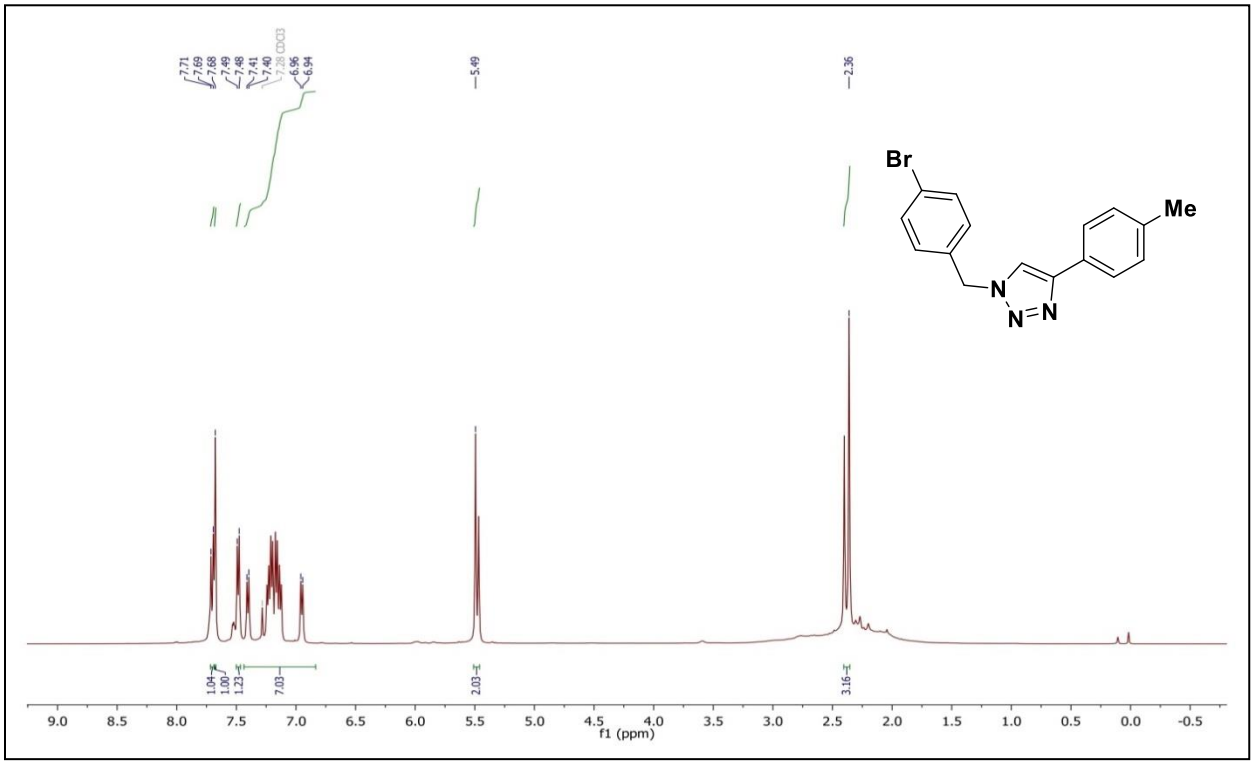


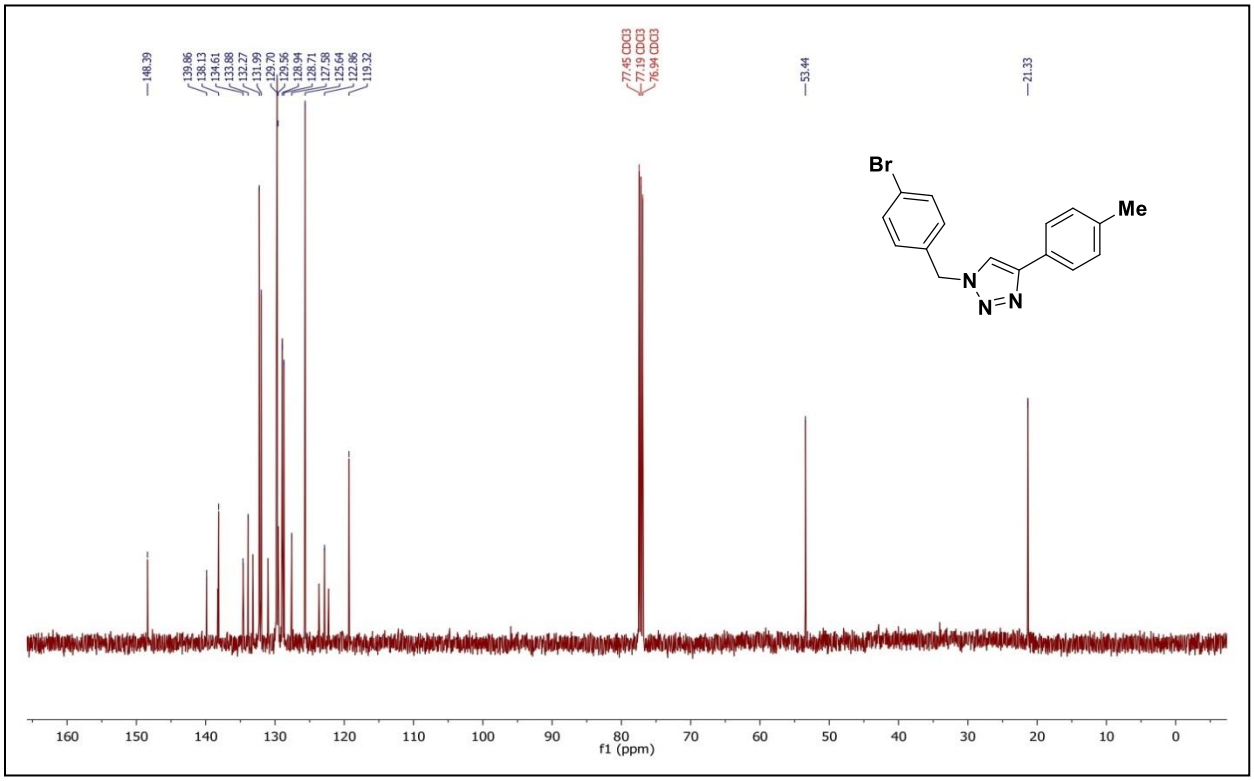


^{19}F NMR spectra of 1-(4-chlorobenzyl)-4-(4-fluorophenyl)-1H-1,2,3-triazole (**Scheme 3, entry 6h**).

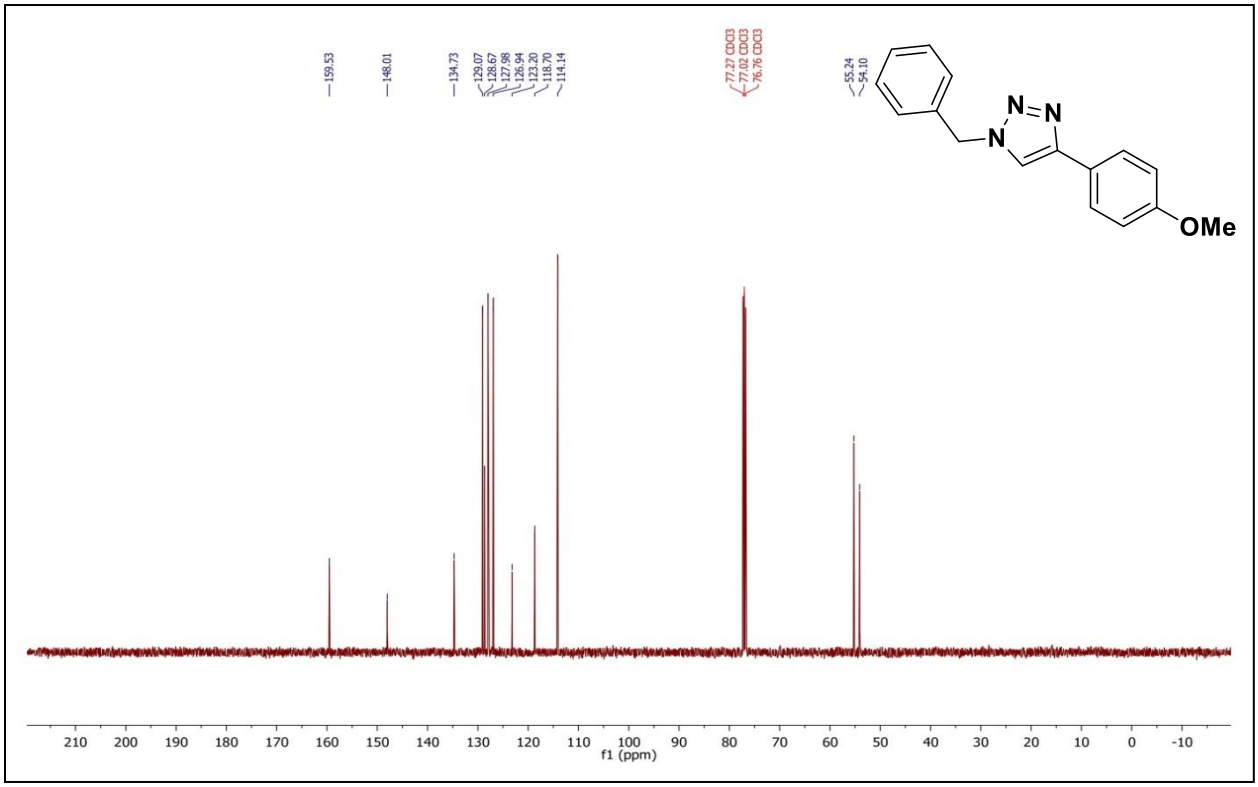


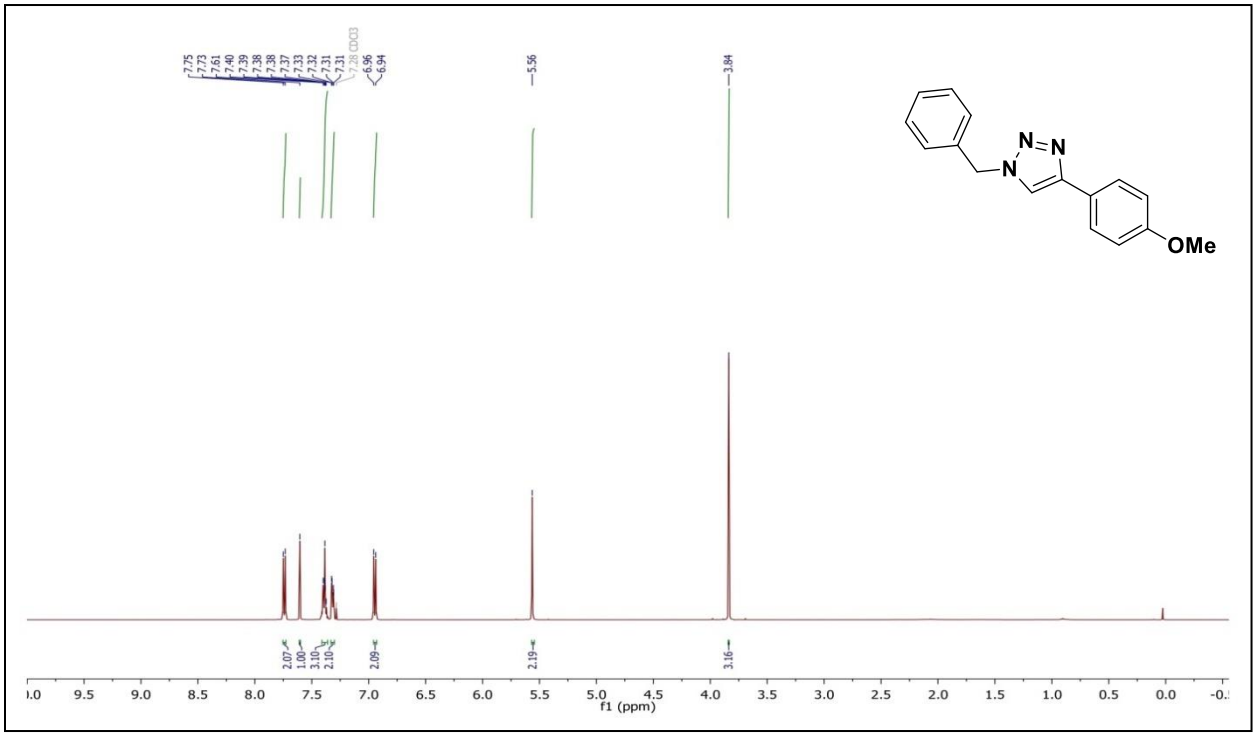
^{1}H NMR and ^{13}C NMR spectra of 1-(4-bromobenzyl)-4-(p-tolyl)-1H-1,2,3-triazole **(Scheme 3, entry 6i)** respectively. **Ref: S4**



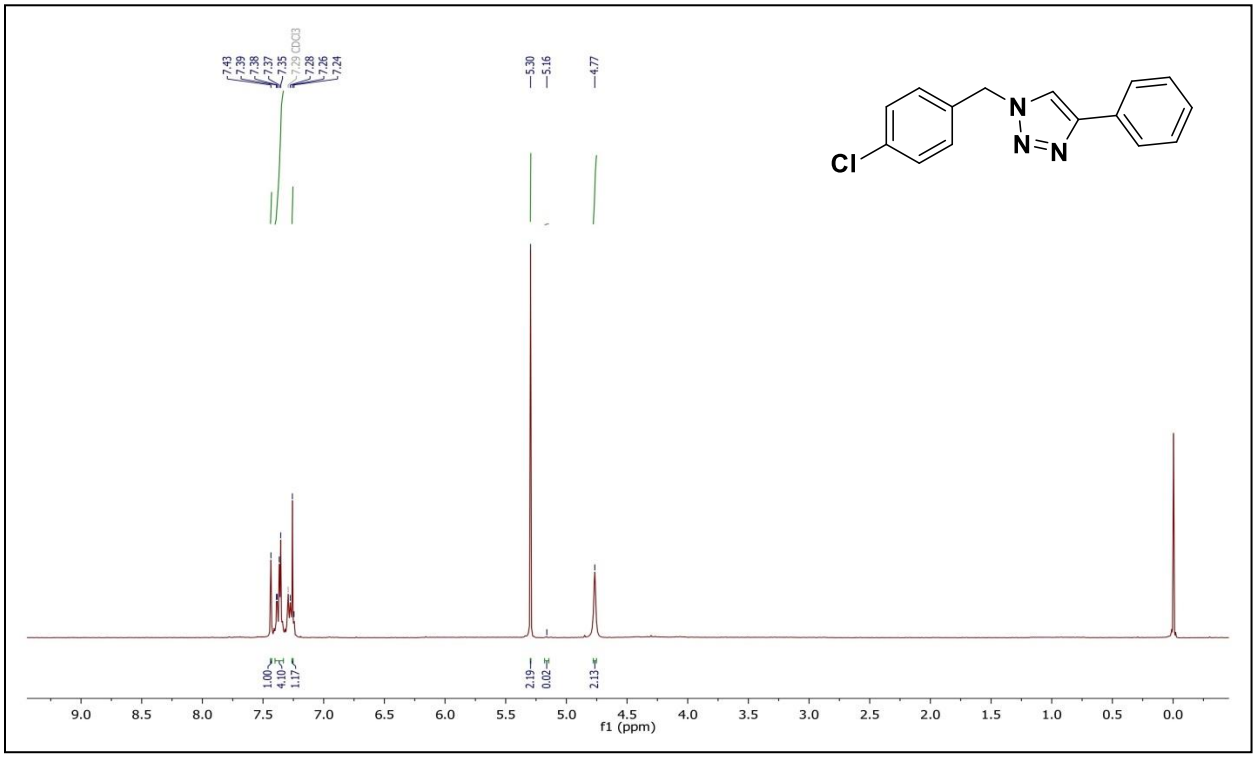


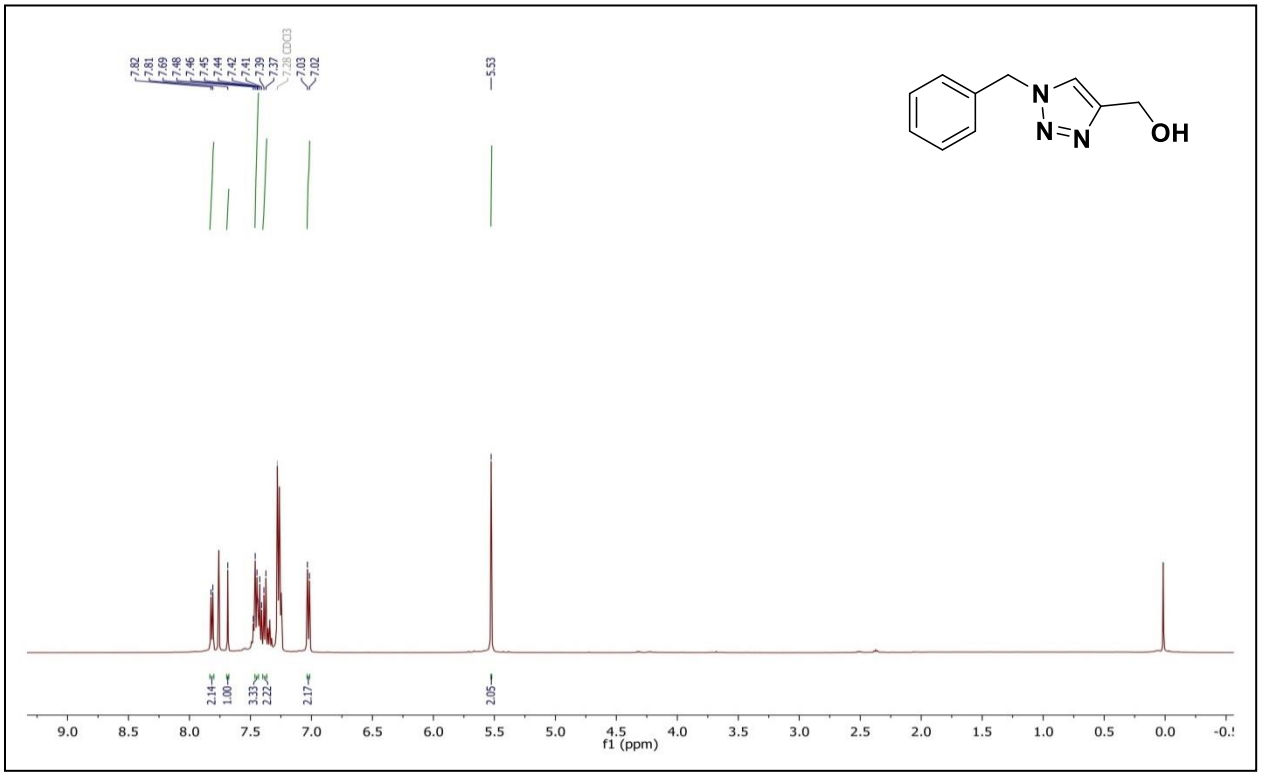
^{1}H NMR and ^{13}C NMR spectra of 1-benzyl-4-(4-methoxyphenyl)-1H-1,2,3-triazole **(Scheme 3, Entry 6j)** respectively. **Ref: S4**



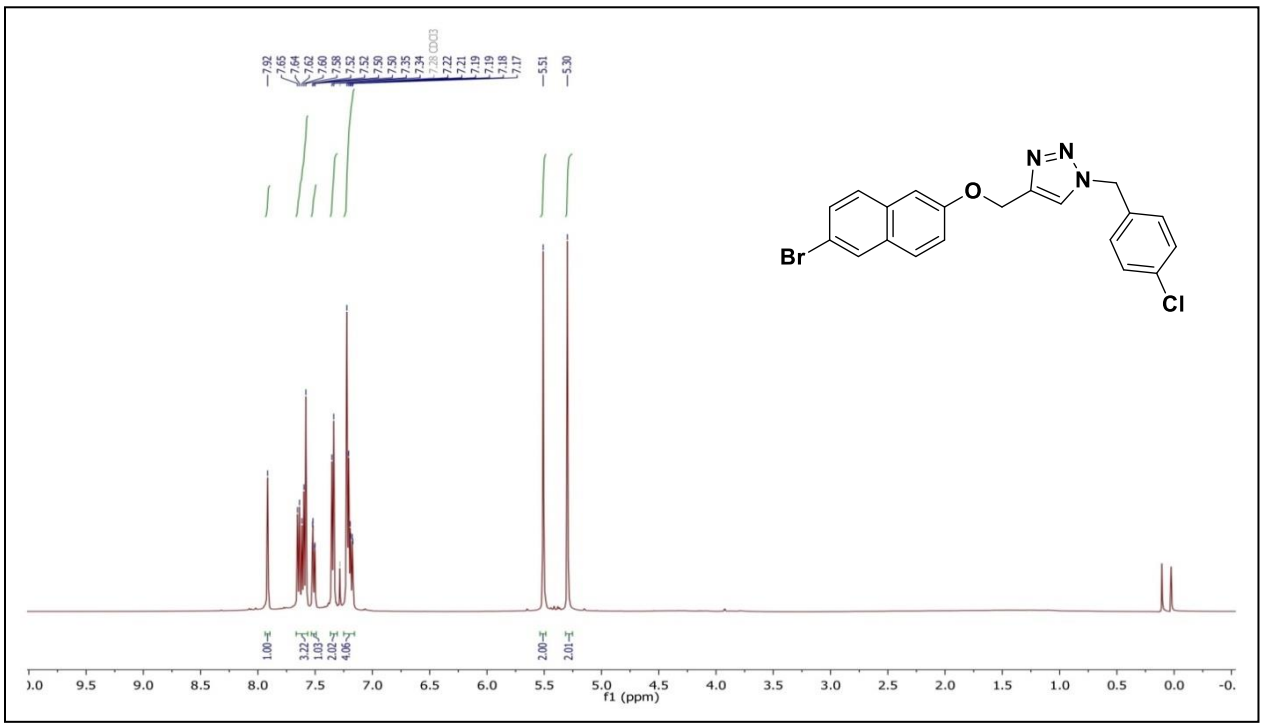


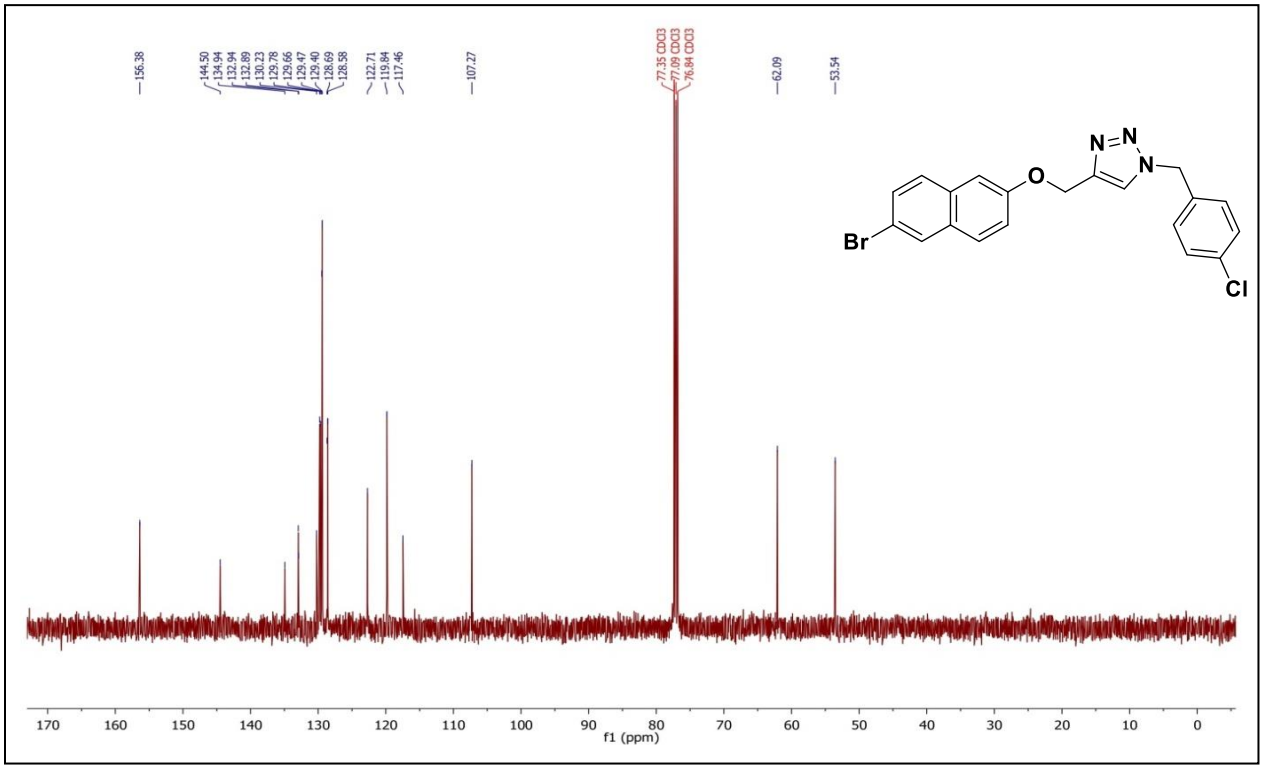
^{1}H NMR spectra of 1-(4-chlorobenzyl)-4-phenyl-1H-1,2,3-triazole **(Scheme 2, Entry 3d)** and (1-benzyl-1H-1,2,3-triazol-4-yl)methanol **(Scheme 3, entry 6l)** respectively.



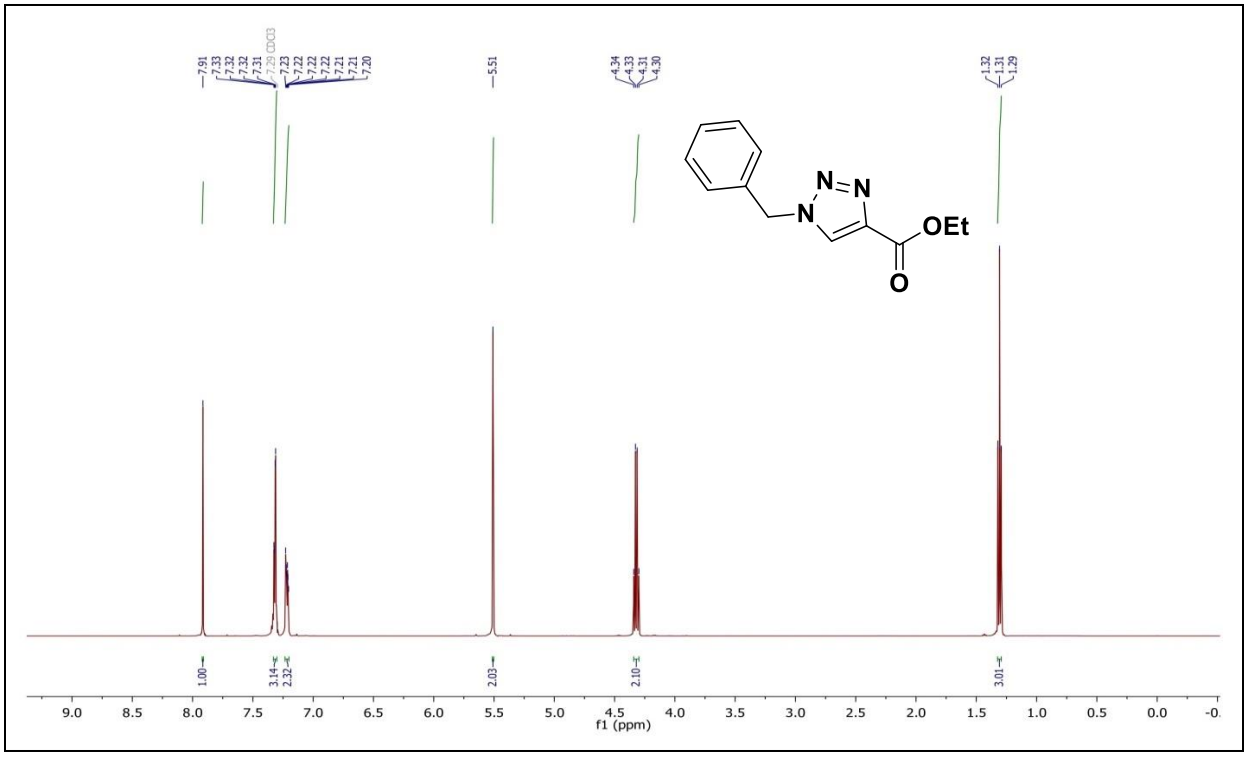


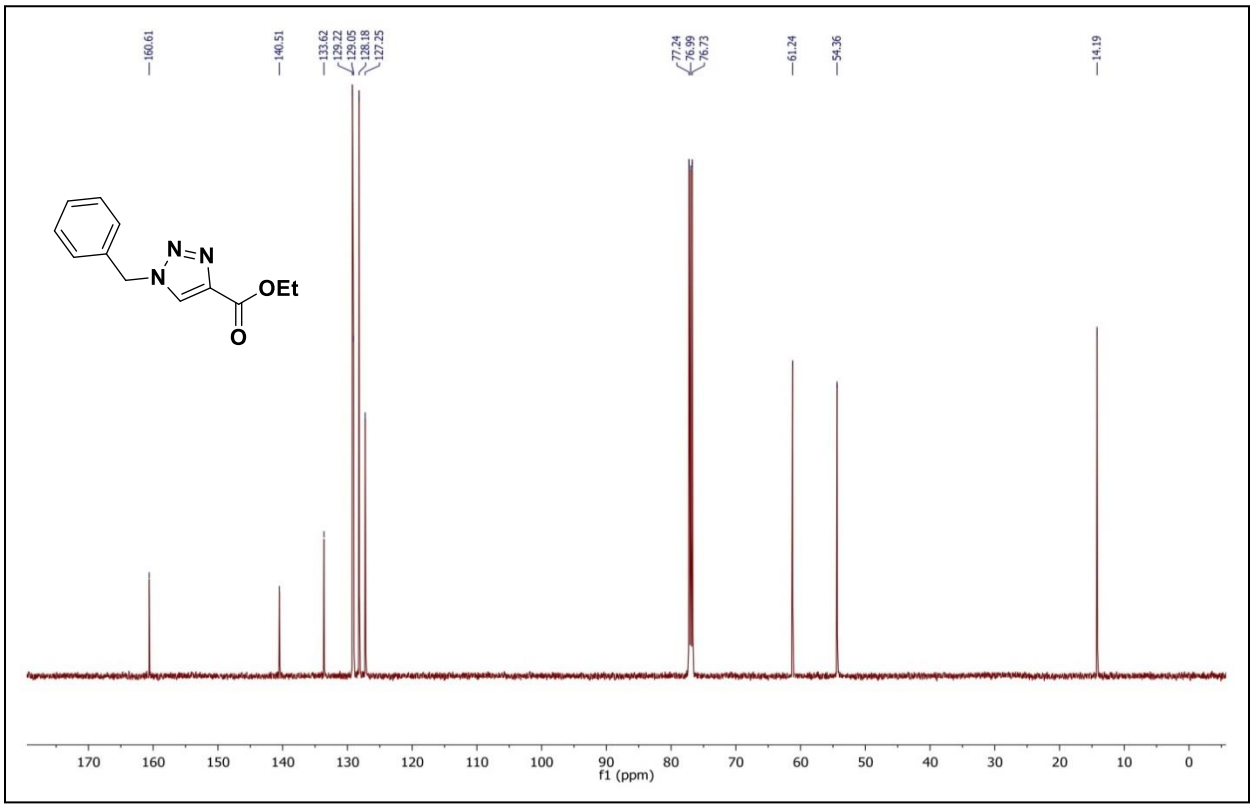
^{1}H NMR and ^{13}C NMR spectra of 4-(((6-bromonaphthalen-2-yl)oxy)methyl)-1-(4-chlorobenzyl)-1H-1,2,3-triazole **(Scheme 3, Entry 6m)** respectively.



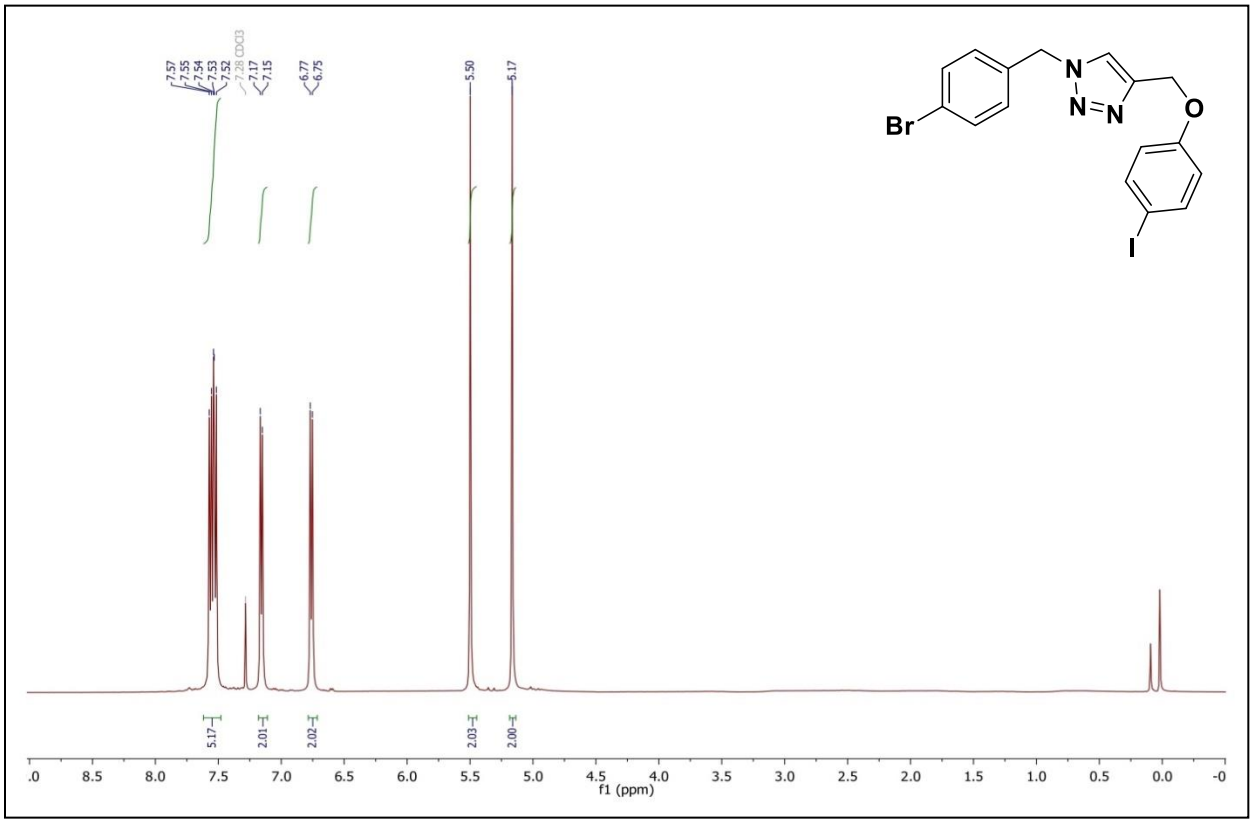


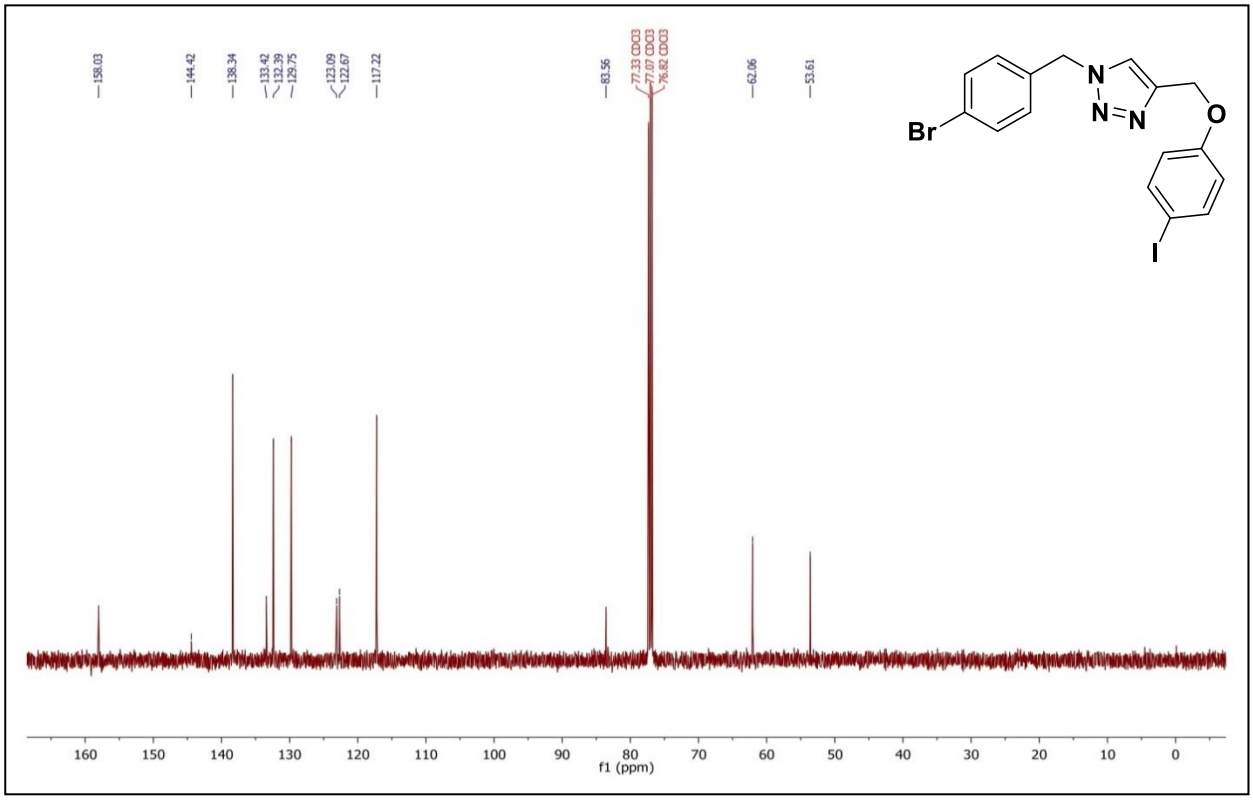
^{1}H NMR and ^{13}C NMR spectra of ethyl 1-benzyl-1H-1,2,3-triazole-4-carboxylate **(Scheme 3 , Entry 6o)** respectively.



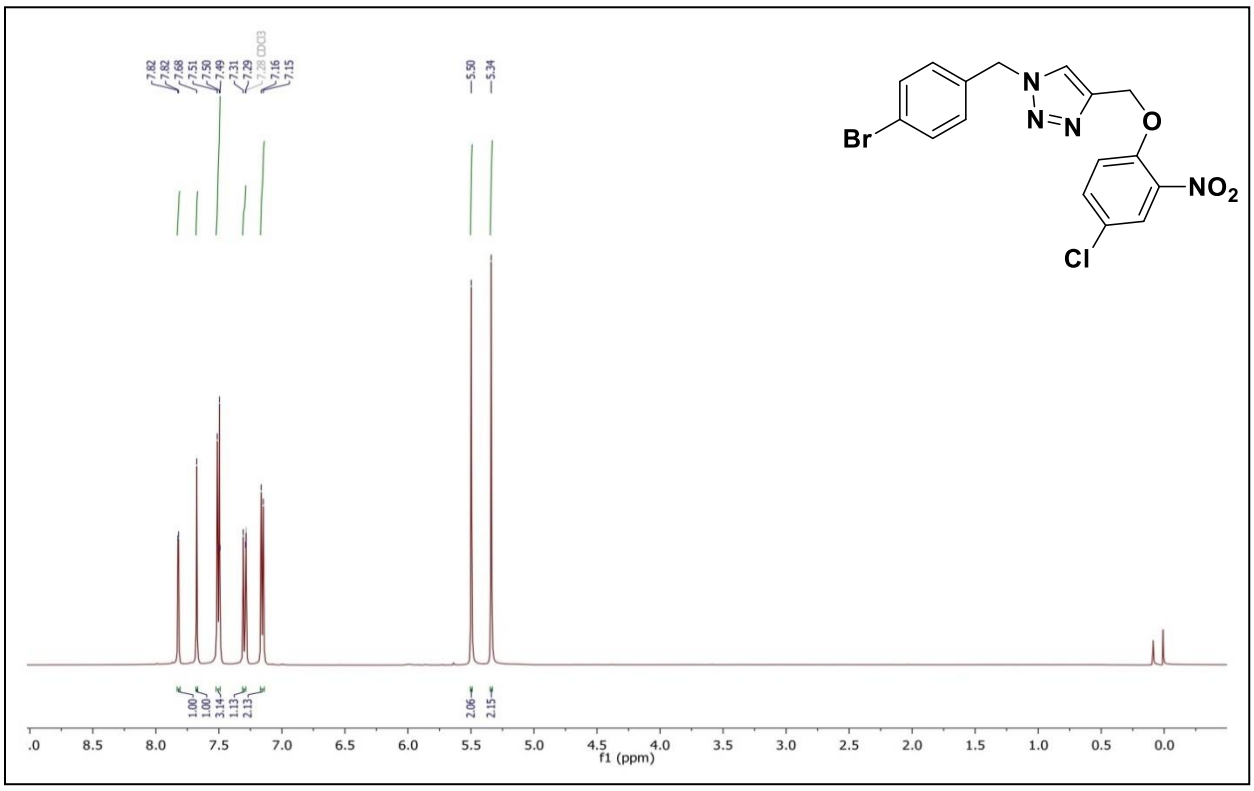


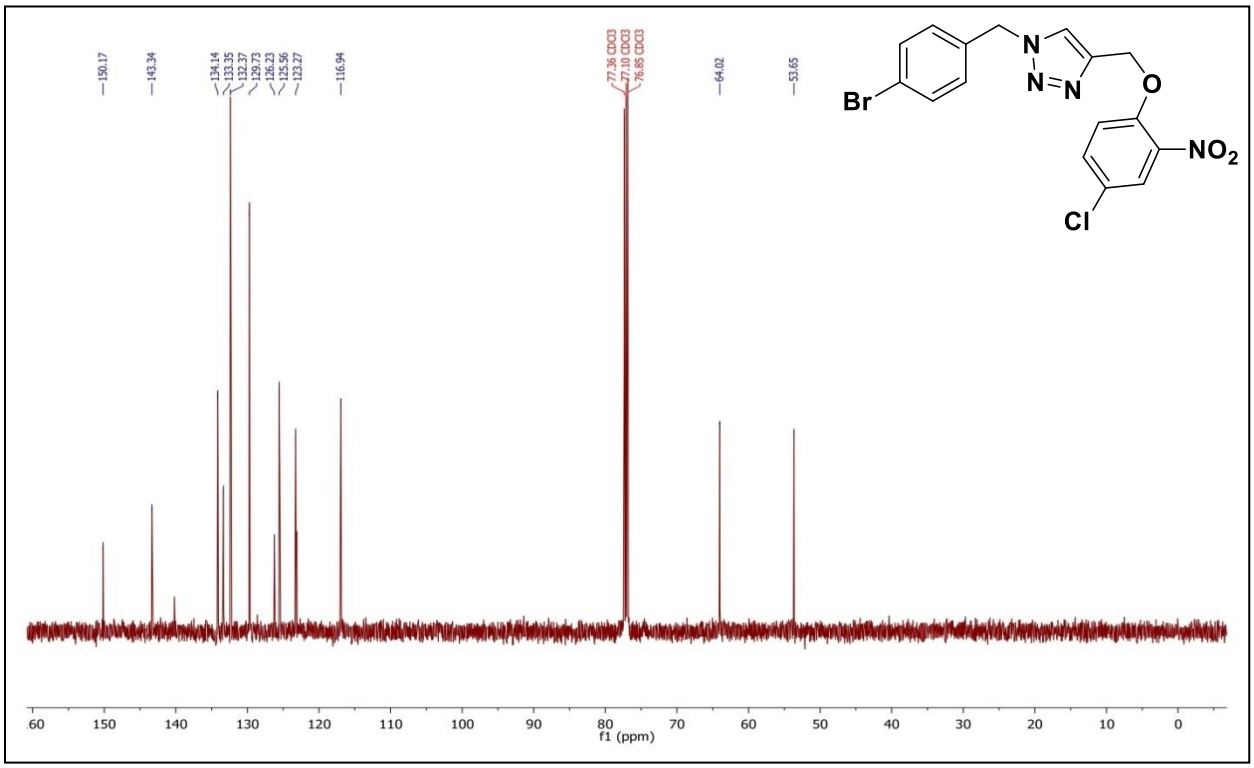
^{1}H NMR and ^{13}C NMR spectra of 1-(4-bromobenzyl)-4-((4-iodophenoxy)methyl)-1H-1,2,3-triazole **(Scheme 3, Entry 6p)** respectively.



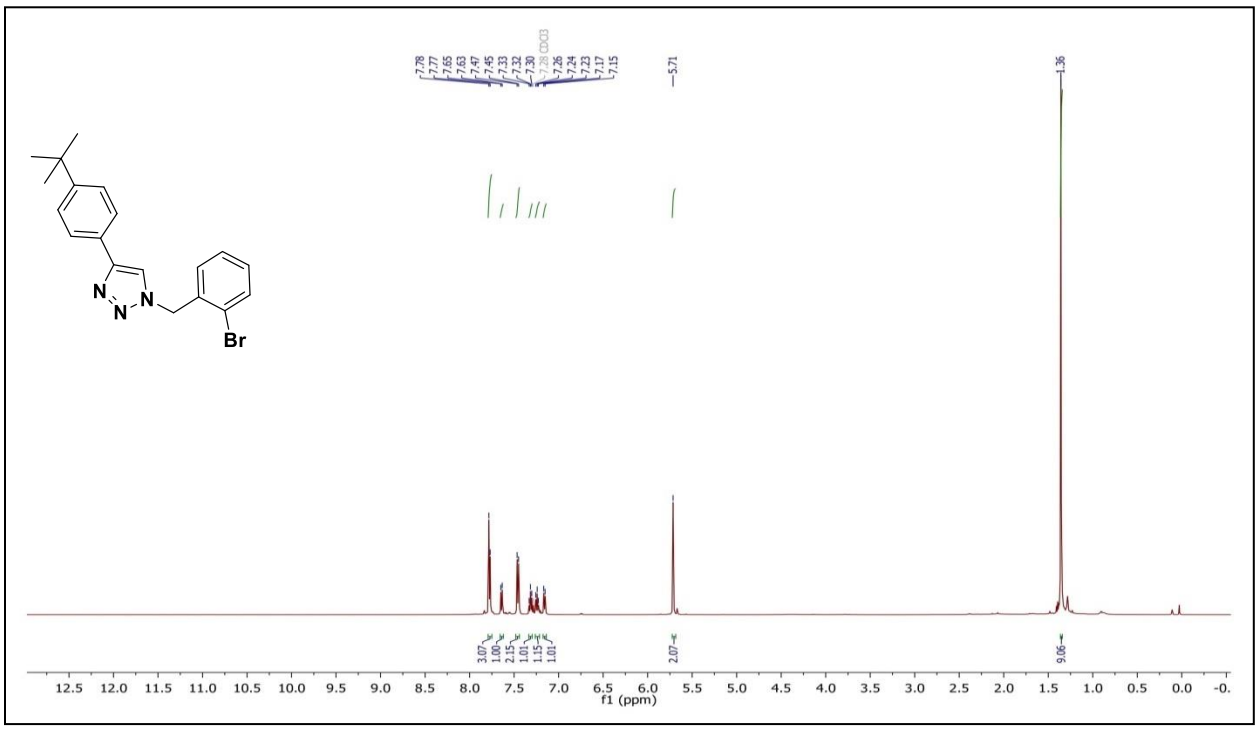


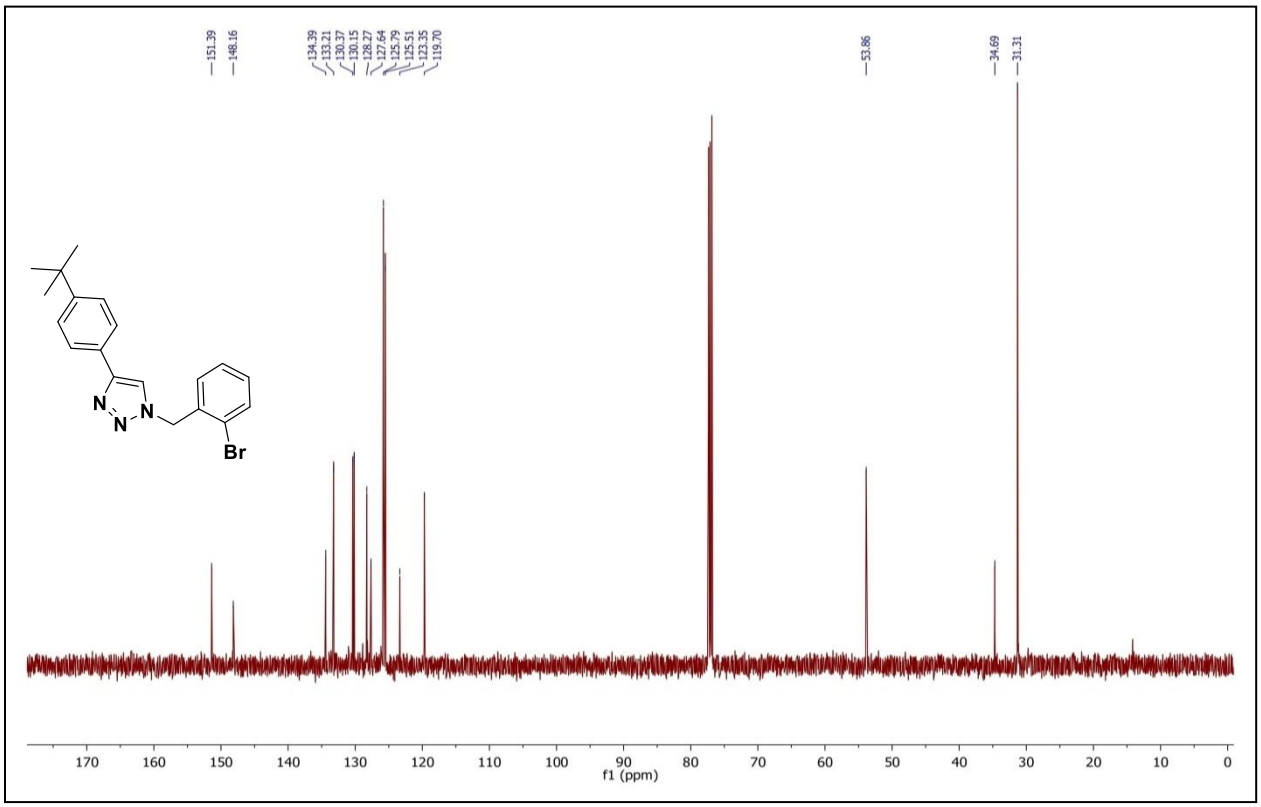
^{1}H NMR and ^{13}C NMR spectra of 1-(4-bromobenzyl)-4-((4-chloro-2-nitrophenoxy)methyl)-1H-1,2,3-triazole **(Scheme 3, Entry 6s)** respectively.



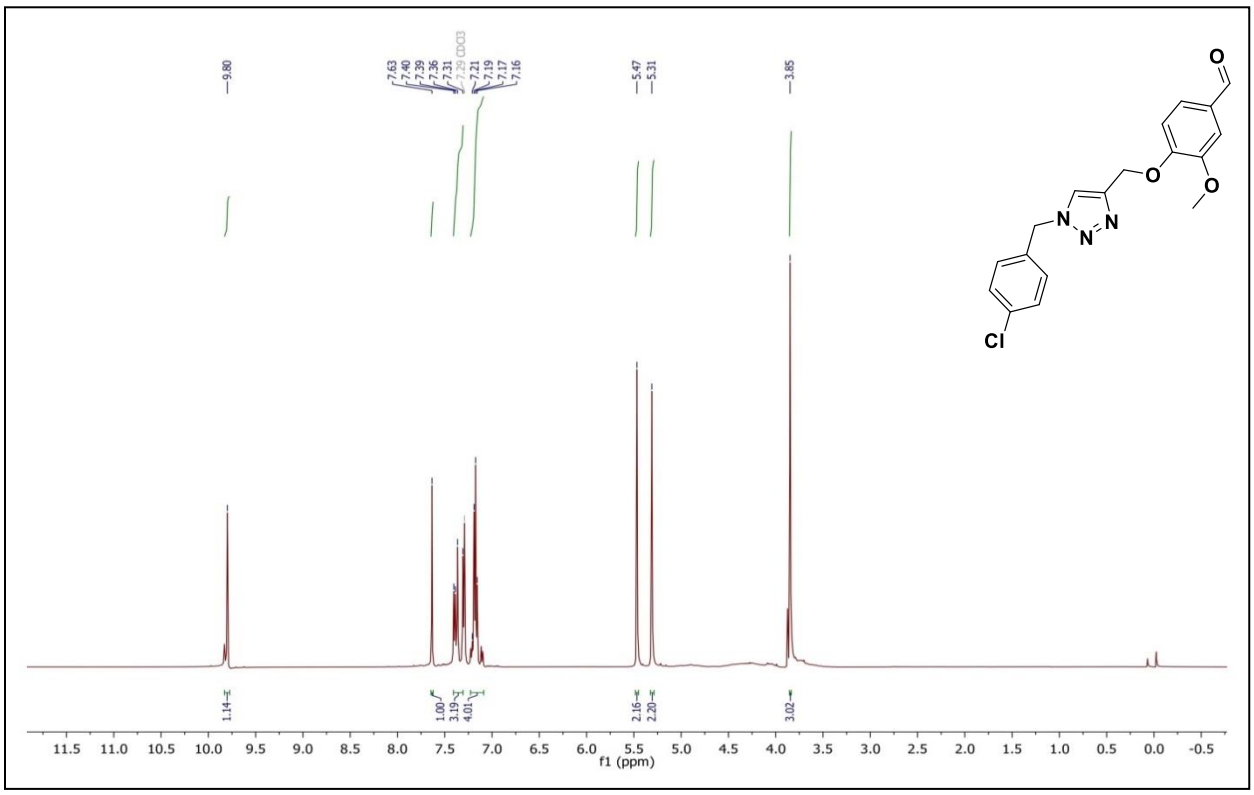


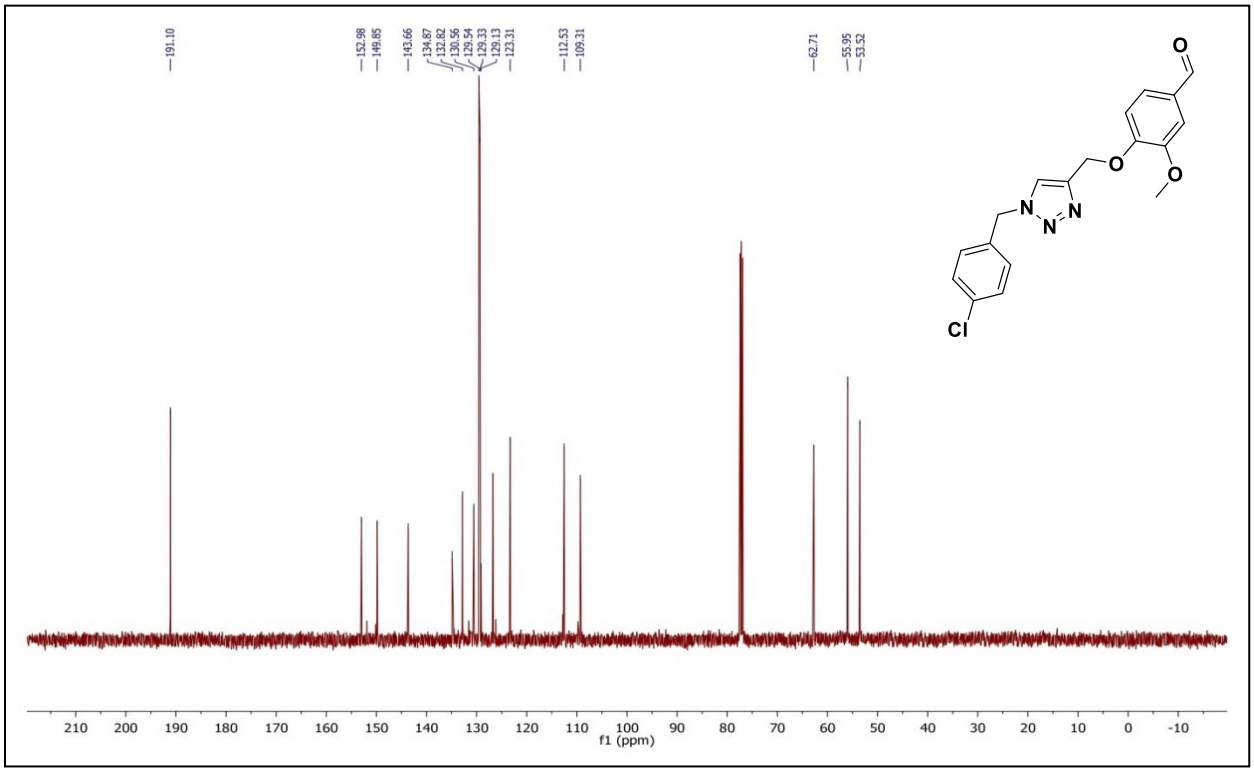
^{1}H NMR and ^{13}C NMR spectra of 1-(2-bromobenzyl)-4-(4-(tert-butyl)phenyl)-1H-1,2,3-triazole **(Scheme 3, Entry 6u)** respectively.



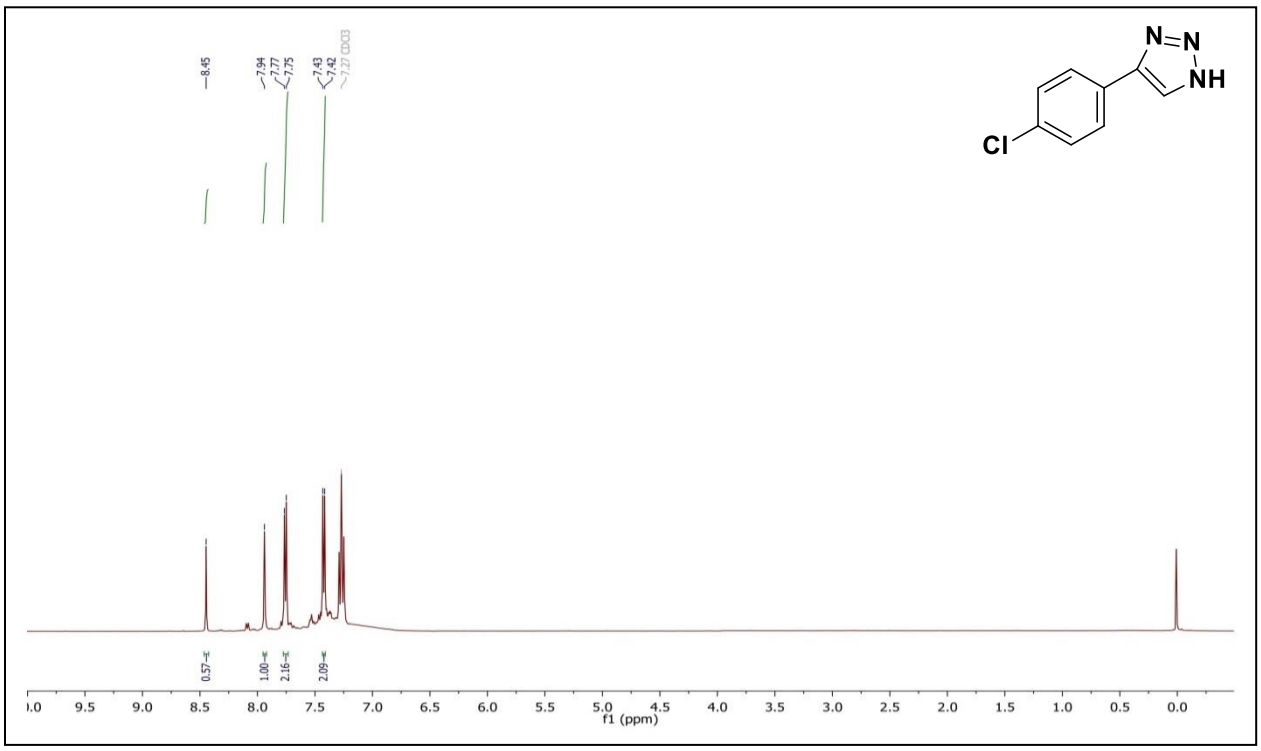


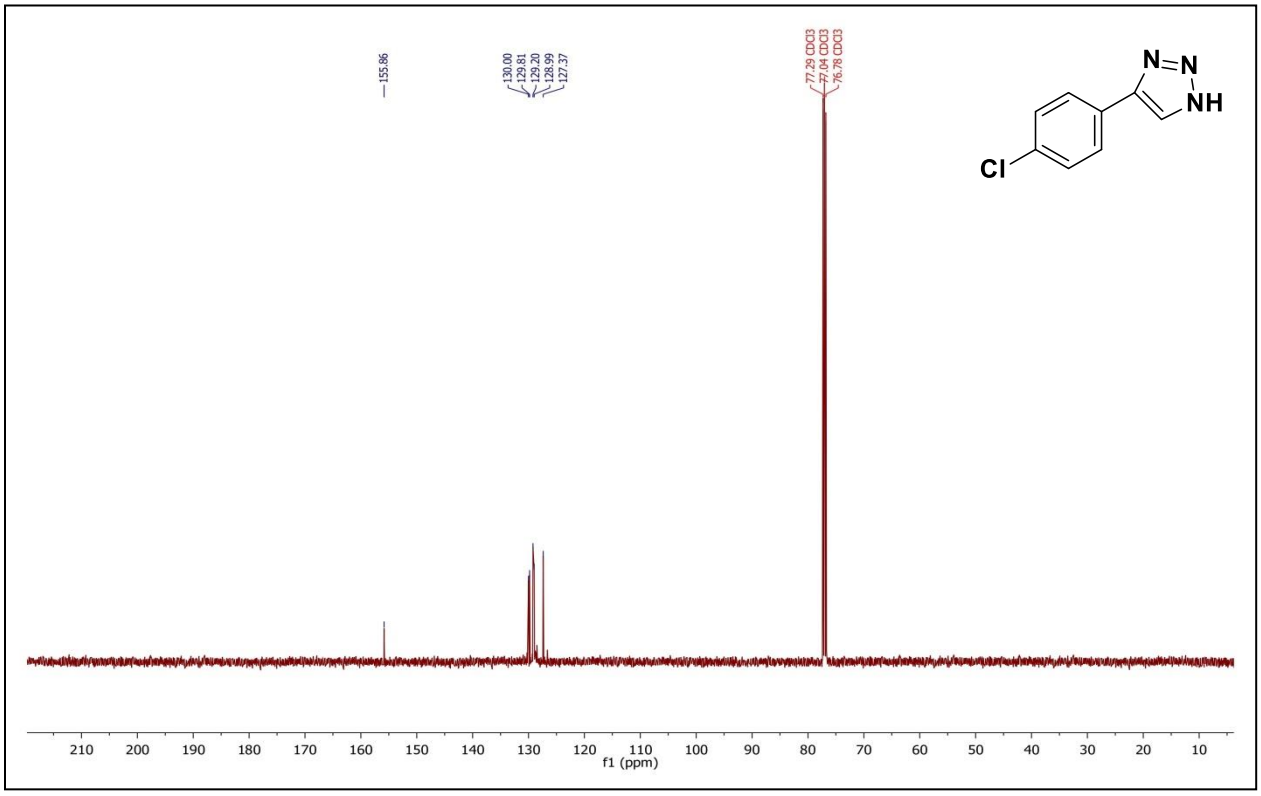
^{1}H NMR and ^{13}C NMR spectra of 4-((1-(4-chlorobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)-3-methoxybenzaldehyde **(Scheme 3, Entry 6v)** respectively.



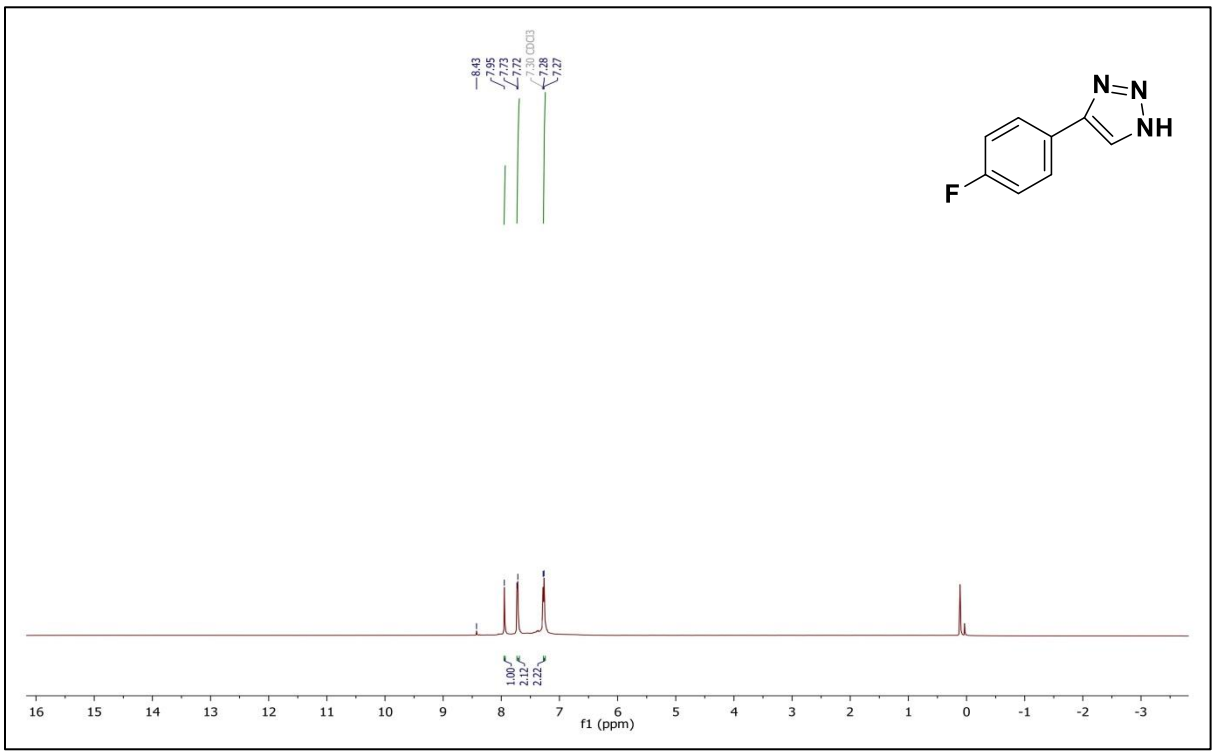


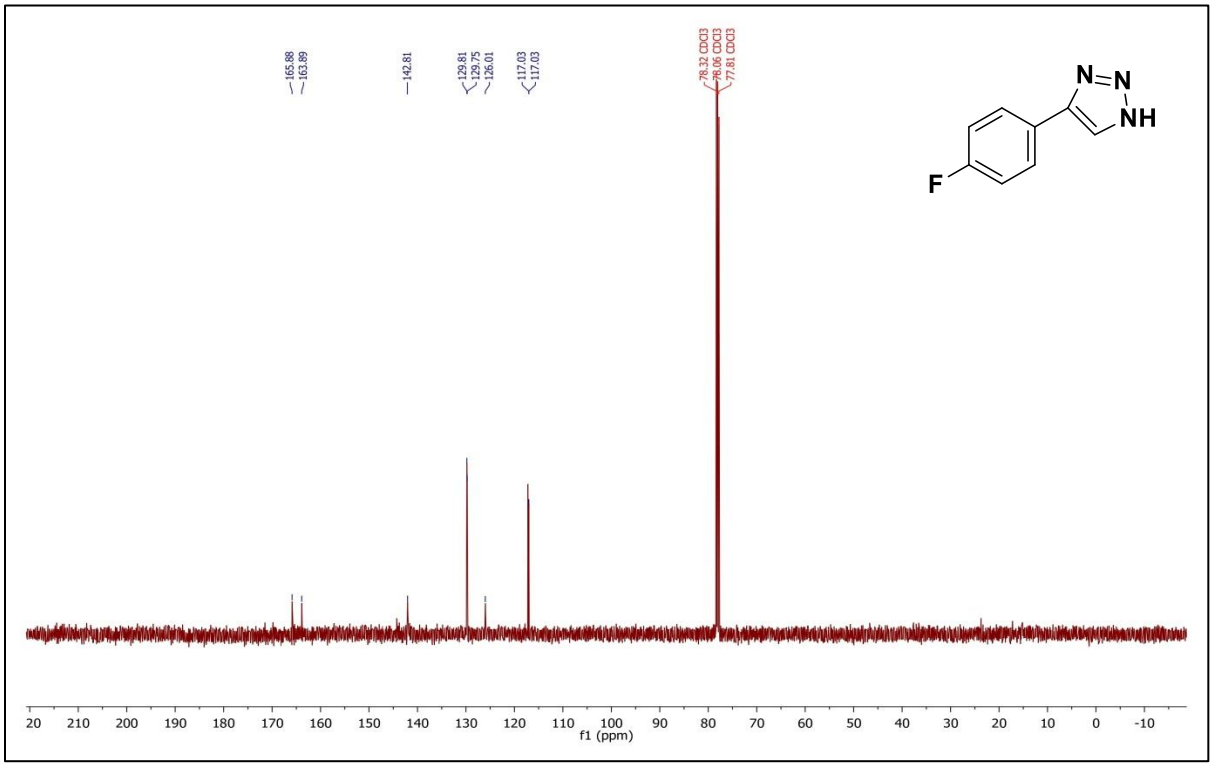
^{1}H NMR and ^{13}C NMR spectra of 4-(4-chlorophenyl)-1H-1,2,3-triazole **(Scheme 5, Entry 14a)** respectively. (**Ref: 29**)



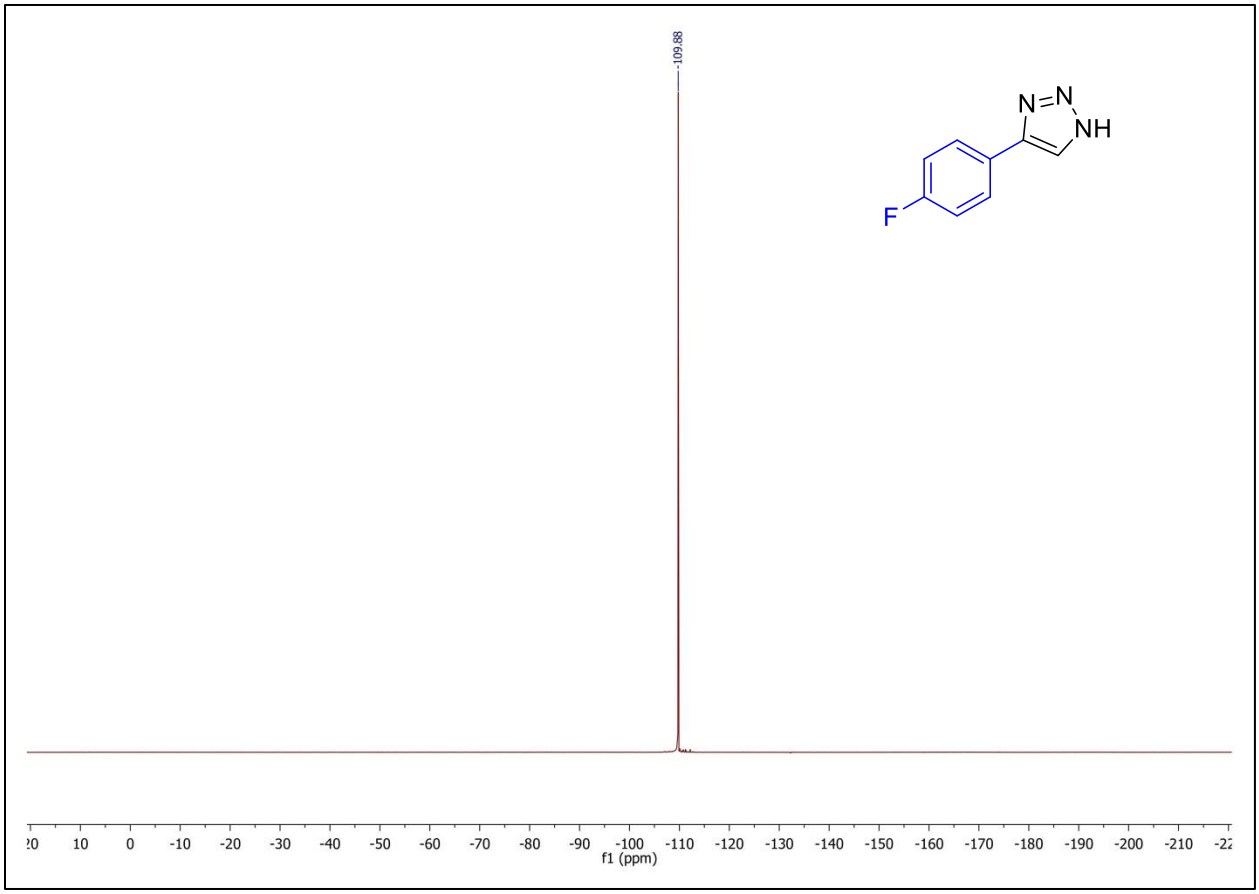


^{1}H NMR and ^{13}C NMR spectra of 4-(4-fluorophenyl)-1H-1,2,3-triazole **(Scheme 5, Entry 14b)** respectively.

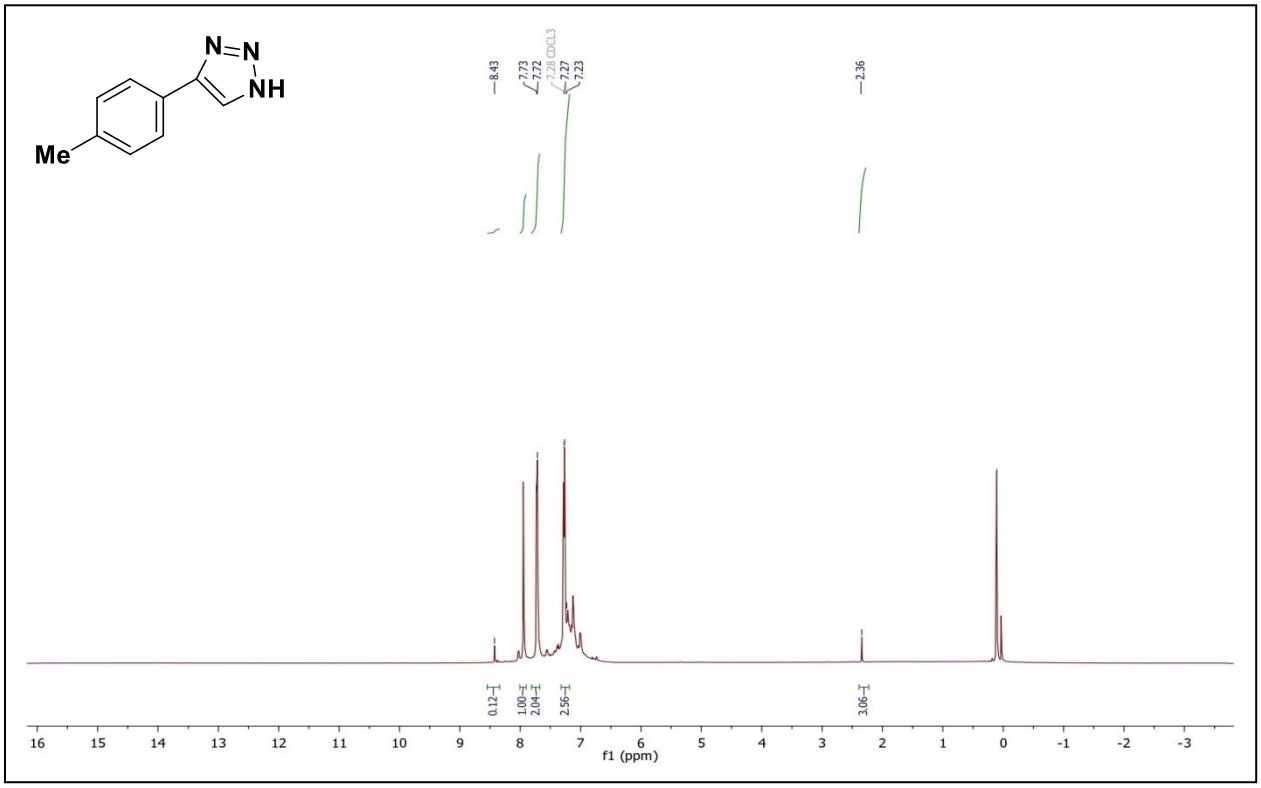


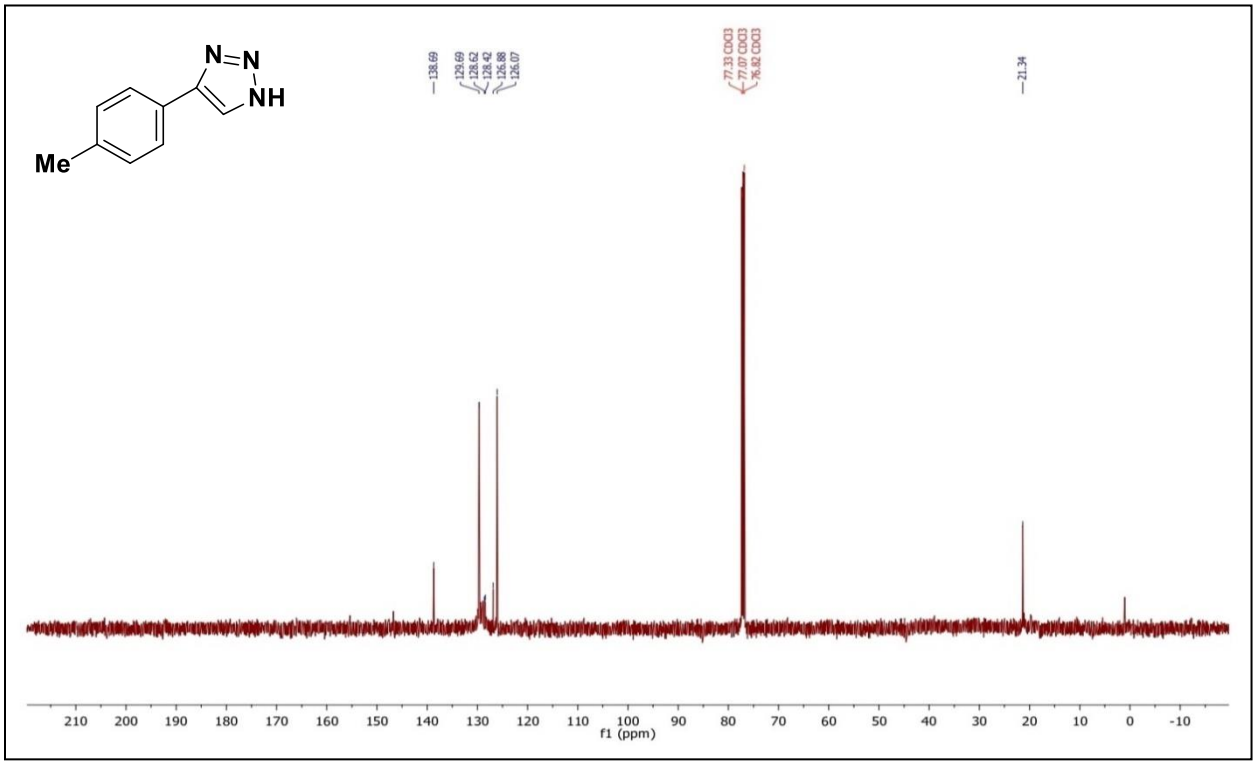


^{19}F NMR spectra 4-(4-fluorophenyl)-1H-1,2,3-triazole (**Scheme 5, entry 14b**)

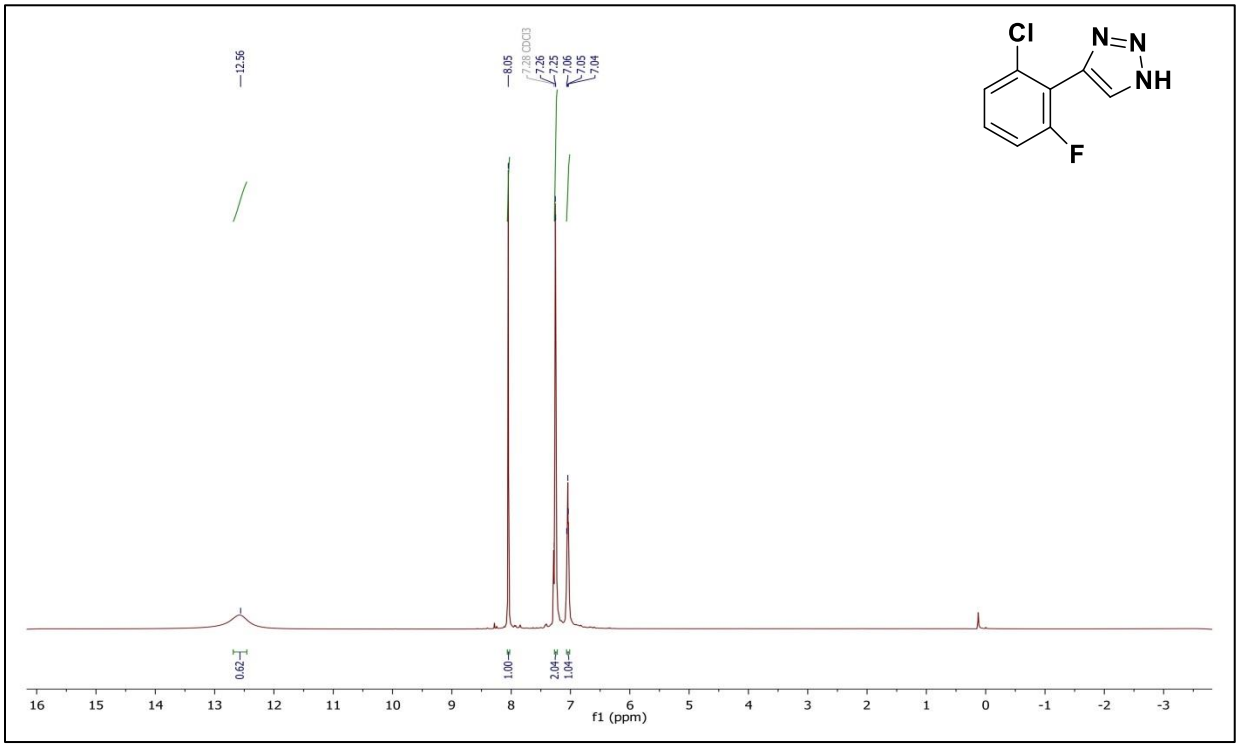


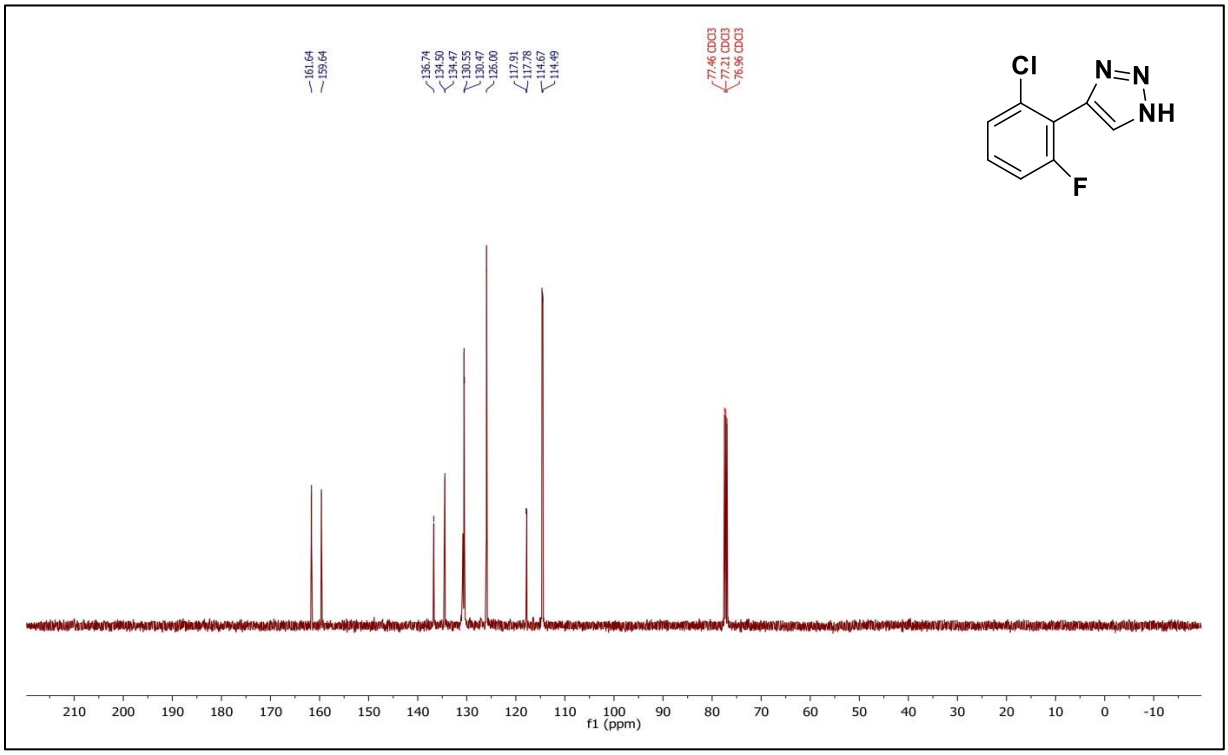
^{1}H NMR and ^{13}C NMR spectra of 4-(p-tolyl)-1H-1,2,3-triazole **(Scheme 5, Entry 14c)** respectively.



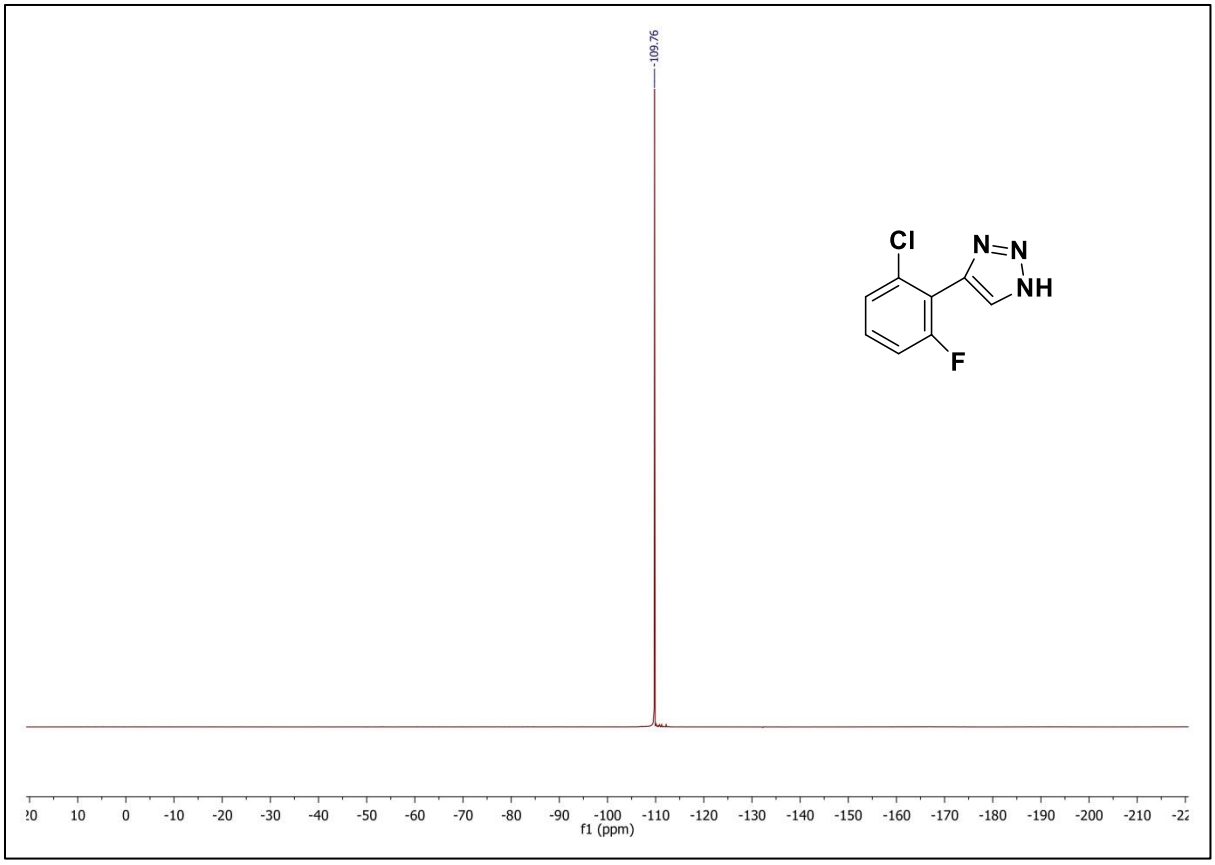


^{1}H NMR and ^{13}C NMR spectra of 4-(2-chloro-6-fluorophenyl)-1H-1,2,3-triazole **(Scheme 5, Entry 14d)** respectively.

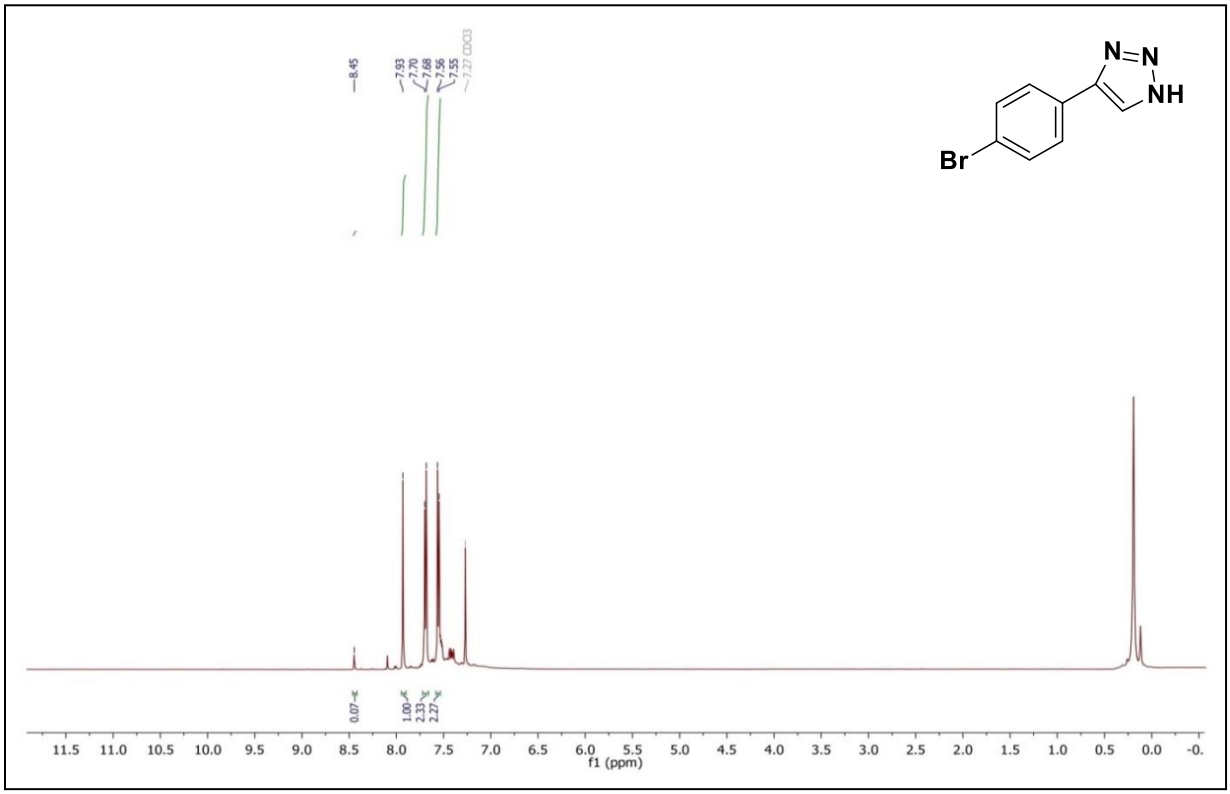


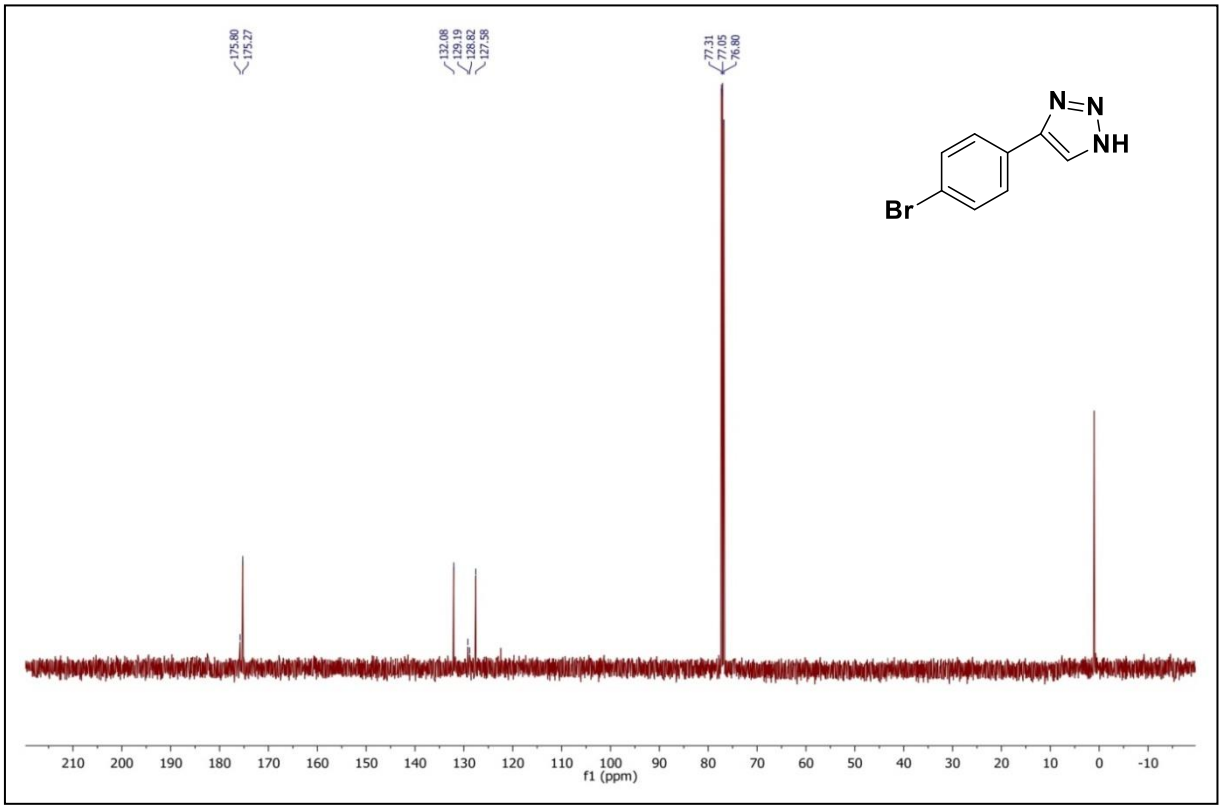


^{19}F NMR spectra of of 4-(2-chloro-6-fluorophenyl)-1H-1,2,3-triazole (**Scheme 5, entry 14d**)

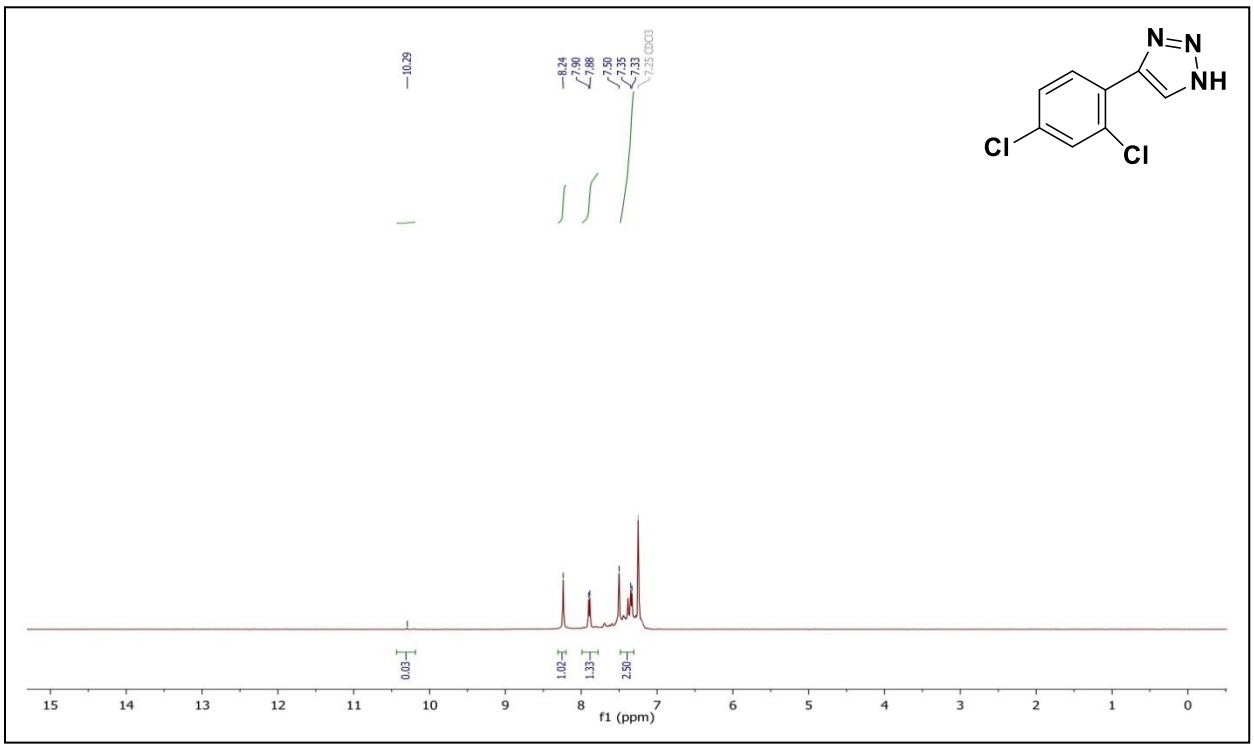


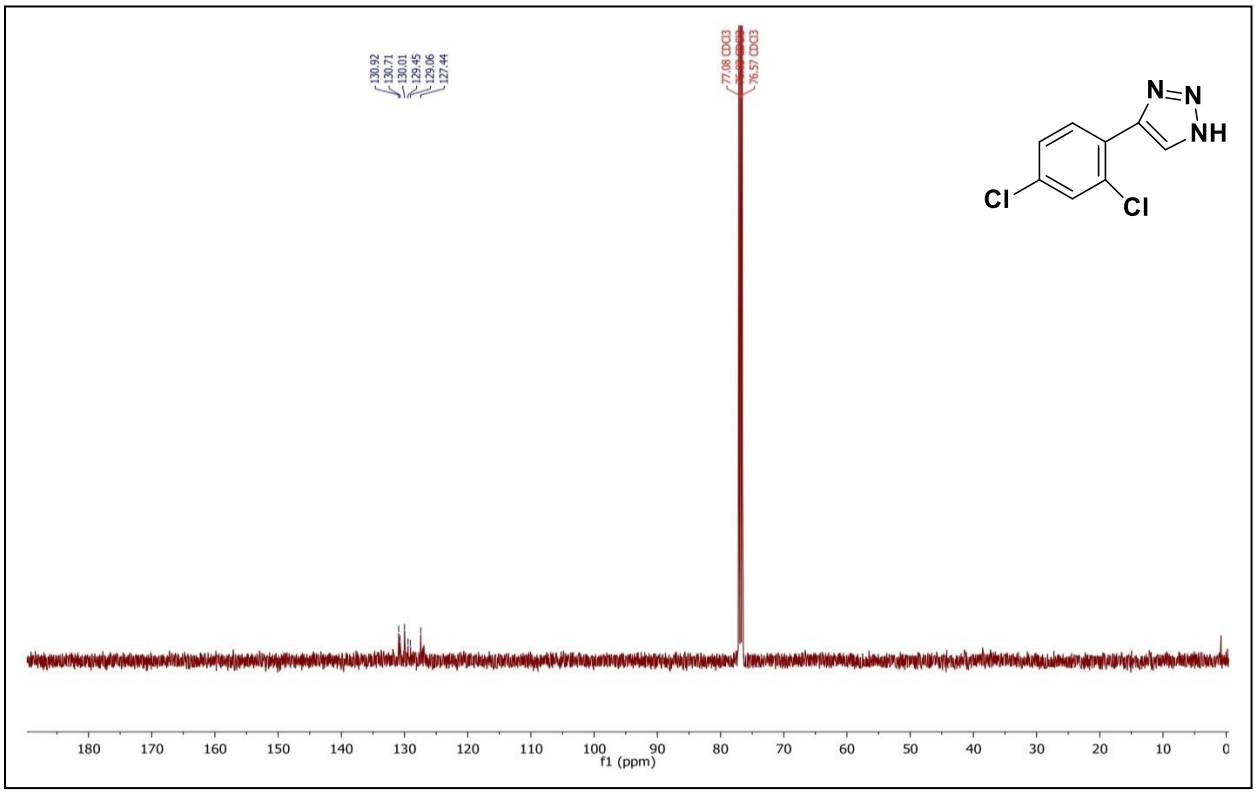
^{1}H NMR and ^{13}C NMR spectra of 4-(4-bromophenyl)-1H-1,2,3-triazole **(Scheme 5, Entry 14e)** respectively. (**Ref: 29**)



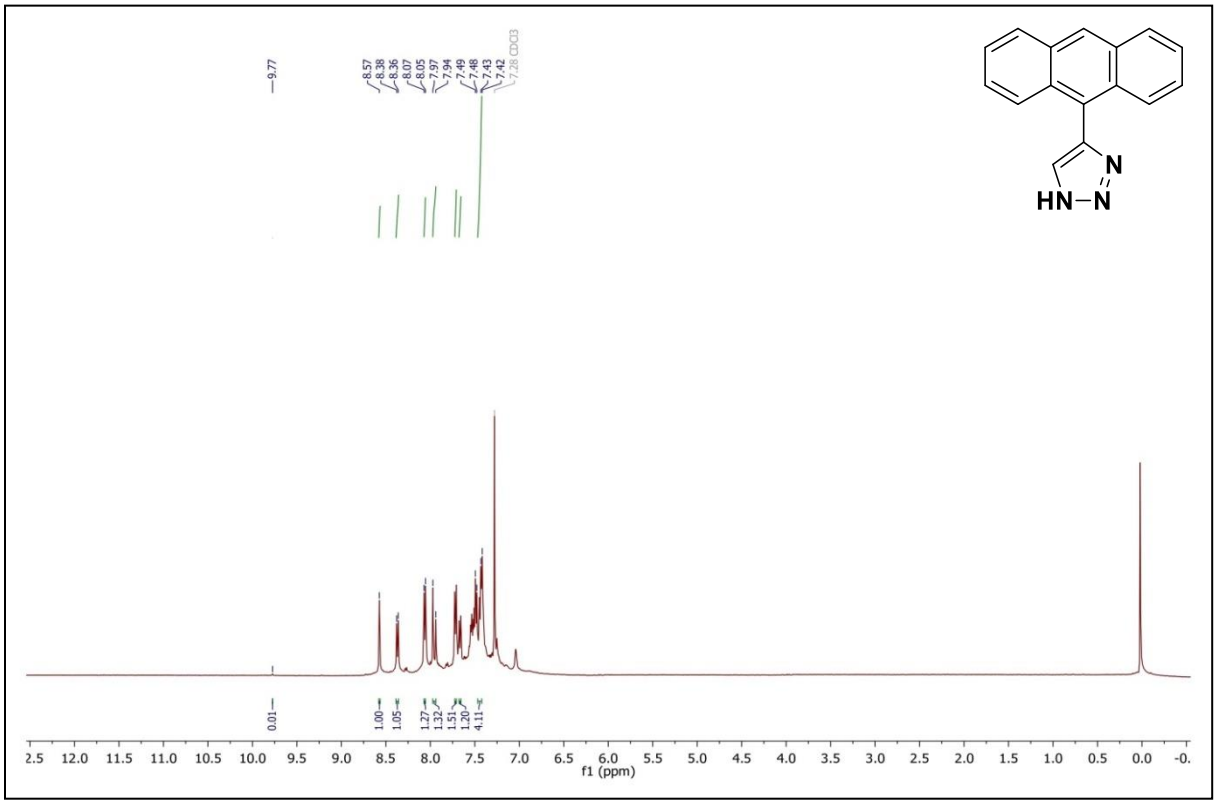


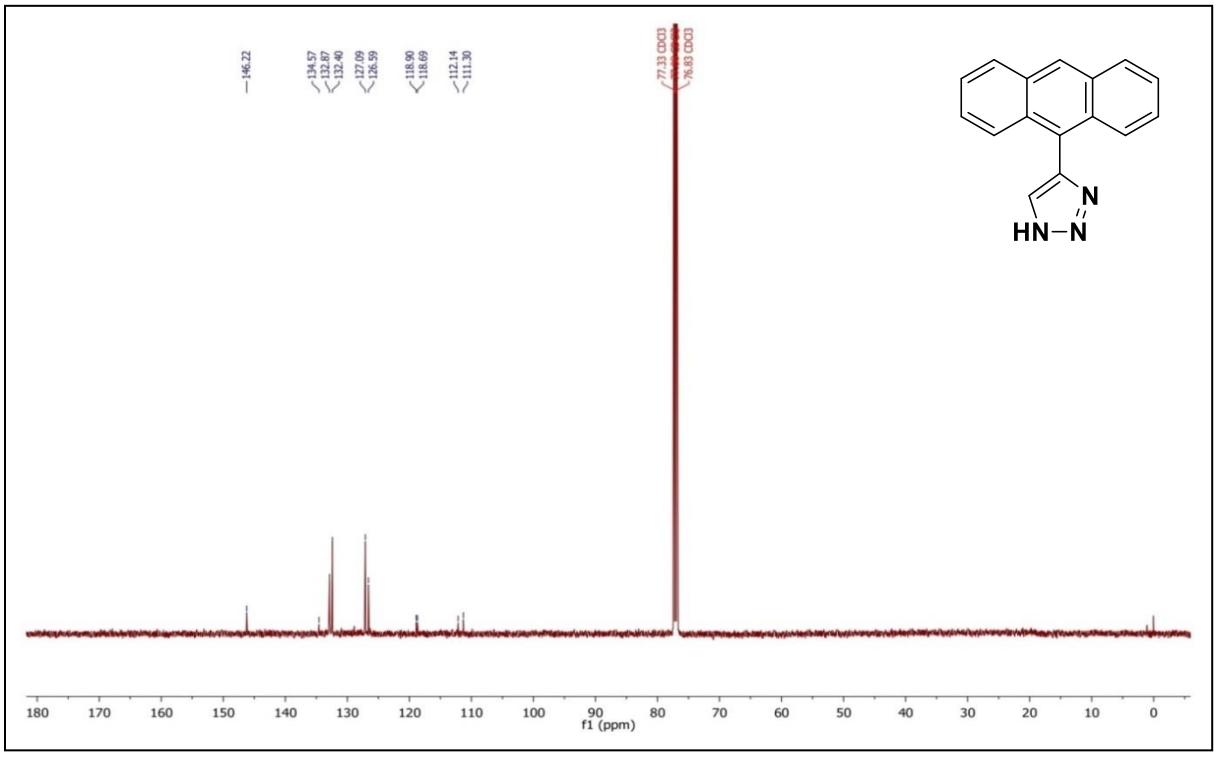
^{1}H NMR and C NMR spectra of 4-(2,4-dichlorophenyl)-1H-1,2,3-triazole **(Scheme 5, Entry 14f)** respectively.



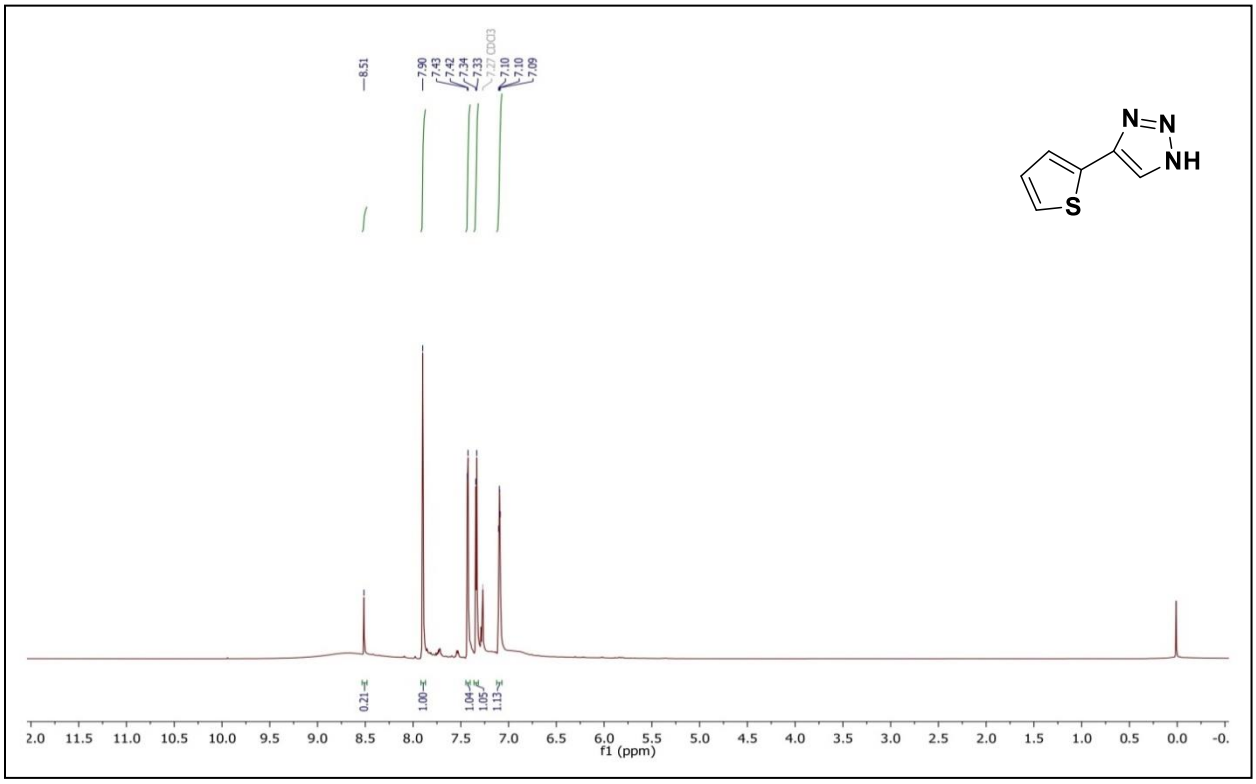


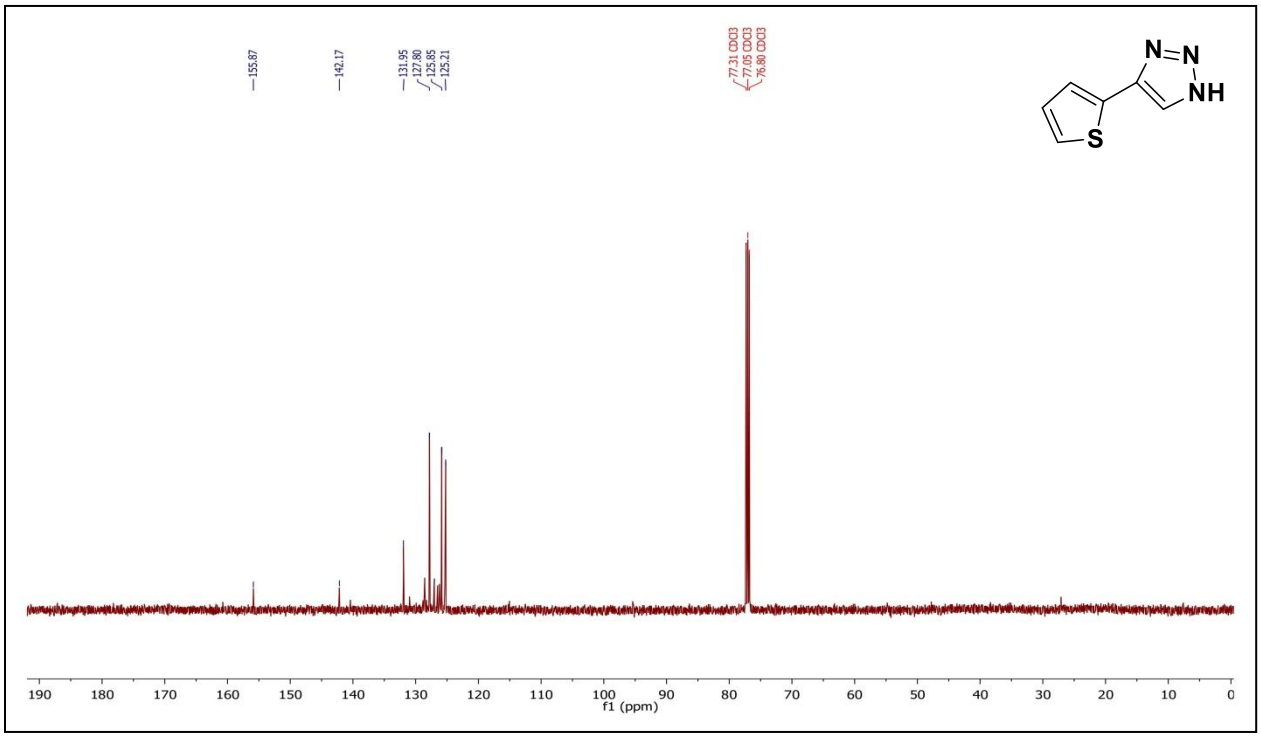
^{1}H NMR and ^{13}C NMR spectra of 4-(anthracen-9-yl)-1H-1,2,3-triazole **(Scheme 5, Entry 14g)** respectively.



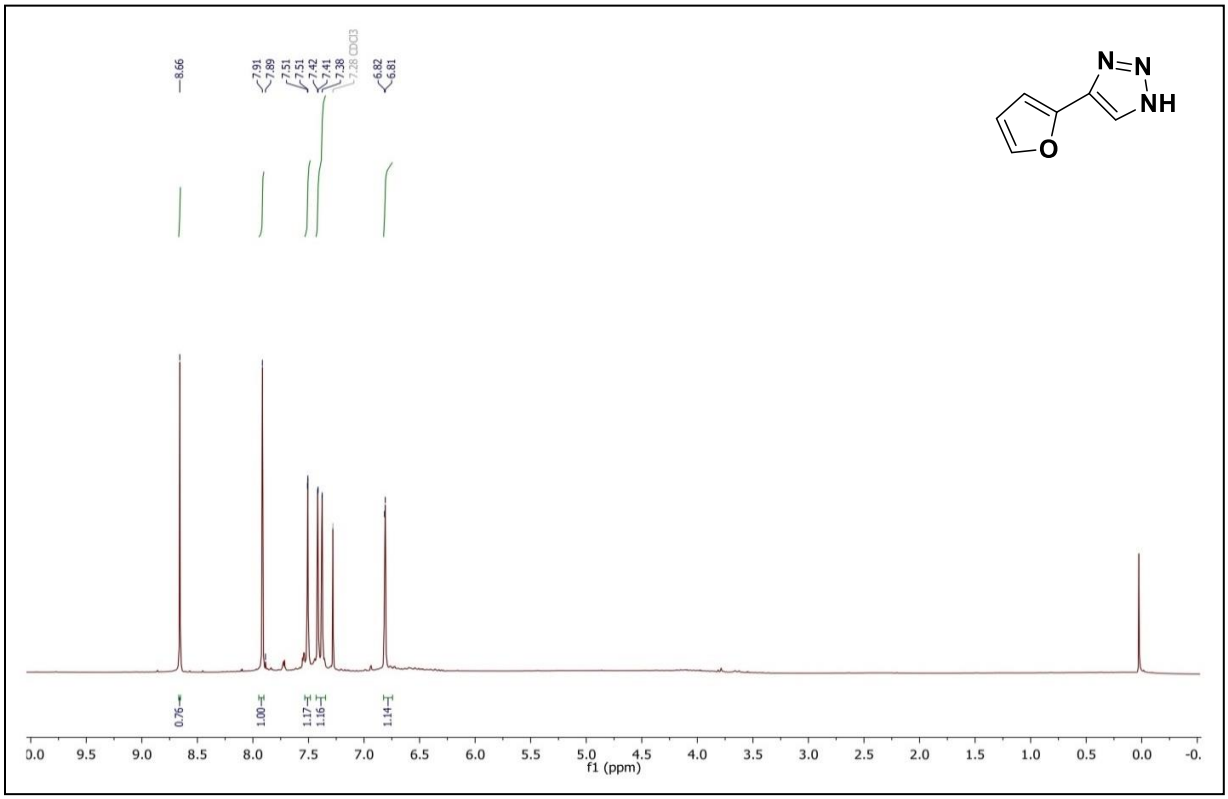


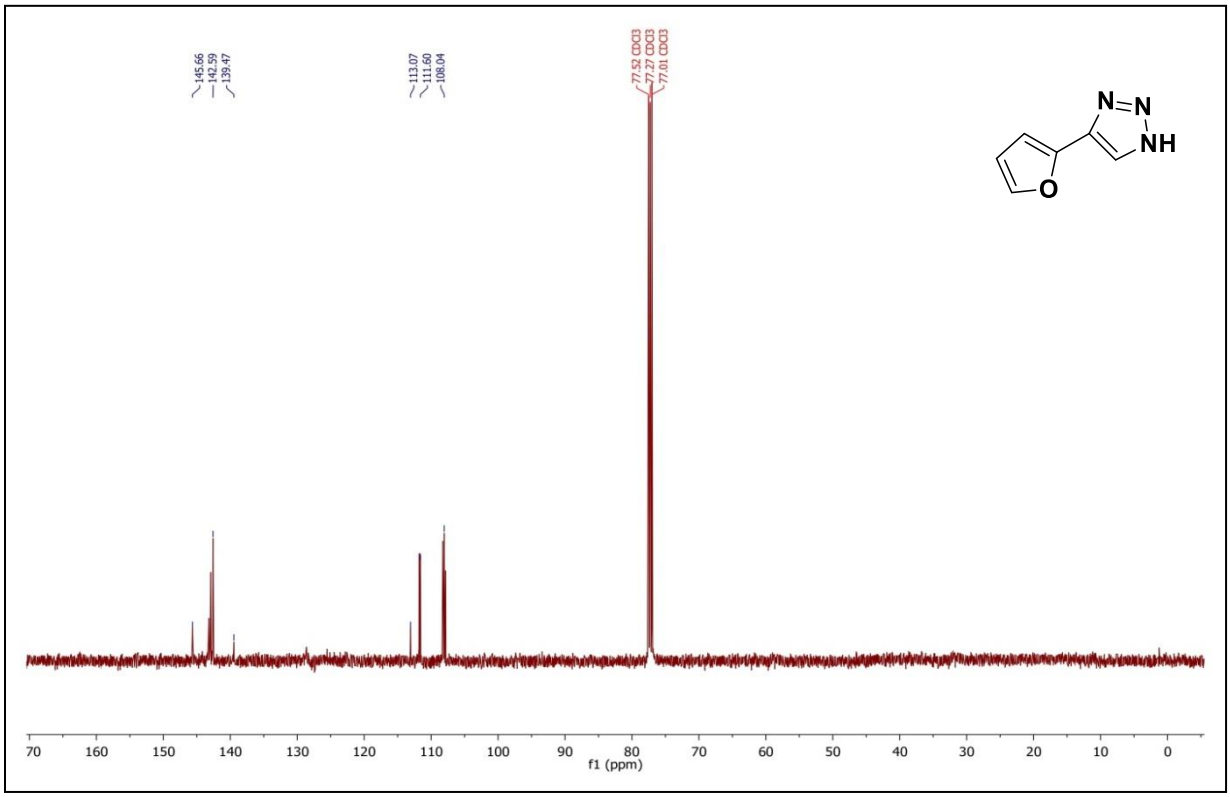
^{1}H NMR and ^{13}C NMR spectra of 4-(thiophen-2-yl)-1H-1,2,3-triazole **(Scheme 5, Entry 14h)** respectively.



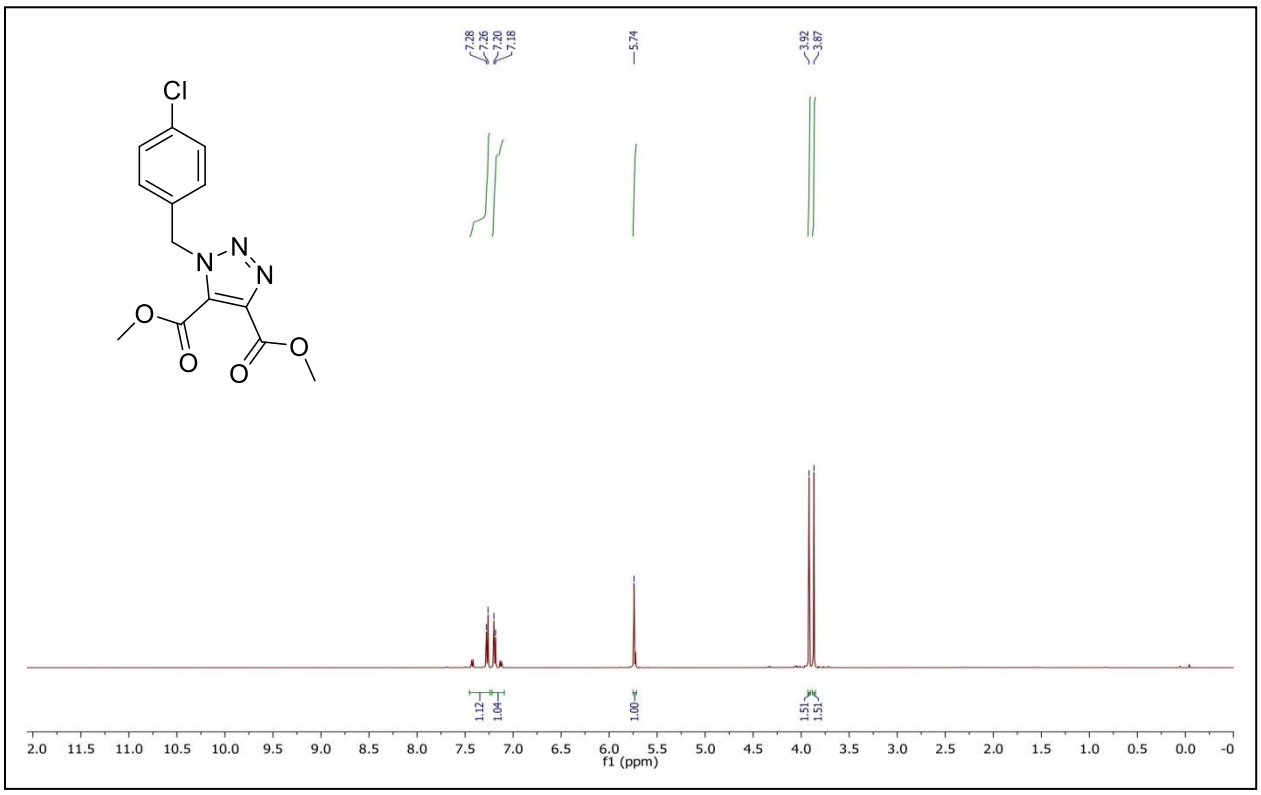


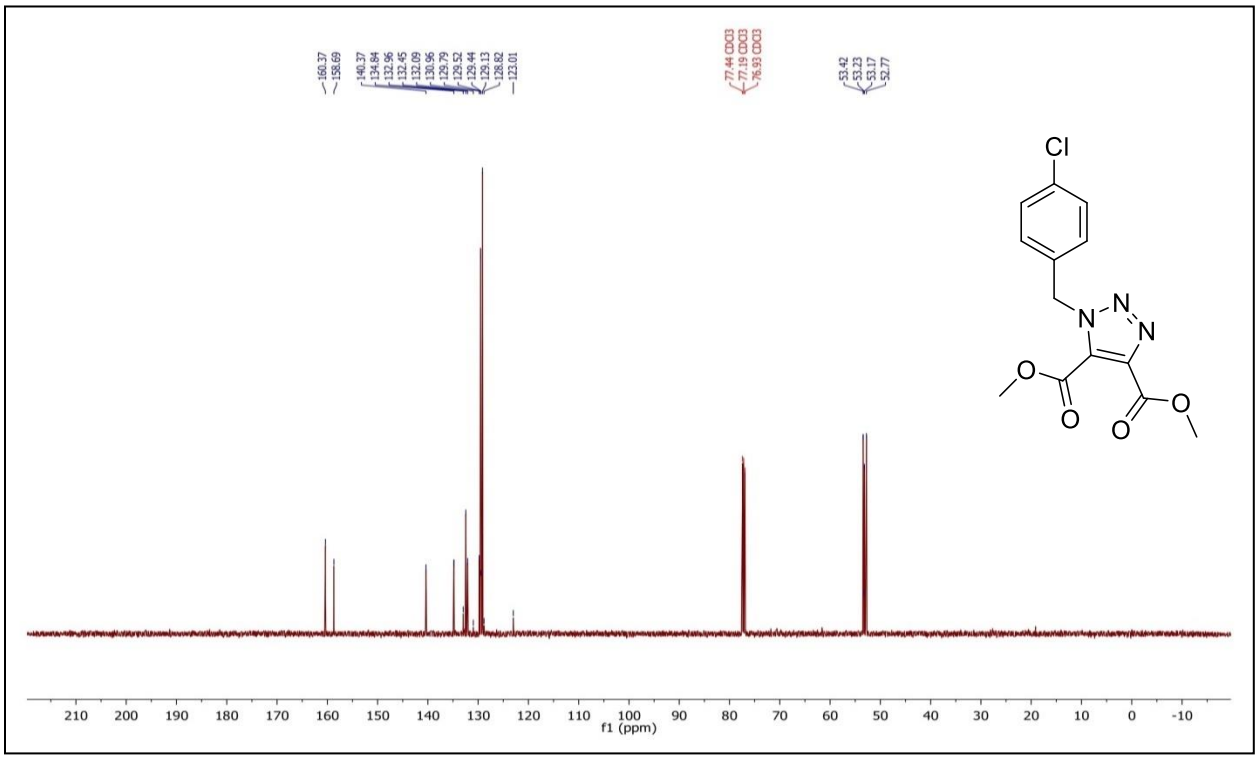
^{1}H NMR and ^{13}C NMR spectra of 4-(furan-2-yl)-1H-1,2,3-triazole **(Scheme 5, Entry 14i)** respectively.



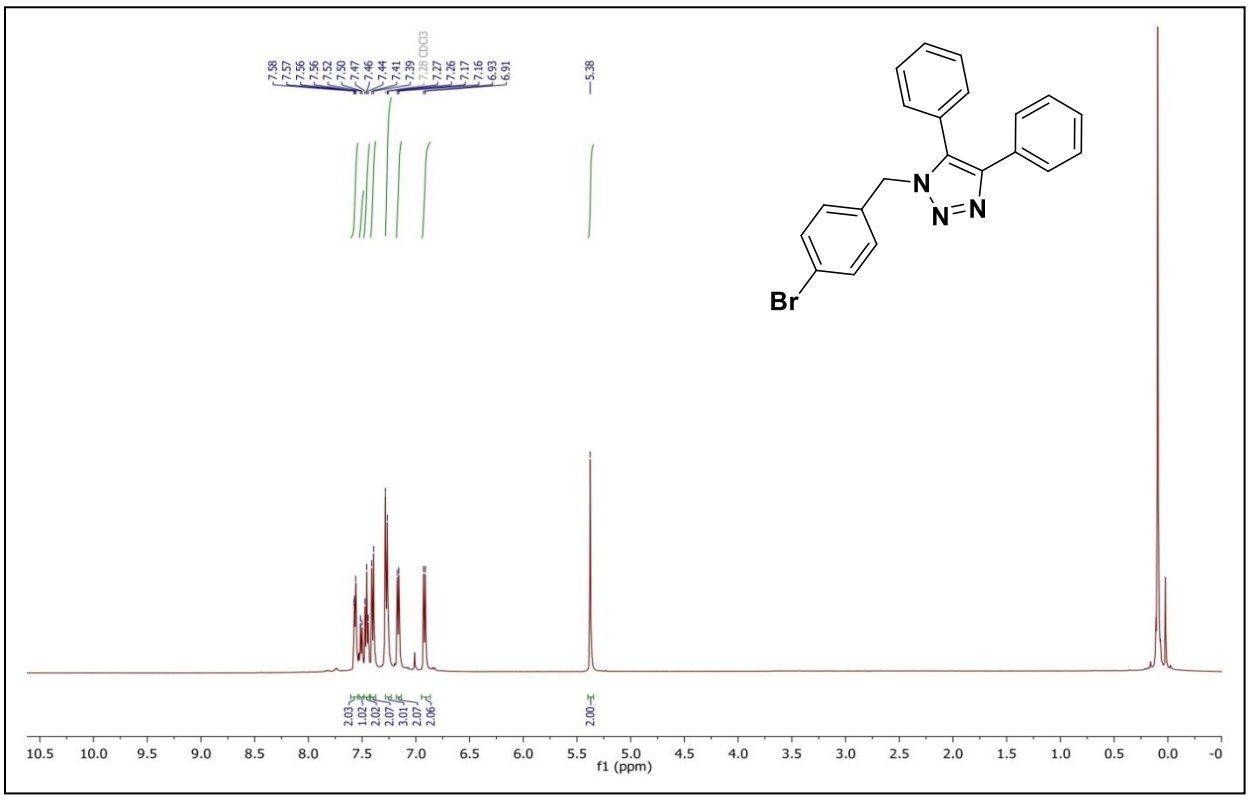


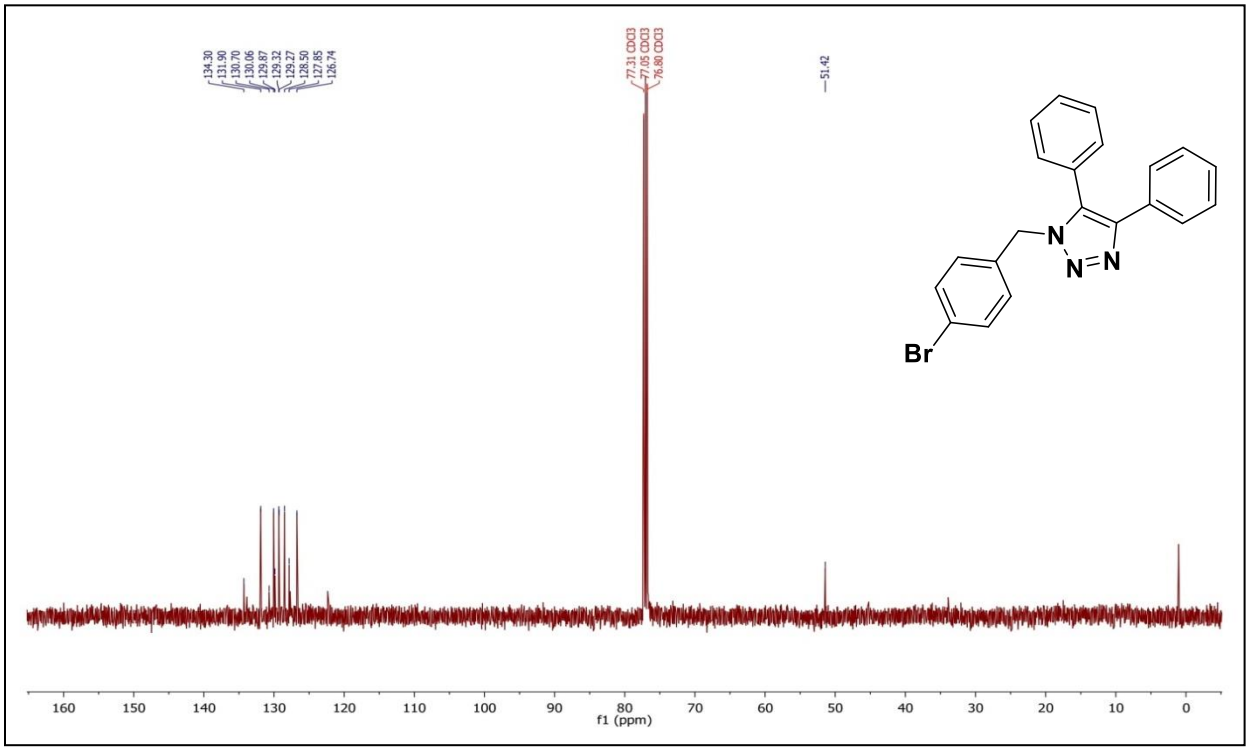
^{1}H NMR and ^{13}C NMR spectra of dimethyl 1-(4-chlorobenzyl)-1H-1,2,3-triazole-4,5-dicarboxylate **(Scheme 6, Entry 17a)** respectively.





^{1}H NMR and ^{13}C NMR spectra of 1-(4-bromobenzyl)-4,5-diphenyl-1H-1,2,3-triazole **(Scheme 6, Entry 17c)** respectively.





References

S1. S. Chassaing, M. Kumarraja, A. S. S. Sani, P. Pale, and J. Sommer, *Org. Lett.* **2007**, *9*, 883–886.

S2. J. –G.Wu, X. -J. Liao, L. Yuan, Y. Wang, Y. X. Zheng, J. L. Zuo and Y. Pan, *Chem. Eur. J.* **2020**, *26*, 5694–5700.

S3. S4. R., Jahanshahi, and B. Akhlaghinia. *RSC Advances*, **2016**, *6*, 29210-29219.

S4. S4. K. V. Aken, L. Strekowski and L. Patiny. *Beilstein J. Org. Chem.*, **2006**, *2*, 3.

CHECK CIF REPORT:

Datablock: H_a

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             alpha=90       beta=90.943(3) gamma=90
Temperature: 297 K
                    Calculated                      Reported
Volume              1316.8(2)                       1316.8(2)
Space group         P 21/c                          P 21/c
Hall group          -P 2ybc                         -P 2ybc
Moiety formula      C15 H12 Cl N3                   ?
Sum formula         C15 H12 Cl N3                   C15 H12 Cl N3
Mr                  269.73                          269.73
Dx,g cm-3           1.361                           1.361
Z                   4                               4
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F000'               560.75
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Nref                2317                            2305
Tmin,Tmax           0.954,0.978
Tmin'               0.951
Correction method= Not given
Data completeness= 0.995        Theta(max)= 24.985
R(reflections)= 0.0412( 2002)                   wR2(reflections)=
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S = 0.880              Npar= 172
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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 C

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.594 11 Report
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PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... 7 Note
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Alert level G

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PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL 2019/3 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 75% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note

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PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 50.0 Degree
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 9.72 Note
Predicted wR2: Based on SigI**2 1.45 or SHELX Weight 16.60
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 5 Info

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

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

PLATON version of 06/01/2024; check.def file version of 05/01/2024

Datablock H_a - ellipsoid plot