Supplementary Information (SI) for New Journal of Chemistry.

Amberlyst-15H Cu(II) Catalyzed Diazotization-Azidation-Cycloaddition: A Streamlined Route to Triazoles from Aliphatic Amines

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Material and Methods

All reactions were conducted using Triple distilled water unless specified otherwise. The reagents were obtained at the highest commercial grade and utilized without additional purification, unless **s**pecified differently. Reactions were stirred using a magnetic stirrer and observed using thin layer chromatography (TLC) on 0.25 mm E. Merck silica gel plates (60F254) under UV light. The visualization was done using an aqueou**s** **s**olution of potassium permanganate with heat. 0.25 mm E. Merck silica gel plates (60 F254) were used for preparative TLC. Column chromatography was performed using 100-200 mesh Silica gel, NMR spectra and were obtained using Bruker AN400. The spectra were calibrated using residual undertreated solvent as an internal reference (for $CDCl_3$, $^1H = \delta$ 7.26 and $^{13}C = \delta$ 77.16, for DMSO-d_6 $^1H = \delta$ 2.50 and $^{13}C = \delta$ 40.6-39.4). These acronyms are used to denote multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, m = multiplet, br = broad, app = evident. High-resolution mass **S**pectrometric data using electrospray ionization (ESI) were obtained with a SCIEX TripleTOF 6600 High Resolution Accurate Mas**S**ystem. IR spectra were recorded on a PerkinElmer FT-IR spectrometer (model: Spectrum Two) in the range of 4000–400 cm^{-1} using KBr pellets or neat samples, as appropriate. The characteristic absorption bands are reported in wavenumbers (cm^{-1}). ESR spectra were obtained using a JEOL JES-FA200 ESR spectrometer operating at X-band frequencies (~9.4 GHz). Spectra were recorded at room temperature or liquid nitrogen temperatures (77 K), depending on the sample's stability. Microwave power, modulation amplitude, and sweep width were optimized to maximize signal resolution and sensitivity. XPS analyses were performed on a Thermo Scientific K-Alpha XPS instrument equipped with a monochromatic Al K_α source (1486.6 eV). Survey spectra were collected to determine elemental composition, and high-resolution spectra were analyzed for oxidation state determination using CasaXPS software. Calibration was performed using the C 1s peak at 284.8 eV as the reference.

General Procedure for the catalysis:

Preparation of Catalyst: 20mg Amberlyst** in 2 ml of TDW was **s**uspended followed by the addition of $CuSO_4.5H_2O$ (5 mg, w/w, or till the point when the $CuSO_4$ colour no more disappears). The obtained Cu@Amberlyst was filtered and allowed to dry at room temperature.

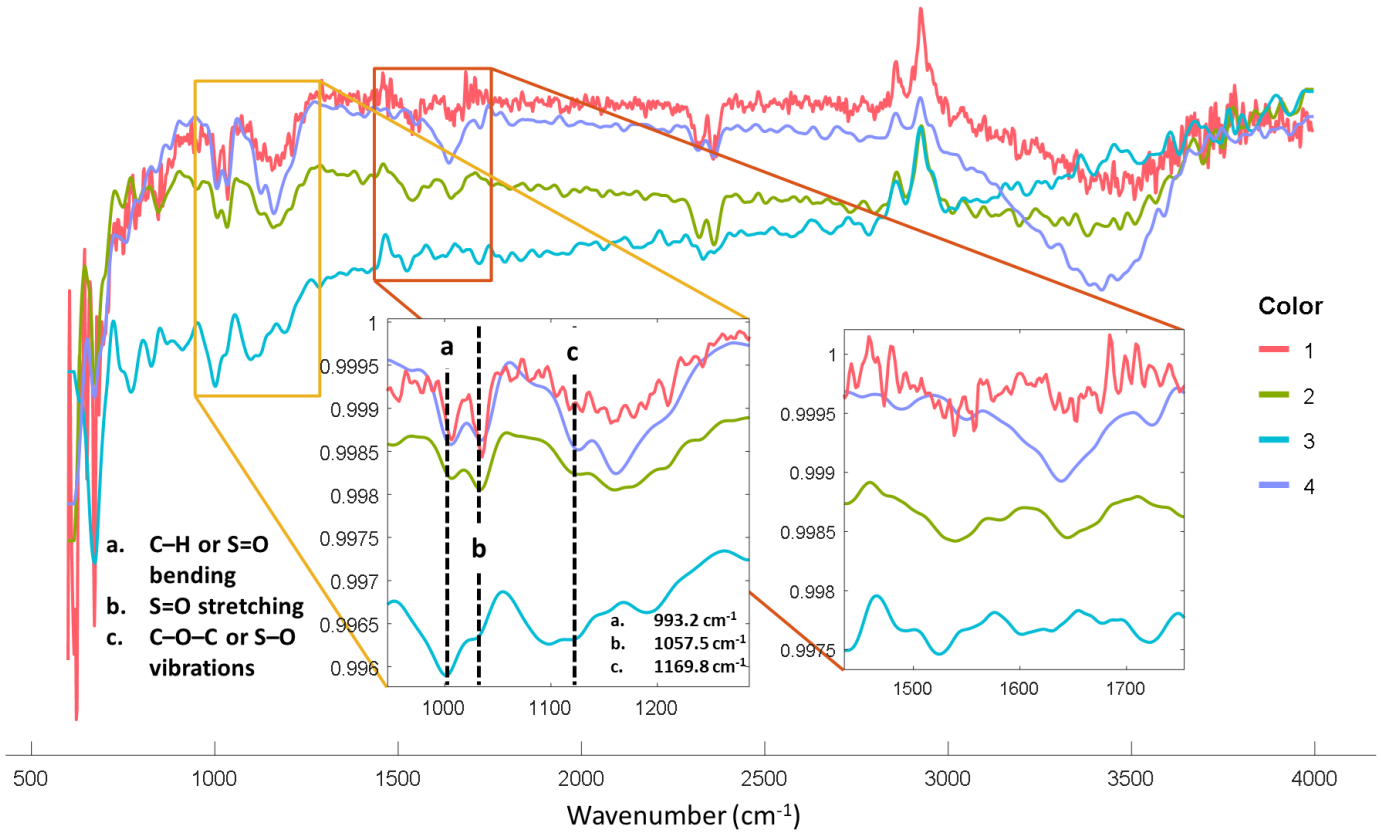


Figure S1. IR study of the sample Cu@Amberlyst catalyst (Cu:Amberlyst (**2, navy blue**) 0:100; (**1, red**) 10:100; (**3, dirty green**) 50:100; and (**4, blue**) 100:100)

Interaction with $CuSO_4$ showed shifts in the characteristic peaks of Amberlyst 15H, at 993.2, 1057.5, 1169.789, 1636.9, 1656.7, 2315.8, 2365.9, 2992.2, 3407.4 cm^{-1} predominantly due Cu^{2+} ions coordinate with functional groups like sulfonic acid groups in the resin. Broadening of Peaks due to increased heterogeneity in the chemical environment of the functional groups is evidenced a**s s**hown in the **Figure** 1 as the loading of the Cu increased from the 10-100:100.

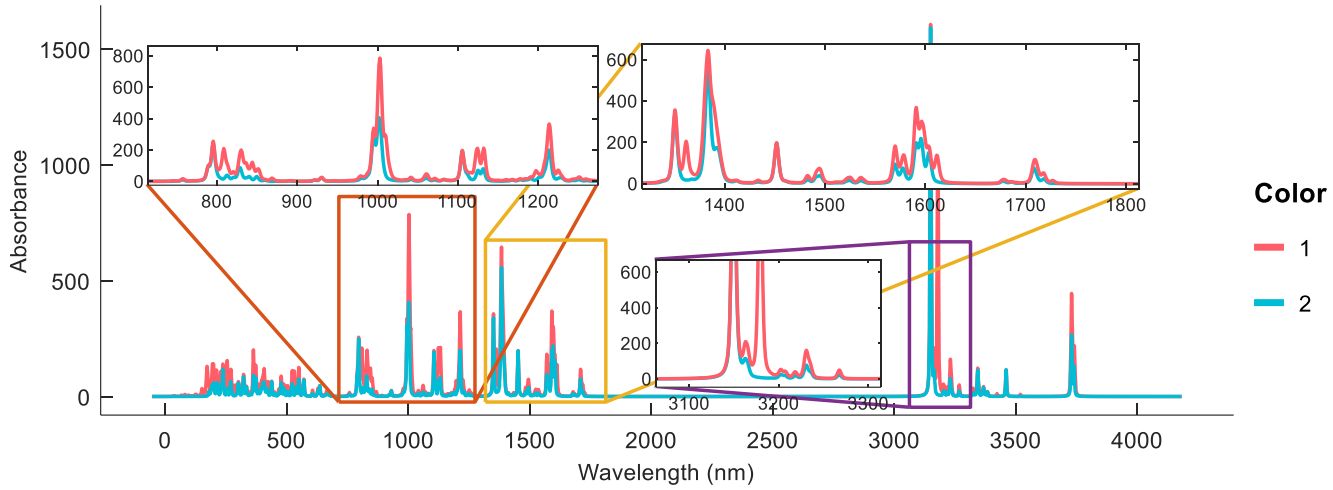


Figure S2. Predicted IR of proposed catalyst (Cu@Amberlyst (2, blue) and Amberlyst (1, red)

Reaction Procedure: A round-bottom flask (*R*.B.) was charged with 1% (w/w) of the catalyst (5 mg), followed by the addition of butylamine (*n*-$BuNH_2$) (50 mg, 0.68 mmol, 1.0 eq). Sodium nitrite (47 mg, 0.68 mmol, 1.0 eq) was then added at 5°C. After 20-30 minutes, sodium azide (47 mg, 0.71 mmol, 1.05 eq) was added, and the

reaction was allowed to proceed at room temperature for 6-8 hours. Upon completion, the reaction mixture was separated, and the mother liquor was treated with 2N K_2CO_3 (6-7 drops) to eliminate residual hydrazoic acid (HN_3). The organic compounds were extracted using ethyl acetate (EtOAc, 10 mL × 3), and the organic layer was separated, dried over anhydrous sodium sulfate (Na_2SO_4, 200 mg), and evaporated under reduced pressure. The crude product was subjected to NMR analysis. (**Note:** (a) In the case of aromatic amines or alkynes, sodium dodecyl sulfate (SDS, 5 mg) was added, whereas this step was omitted for aliphatic partners. (b) Notably, while this step can tolerate up to 15°C, an increase in temperature significantly affects the yield of the coupling reaction. (c) Direct freeze-drying of the mother liquor post-filtration resulted in a 5-7% increase in yield.) **^{1}H NMR (500 MHz, $CDCl_3$, δ, ppm):** 8.03 (s, 2H), 5.13 (m, *J* = 7.7, 4.3 Hz, 2H), 4.68 (d, *J* = 7.0 Hz, 4H), 3.56 – 3.49 (t, 2H), 2.78 (m, *J* = 12.2, 4.0 Hz, 2H), 2.62 (m, *J* = 12.5, 8.6, 4.5 Hz, 2H), 2.10 (m, *J* = 13.4, 4.1 Hz, 2H), 1.56 (m, *J* = 13.4, 9.0, 4.0 Hz, 2H).

Alternative Workup procedure for solid products: The obtained precipitate was filtered and recrystallised using Ethanol:Et_2O (1:5), to obtain solid pure products.

Conditions for the Preparation of Compound 3: A round-bottom flask was charged with 1% (w/w) of the catalyst (5 mg) and *n*-butylamine (*n*-$BuNH_2$) (50 mg, 0.68 mmol, 1.0 eq). Sodium nitrite (47 mg, 0.68 mmol, 1.0 eq) was added at 5°C. (**Note:** SDS (5 mg) was added for aromatic amines or alkynes, but this step was omitted for aliphatic partners. While the reaction can tolerate up to 15°C, an increase in temperature significantly affects the yield.) After 20-30 minutes, sodium azide (47 mg, 0.71 mmol, 1.05 eq) and the alkyne (74 mg, 0.75 mmol, 1.1 eq) were added, and the reaction was allowed to proceed at room temperature for 20-50 minutes. **^{1}H NMR (400 MHz, $CDCl_3$, ppm):** δ 7.75 (s, 1H, Triazole-**H**), 4.70 (d, *J* = 7.0 Hz, 2H, C**H**$_2$OH), 4.08 (t, *J* = 7.2 Hz, 2H, NC**H**$_2$$(CH_2)_2CH_3$), 1.90 – 1.76 (m, 2H, NCH_2C**H**$_2$Et), 1.31 (q, *J* = 7.4 Hz, 2H, $N(CH_2)_2$C**H**$_2CH_3$), 0.94 (t, *J* = 7.2 Hz, 3H, $N(CH_2)_2CH_2$C**H**$_3$); **^{13}CNMR (100 MHz, $CDCl_3$ + DMSO-d_6, ppm):** δ 143.3, 124.3, 54.8, 50.5, 31.2, 19.3, 13.7; **ESI-MS ($M+H^+$):** Calculated for $C_7H_{13}N_3O$: 155.1058, observed: 156.1131.

Alternative Workup procedure for solid products: The obtained precipitate was filtered and recrystallised using Ethanol:Et_2O (1:5), to obtain solid pure products.

Ex-situ NMR analysis:

Prepared 68.0 mM solution by dissolving *n*-$BuNH_2$ (3g) in 60 mL water, for 0.2 equiv 0.39mL, 0.4 equiv 0.79mL, 0.5 equiv 0.98 mL, 0.8 equiv 1.58mL, 1.0 equiv. 1.97 mL and 1.6 equiv, 3.16 ml of stock solution was added to 0.38ml (0.2 equiv), 0.77mL (0.4 equiv), 0.97mL (0.5), 1.552 mL (0.8 equiv), 1.94 mL (1.0 equiv) and 3.1mL (1.6 equiv.) of Propargyl alcohol from its respective stock solution prepared by adding 1.8g of Propargyl alcohol in 60 mL of water, followed by addition of NaN_3 (0.4mL, 0.81mL, 1.02 mL, 1.63mL, 2.04 mL and 3.26mL from the stock solution prepared using 2.1g in 60 mL) and $NaNO_2$ (0.43mL, 0.87 mL, 1.08mL, 1.73mL, 2.17mL and 3.47 mL from the stock solution prepared using 2.1 g in 60 mL water) The total volume of the reaction was made to 15 mL by adding additional water. And reaction sample were then operated under optmised reaction condition, and NMR sample were prepared every 10 min for a period of 2hrs

Table S1. Screening of various copper salts as catalysts for the click reaction

Entry[a]	Catalyst (*w/w*)[b]	Time (hr)	Temp(°C)	Yield (3 in %)
1.	Chitosan/$CuSO_4$	16	80	0
2.	Hyaluronic acid/$CuSO_4$	16	80	0
3.	Glucosamine/$CuSO_4$	16	80	5
4.	Amberlyst/$CuSO_4$ (1:0.05)	16	80	96
5.	Amberlyst/$CuSO_4$ (1:0.05)	16	27	88
6.	Amberlyst/CuI (1:0.05)	16	27	74
7.	Amberlyst/Cu_2O(1:0.05)	16	80	64
8.	Amberlyst/Cu_2O (1:0.02)	16	27	72
9.	Amberlyst/$CuSO_4$ (1:0.02)	16	64	92
10.	Amberlyst/$CuSO_4$ (1:0.05)	8	27	96
11.	Amberlyst/$CuSO_4$ (1:0.02)	8	27	94
12.	Amberlyst/$CuSO_4$ (1:0.01)	8	27	94
13.	Amberlyst 70/$CuSO_4$	8	58	10
14.	Amberlyst 35/$CuSO_4$	8	58	75
15.	Amberlyst 36/$CuSO_4$	8	58	8
16.	Amberlyst 15[##]/$CuSO_4$	4	27	96
17.	Amberlyst 15[#]/$CuSO_4$	4	27	92
18.	Amberlyst 15[#]/Cu	4	27	32
19.	Amberlyst 15[#]/CuI	4	27	29
20.	Amberlyst 15H**/$CuSO_4$	3	20	84
21.	Amberlyst 15H*/$CuSO_4$	3	20	72
22.	Amberlyst/$CuBr_2$ (1:0.05)	8	27	68
23.	Amberlyst/$Cu(OAc)_2$ (1:0.05)	16	80	51
24.	Amberlyst/$Cu(OAc)_2$ (1:0.02)	8	27	40
25.	Amberlyst/CuCl (1:0.05)	8	27	64
26.	Amberlyst/$Cu(OTf)_2$ (1:0.05)	8	27	61
27.	Amberlyst/$Cu(OTf)_2$ (1:0.02)	8	27	55
28.	Amberlyst/CuBr (1:0.05)	8	27	48
29.	Amberlyst/$Cu(OH)_2$ (1:0.05)	8	27	42
30.	Amberlyst/$Cu_2CO_3(OH)_2$ (1:0.05)	8	27	50
31.	Amberlyst/$Cu(NO_3)_2$ (1:0.05)	8	27	38
32.	Amberlyst/CuF_2 (1:0.05)	8	27	45
33.	Amberlyst/Cu(acetylacetonate)$_2$ (1:0.05)	8	27	57
34.	Amberlyst/$Cu(OTf)_2$ (1:0.01)	8	27	52

[a.] All reactions were carried out using H_2O as solvent, on completion of the reaction EtOAc was added and organic layer was separated dried and evaporated to obtain the desired 1,2,3-triazole.

[b.]ligand /Cu (1:0.05) for Entry 1-3 and 15-23

[#]Amberlyst was treated with conc. H_2SO_4 at 50°C for 16h for increasing the sulphonation degree. The activated catalyst was filtered and washed repeatedly with distilled water and was elucidated using the IR.

[##] Amberlyst was treated with conc. H_2SO_4 at 20°C for 16h

* Amberlyst was treated with conc. H_2SO_4 at 50°C for 3h

** Amberlyst was treated with conc. H_2SO_4 at 20°C for 3h

Table S2: Optimization of Solvent and Reaction Temperature

Entry	Solvents	4	@60°C
1	*tert-BuOH*	68	72
2	EtOH	32	35
3	CH_3CN	11	10
4	THF	46	50
5	DMF	82	85
6	Water	88	90

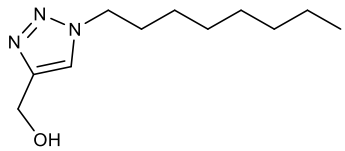
Table S3: Optimization of Azidation reaction condition

Entry	Reagent Conditions	Solvent	Yield (%)
1	BuONO & $TMSN_3$	THF	45
2		DMF	52
3		Acetonitrile	40
4		*tert*-BuOH	60
5		Water	70
6		EtOH	55
7	BuONO & NaN_3	THF	50
8		DMF	48
9		Acetonitrile	45
10		*tert*-BuOH	58
11		Water	72
12		EtOH	65
13	$NaNO_2$ & $TMSN_3$	THF	55
14		DMF	60
15		Acetonitrile	52
16		*tert*-BuOH	68
17		Water	75
18		EtOH	63
19	$NaNO_2$ & NaN_3	THF	62
20		DMF	70
21		Acetonitrile	65
22		*tert*-BuOH	78
23		Water	95
24		EtOH	85

Table S4: Role of pH and fate of reaction

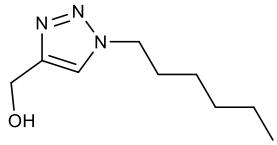
pH	4d	4c	4d (in polyethylene glycol (PEG))	4c (in PEG)
3	24	76	6	60
4	18	80	4	62
5	12	86	0	76
6	38	47	8	45
7	22	25	3	18
8	20	22	3	20

Spectral detail of the Synthesised Compounds

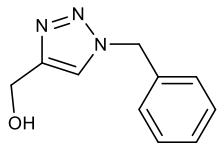


(1-octyl-1*H*-1,2,3-triazol-4-yl) methanol (3a): The method adheres to same protocol as mentioned in general procedure by adding octylamine (156µl,1.0 mmol) and propargyl alcohol (58.2 µl,1.0mmol.). On completion of the reaction the reaction mixture was extracted with EtOAc (3 x 5 mL) dried over Na_2SO_4 and evaporated under vacuo to obtain the desired **3a.** The product was isolated as white solid (203mg, 96%),

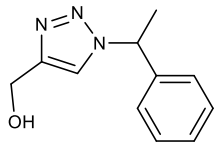
m.p:74-76º*C;* ^{1}*H* NMR (CDCl$_3$, 400MHz, ppm): δ 7.74 (s, 1H, Triazole-H), 4.70 (s, 2H, C**H**$_2$OH), 4.07 (t, *J* = 6.5 Hz, 2H, N-C**H**$_2$), 3.80 (brs, 1H, O**H**), 1.84 (p, *J* = 6.8 Hz, 2H, N-C**H**$_2$(CH$_2$)$_2$), 1.43 (p, *J* = 7.1 Hz, 2H, N-(CH$_2$)$_2$C**H**$_2$), 1.26 (q, *J* = 6.8 Hz, 10H, -(C**H**$_2$)$_4$-CH$_3$), 0.87 (t, *J* = 6.8 Hz, 3H, -(CH$_2$)$_4$-C**H**$_3$); **^{13}*C* NMR (CDCl$_3$, 100MHz, ppm)):** δ 143.1, 123.4, 54.8, 51.2, 31.7, 31.3, 29.4, 29.2, 26.1, 22.7,14.0; **ES$^-$MS:** [M$^+$*H*]$^+$ calculated for $C_{11}H_{22}N_3O^+$: 212.17 *m/z,* found 212.25 *m/z.* **HRMS (ESI+):** [M+H]$^+$ calculated for $C_{11}H_{22}N_3O$ *m/z* 212.1763; found 212.1757(experimental).



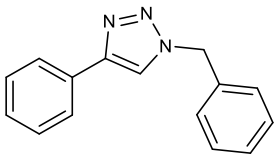
(1-hexyl-1*H*-1,2,3-triazol-4-yl) methanol (3b): The method adheres to same protocol as mentioned in general procedure by adding hexylamine (132µl, 1.0mmol.) and propargyl alcohol (58.2 µl, 1.0mmol.). The product was isolated as yellow thick liquid (174mg,95%); **^{1}*H* NMR (CDCl$_3$, 400MHz, ppm):** δ 7.74 (s, 1H, Triazole-**H**), 4.70 (s, 2H, C**H**$_2$OH), 4.07 (t, *J* = 6.5 Hz, 2H, N-C**H**$_2$), 1.91 – 1.78 (m, 2H, NCH$_2$C**H**$_2$), 1.47 – 1.31 (m, 6H, (C**H**$_2$)$_3$CH$_3$), 0.90 (d, *J* = 5.7 Hz, 3H, (CH$_2$)$_3$C**H**$_3$). **^{13}*C* NMR (CDCl$_3$, 100MHz, ppm)):**δ 143.1, 123.4, 54.8, 51.0, 31.1, 30.6,25.6, 22.1, 13.6; **ES$^-$MS:** [M$^+$*H*]$^+$ calculated for $C_9H_{18}N_3O^+$:184.14*m/*found 184.20*m/z*. **HRMS (ESI+):** [M+H]$^+$ calculated for $C_9H_{18}N_3O$ *m/z* 184.1450; found 184.1472 (experimental).



(1-benzyl-1*H*-1,2,3-triazol-4-yl) methanol (3c): The method adheres to same protocol as mentioned in general procedure by adding benzylamine(109 µl, 1.0mmol) and propargyl alcohol(58.2 µl, 1.0mmol).The product was isolated as white solid (172mg,91%);m.p:74-76^0*C*;**^{1}*H* NMR (CDCl$_3$, 400MHz, ppm):** δ 7.94 (s, 1H, Triazole-**H**), 7.35 (s, 5H, Ar**H**), 5.53 (s, 2H, C**H**2OH), 4.73 – 4.57 (s, 2H, Benzyl-**H**). **^{13}*C* NMR (CDCl$_3$, 100MHz, ppm)):** δ 146.1, 133.8, 129.3, 129.2, 128.4, 125.6, 77.3, 77.0, 76.7, 54.7, 54.1; **ES$^-$MS:** [M$^+$*H*]$^+$ calculated for $C_{10}H_{12}N_3O^+$: 190.09*m/z* found 190.15*m/z.* ; **HRMS (ESI+):** [M+H]$^+$ calculated for $C_{10}H_{12}N_3O$ *m/z* 190.0980; found 190.0975(experimental).

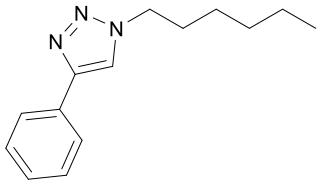


±(1-(1-phenylethyl)-1*H*-1,2,3-triazol-4-yl)methanol (3d): The method adheres to same protocol as mentioned in general procedure by adding 1phenylethylamine(129 µl, 1.0mmol) and propargyl alcohol(58.2 µl, 1.0mmol).The product was isolated as white solid (179mg,88%); m.p:78^0*C*; **^{1}*H* NMR (CDCl$_3$, 400MHz, ppm):** δ 7.86 (s, 1H, Triazole-**H**), 7.36 (q, *J* = 8.2 Hz, 5H, Ar-**H**), 5.27 – 5.18 (m, 1H, BnC**H**CH$_3$), 4.76 (s, 2H, C**H**$_2$OH), 1.98 (d, *J* = 7.2 Hz, 3H, C**H**$_3$). **^{13}*C* NMR (CDCl$_3$, 100MHz, ppm)):** δ 141.9, 141.1, 129.5, 128.4, 128.3, 117.5, 77.3, 77.0, 76.7, 59.5, 53.9, 21.4 **ES$^-$MS:** [M$^+$*H*]$^+$ calculated for $C^{11}H^{14}N^3O^+$: 204.11*m/z,* found 204.18*m/z.* ; **HRMS (ESI+):** [M+H]$^+$ calculated for $C_{11}H_{14}N_3O$ *m/z* 204.1137; found 204.1131(experimental).



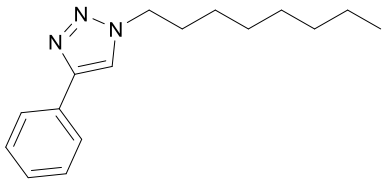
1-benzyl-4-phenyl-1*H*-1,2,3-triazole (3e): The method adheres to same protocol as mentioned in general procedure by adding benzyl amine(109 µl, 1.0mmol) and phenylacetylene (110 µl, 1.0mmol). The product was isolated as white solid; m.p:128-130^0*C*;**^{1}*H* NMR (CDCl$_3$, 400MHz, ppm):** δ 7.97 (s, 1H, Triazole-**H**), 7.90 (d, *J* = 7.4 Hz, 2H, Ar**H**), 7.40 – 7.33 (m, 4H, Ar**H**), 7.30 (d, *J* = 7.5 Hz, 4H, Ar**H**), 5.60 (s, 2H, BnC**H**2). **^{13}*C* NMR (CDCl$_3$,**

100MHz, ppm)): δ 144.3, 133.9, 129.3, 129.2, 128.7, 128.2, 127.8, 126.5, 126.4, 122.5, 55.5; **ES$^-$MS:** $[M^+H]^+$ calculated for $C_{15}H_{12}N^+$: 234.10*m/z*, found 234.15*m/z*. **HRMS (ESI+):** $[M+H]^+$ calculated for $C_{15}H_{14}N_3$ *m/z* 236.1188; found 236.1169 (experimental).

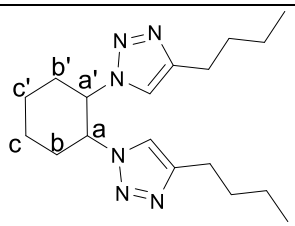


1-hexyl-4-phenyl-1*H*-1,2,3-triazole (3f): The method adheres to same protocol as mentioned in general procedure by adding hexyl amine (137 µl, 1.0mmol) and phenylacetylene (110 µl, 1.0mmol). The product was isolated as white solid (218mg,95%); m.p:70^0*C*;

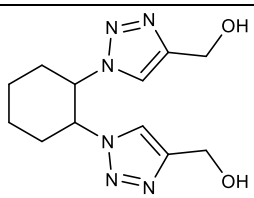
^{1}*H* NMR (CDCl$_3$, 400MHz, ppm): δ 7.85 (d, *J* = 7.0 Hz, 3H, ArH, Triazole-**H**), 7.39 (d, *J* = 6.5 Hz, 3H, Ar**H**), 4.13 (t, *J* = 6.5 Hz, 2H, NC**H**$_2$), 1.90 – 1.73 (m, 2H, NCH$_2$C**H**$_2$), 1.37 (dd, *J* = 14.7, 7.8 Hz, 6H, N-(CH$_2$)$_2$(C**H**$_2$)$_3$CH$_3$), 0.89 (t, *J* = 6.3 Hz, 3H, N-(CH$_2$)$_2$(CH$_2$)$_3$C**H**$_3$).); **^{13}*C* NMR (CDCl$_3$, 100MHz, ppm)):** δ 142.5, 129.7, 128.8, 128.7, 124.9, 120.1, 77.3, 77.0, 76.7, 51.9, 30.9, 30.6, 26.0, 22.1, 13.6; **ES$^-$MS:** $[M^+H]^+$ calculated for $C_{14}H_{18}N_3^+$:228.14*m/z*, found 228.18*m/z*. ; **HRMS (ESI+):** $[M+H]^+$ calculated for $C_{14}H_{20}N_3$ *m/z* 230.1657; found *m/z* 230.1652(experimental).



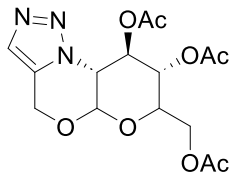
1-octyl-4-phenyl-1*H*-1,2,3-triazole (3g) : The method adheres to same protocol as mentioned in general procedure by adding octyl amine (165 µl ,1.0mmol) and phenylacetylene (110 µl,1.0mmol).The product was isolated as white solid (219mg,85%); m.p: 90-92^0*C*; **^{1}*H* NMR (CDCl$_3$, 400MHz, ppm):** δ 7.85 (d, *J* = 7.1 Hz, 3H, Triazole-H, ArH), 7.42 – 7.35 (m, 3H, ArH), 4.13 (t, *J* = 6.5 Hz, 2H, N-C**H**$_2$), 1.85 – 1.77 (m, 2H, NCH$_2$C**H**$_2$), 1.41 (m, *J* = 7.2 Hz, 2H, NCH$_2$CH$_2$C**H**$_2$), 1.32 – 1.21 (m, 8H, N(CH$_2$)$_3$(C**H**$_2$)$_4$CH$_3$, 0.87 (t, *J* = 6.8 Hz, 3H, N(CH$_2$)$_3$(CH$_2$)$_4$C**H**$_3$); **^{13}*C* NMR (CDCl$_3$, 100MHz, ppm)):** δ 142.5, 129.7, 128.8, 128.7, 124.9, 120.1, 77.3, 77.0, 76.7, 52.1, 31.7, 31.1, 29.4, 29.2, 26.5, 22.7, 14.1; **ES$^-$MS:** $[M^+H]^+$ calculated for $C_{16}H_{22}N_3^+$:256.18*m/z*,found:256.25 *m/z*. **HRMS (ESI+):** $[M+H]^+$ calculated for $C_{16}H_{24}N_3$ *m/z* 258.1970; found *m/z* 258.1965(experimental).



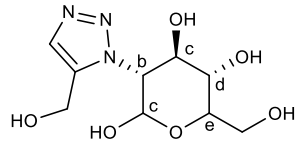
1,2-bis(4-butyl-1*H*-1,2,3-triazol-1-yl) cyclohexane (3h): The method adheres to same protocol as mentioned in general procedure by adding cyclohexane-1,2-diamine (123 µl, 1.0mmol) and 1-hexyne (230 µl,2.00mmol). The product was isolated as yellow thick liquid (259mg,78%); **^{1}*H* NMR (CDCl$_3$, 400MHz, ppm):** δ 7.72 (s, 2H, Triazole-H), 5.03 (dd, *J* = 7.6, 4.5 Hz, 2H, 2N-C**H**^{a}), 2.82 (d, *J* = 11.8 Hz, 2H, 2NCH^{a}C**H**$^b_{ax}$H$^b_{eq}$), 2.65 (d, *J* = 8.2 Hz, 2H, 2NCH^{a}CH$^b_{ax}$**H**$^b_{eq}$), 2.56 (t, *J* = 7.8 Hz, 4H, 2-C**H**$_2$CH$_2$CH$_2$CH$_3$), 2.13 (d, *J* = 13.6 Hz, 2H, C**H**$^c_{ax}$H$^c_{eq}$), 1.75 (p, *J* = 7.5 Hz, 4H, 2-CH$_2$C**H**$_2$CH$_2$CH$_3$), 1.65 – 1.49 (m, 2H, CH$^c_{axial}$**H**$^c_{eq}$), 1.32 (p, *J* = 7.2 Hz, 4H, 2-CH$_2$CH$_2$C**H**$_2$CH$_3$), 0.94 (t, *J* = 6.9 Hz, 6H, 2-CH$_2$CH$_2$CH$_2$C**H**$_3$); **^{13}*C* NMR (CDCl$_3$, 100MHz, ppm)):** δ 140.7, 122.6, 67.1, 36.6, 30.3, 27.6, 25.0, 22.2, 13.9; **ES$^-$MS:** $[M^+H]^+$ calculated for $C_{18}H_{29}N_6^+$:329.24*m/z*,found:329.30*m/z*. **HRMS (ESI+):** $[M+H]^+$ calculated for $C_{18}H_{31}N_6$ *m/z* 331.2610; found *m/z* 331.2605(experimental).



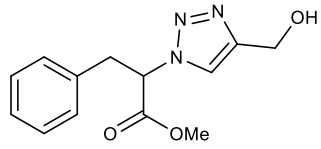
(Cyclohexane-1,2-diylbis(1*H*-1,2,3-triazole-1,4-diyl)) dimethanol (3i): The method adheres to same protocol as mentioned in general procedure by adding cyclohexane 1,2 diamine (123 µl, 1.0mmol) and propargyl alcohol (116 µl,2.0 mmol). The product was isolated as thick yellow liquid (267mg,96%).**^{1}*H* NMR (CDCl$_3$, 400MHz, ppm):** δ 8.03 (s, 2H, Triazole-H), 5.11 (dd, *J* = 7.6, 4.5 Hz, 2H), 4.68 (s, 4H, CH2OH), 3.08 (brs, 1H, OH), 2.77 (s, 2H, 2NCH^{a}C**H**$^b_{ax}$H$^b_{eq}$), 2.62 (m, 2H, 2NCH^{a}CH$^b_{ax}$**H**$^b_{eq}$), 2.09 (d, *J* = 16.5 Hz, 2H, C**H**$^c_{ax}$H$^c_{eq}$), 1.73 – 1.43 (m, 2H, CH$^c_{axial}$**H**$^c_{eq}$). **^{13}*C* NMR (CDCl3, 100MHz, ppm)):** δ 145.0, 125.1, 67.8, 54.7, 36.5, 24.5. **^{13}*C* NMR (CDCl$_3$, 100MHz, ppm)):** δ 145.0, 125.1, 77.3, 77.0, 76.7, 67.8, 54.7, 36.5, 24.5; **ES$^-$MS:** $[M^+H]^+$ calculated for $C_{12}H_{19}N_6O_2^+$:279.15*m/z*, found:279.20m/z. **HRMS (ESI+):** $[M+H]^+$ calculated for $C_{12}H_{19}N_6O_2$ *m/z* 279.1569; found *m/z* 279.1563(experimental).



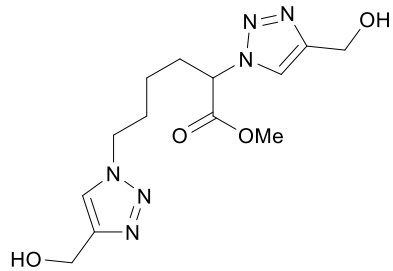
(2*S*)-3-(((1*H*-1,2,3-triazol-5-yl) methoxy) methoxy) butane-1,2,4-triyl triacetate (3j) : The method adheres to same protocol as mentioned in general procedure by adding galactose azide (221mg, 1.0mmol) and propargyl alcohol (58.2 µl, 1.0mmol).The product was isolated as y*e*llow thick liquid (342mg, 95%).**^{1}*H* NMR (CDCl$_3$+*D*MSO-d$_6$, 400MHz, ppm):** δ 7.85 (s, 1H, Triazole-**H**), 5.64 (t, *J* = 7.6 Hz, 1H, N-C**H**), 5.28 (d, *J* = 6.1 Hz, 2H, C**H**2O), 5.20 – 4.96 (m, 2H, C**H**$_2$OAc), 4.87 (m, 1H, OC**H**O), 4.38 (dd, *J* = 11.9, 2.3 Hz, 1H, C**H**OAc), 4.17 (dd, *J* = 11.9, 5.6 Hz, 1H, C**H**OAc), 4.10 – 4.01 (m, 1H, C**H**CH$_2$OAc), 2.10 (s, 3H, Ac), 2.06 (s, 3H, Ac), 2.04 (s, 3H, Ac). **^{13}*C* NMR (CDCl$_3$+DMSO-d$_6$, 100MHz, ppm)):** δ 170.6, 169.7, 169.3, 137.5, 128.53, 94.3, 77.3, 77.0, 76.7, 72.1, 71.2, 69.1, 62.7, 62.1, 59.1, 20.9, 20.6, 20.5; **ES$^-$MS:**[M$^+$*H]*$^+$calculated for $C_{14}H_{22}N_3O_8^+$:360.14*m/z*,found:360.25*m/z*. ; **HRMS (ESI+):** [M+H]$^+$ calculated for $C_{15}H_{20}N_3O_8$ *m/z* 370.1250; found *m/z* 370.1245(experimental).



(3*R*,4*R*,5*S*)-6-(hydroxymethyl)-3-(5-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl) tetrahy -dro-2*H*-pyran-2,4,5-triol (3k): Compound 3k was prepared using the same protocol as mentioned in general procedure by adding glucosamine (179mg,1.0mmol) and propargyl alcohol (58.2 µl, 1.0mmol). The product was isolated as Yellow thick liquid (238mg,91%). **^{1}*H* NMR (DMSO-d$_6$, 400MHz, ppm):** δ 7.91 (s, 1H, Triazole-**H**), 5.29 (dd, *J* = 7.4, 4.1 Hz, 1H, C$_c$**H**), 4.86 (m, *J* = 6.9 Hz, 2H, C$_a$**H**,C$_b$**H**), 4.24 – 4.00 (m, 3H, Triazole-C**H**$_2$OH, C$_e$**H**), 3.84 – 3.62 (m, 3H, C**H**$_2$OH, C$_d$**H**). **^{13}*C* NMR (DMSO-d$_6$, 100MHz, ppm)):**δ 142.1, 122.1, 97.5, 77.3, 77.0, 76.7, 74.7, 73.7, 72.4, 65.8, 65.5, 55.2; **ES$^-$MS:** [M$^+$*H*] $^+$ calculated for $C_9H_{16}N_3O_6^+$:262.24*m/z*,found:262.30*m/z*. **HRMS (ESI+):** [M+H]$^+$ calculated for $C_9H_{16}N_3O_6$ *m/z* 258.1970; found *m/z* 258.1965(experimental).

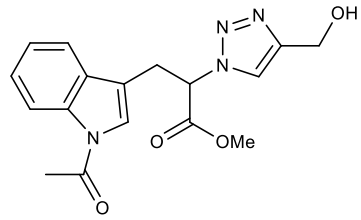


methyl 2-(4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)-3-phenylpropanoate (3l):The method adheres to same protocol as mentioned in general procedure by adding methylphenylalaniate(193 µl,1.0mmol) and propargyl alcohol(58.2 µl, 1.0mmol).The product is isolated as thick yellow liquid (230mg,88%).**^{1}*H* NMR (DMSO-d$_6$, 400MHz, ppm):** δ 7.55 – 7.48 (s, 1H, Triazole-H), 7.35 – 7.27 (m, 2H, Ar**H**), 7.15 (d, *J* = 7.0 Hz, 2H, Ar**H**), 4.91 (dd, *J* = 10.9, 5.8 Hz, 1H, C**H**COOMe), 4.70 (s, 2H, C**H**$_2$OH), 3.76 (s, 3H, COOC**H**$_3$), 3.65 (dd, *J* = 14.1, 5.6 Hz, 1H, BnC**H**H), 3.41 (dd, *J* = 13.7, 10.9 Hz, 1H, BnCH**H**). **^{13}*C* NMR (DMSO-d$_6$, 100MHz, ppm)):** δ 167.7, 145.7, 137.1, 129.3, 129.1, 127.1, 124.5, 77.3, 77.0, 76.7, 62.3, 55.7, 53.2, 36.7; **ES$^-$MS:** [M$^+$*H*] $^+$ calculated for $C_9H_{16}N_3O_6^+$:262.24*m/z*, found:262.30*m/z*. **HRMS (ESI+):** [M+H]$^+$ calculated for $C_{13}H_{16}N_3O_3$ *m/z* 262.1192; found *m/z* 262.1186(experimental).

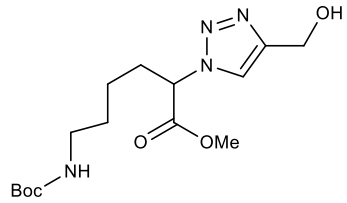


Methyl 2,6-bis(4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl) hexanoate (3m): The method adheres to same protocol as mentioned in general procedure by adding methyllysinate (156µl,1.0mmol) and propargyl alcohol (58.2 µl, 1.0mmol).The product was isolated as yellow thick liquid (268mg,82%).**^{1}*H* NMR (CDCl$_3$, 400MHz, ppm):** δ 7.82 (s, 1H, Triazole-**H**), 7.76 (s, 1H, Triazole-**H**), 4.74 (t, *J* = 10.5 Hz, 1H, NC**H**COOCH$_3$), 4.725(s, C**H**$_2$OH), 4.69(s, C**H**$_2$OH), 4.14 (t, *J* = 6.4 Hz, 2H, NC**H**$_2$(CH$_2$)$_3$-), 2.42 – 2.15 (m, 2H, N(CH$_2$)$_3$C**H**$_2$-), 2.01 (p, *J* = 6.8 Hz, 2H, NCH$_2$C**H**$_2$(CH$_2$)$_2$-), 1.77 (p, *J* = 7.5 Hz, 2H, N(CH$_2$)$_2$C**H**$_2$CH$_2$-). **13C NMR (CDCl$_3$, 100MHz, ppm)):** δ 168.3, 143.2, 142.9, 123.1, 122.7, 77.3, 77.0, 76.7, 61.4, 54.9, 54.8, 53.0, 50.1, 31.1, 30.3, 23.8; **ES$^-$MS:** [M$^+$*H*] $^+$ calculated for

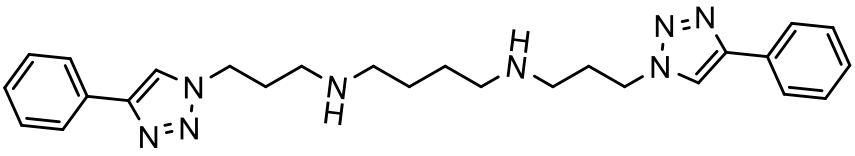
$C_{13}H_{21}N_6O_4^+$:325.16*m/z*,found:325.23*m/z*. **HRMS (ESI+):** $[M+H]^+$ calculated for $C_{13}H_{21}N_6O_4$ *m/z* 325.1624; found *m/z* 325.1618(experimental).



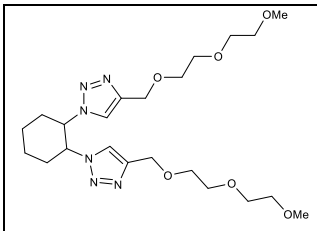
methyl 3-(1-acetyl-1*H*-indol-3-yl)-2-(4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)propanoate (3n):The method adheres to same protocol as mentioned in general procedure by adding methylacetyltryptophanate(260mg,1.0mmol) and propargyl alcohol (58.2 µl,1.0mmol).The product was isolated as yellow thick liquid (322mg, 94%).**^{1}*H* NMR (CDCl$_3$, 400MHz, ppm):** ^{1}H NMR (400 MHz,) δ 8.33 (t, *J* = 4.7 Hz, 1H, ArH), 7.67 (s, 1H, Triazole-**H**), 7.59 (s, 1H, Ar**H**), 7.50 – 7.44 (m, 1H, Ar**H**), 7.35 (dd, *J* = 5.6, 3.6 Hz, 2H, Ar**H**), 4.95 (dd, *J* = 10.8, 5.7 Hz, 1H, NC**H**COOCH$_3$), 4.70 (s, 2H, C**H**$_2$OH), 3.87 (dd, *J* = 14.2, 5.8 Hz, 1H, C**H**H), 3.76 (s, 3H, COOCH$_3$), 3.63 (dd, *J* = 14.5, 10.6 Hz, 1H, CH**H**), 2.55 (s, 3H, COC**H**$_3$). **^{13}C NMR (CDCl$_3$, 100MHz, ppm)):** δ 171.2, 166.1, 145.7, 137.5, 128.1, 126.6, 124.7, 124.6, 124.2, 119.0, 116.8, 113.5, 77.3, 77.0, 76.7, 62.0, 55.7, 53.2, 25.7, 24.2; **ES$^-$MS:** $[M^+H]^+$ calculated for $C_{17}H_{19}N_4O_4^+$:343.14*m/z*,found:343.19*m/z*. **HRMS (ESI+):** $[M+H]^+$ calculated for $C_{13}H_{21}N_6O_4$ *m/z* 325.1624; found *m/z* 325.1618(experimental).



methyl 6-((*tert*-butoxy carbonyl) amino)-2-(4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl) hexanoate (3o): The method adheres to same protocol as mentioned in general procedure by adding methyl-N_6 (tertbutoxycarbonyl)lysinate(260mg,1.0mmol) and propargyl alcohol (58.2 µl,1.0mmol). The product was isolated as yellow thick liquid (223mg, 65%); **^{1}*H* NMR (CDCl$_3$, 400MHz, ppm):** δ 7.85 (s, 1H, Triazole-H), 4.73 (s, 2H, CH$_2$OH), 4.64 (t, *J* = 7.8 Hz, 1H, NC**H**COOCH$_3$), 3.78 (s, 3H, COOC**H**$_3$), 3.22 (t, *J* = 6.9 Hz, 2H, NHC**H**$_2$(CH$_2$)$_3$-), 2.27 – 2.08 (m, 2H, NH(CH$_2$)$_3$C**H**$_2$-), 1.71 (p, *J* = 6.5 Hz, 2H, NH(CH$_2$)$_2$C**H**$_2$CH$_2$-), 1.52 – 1.44 (m, 2H, NHCH$_2$C**H**$_2$(CH$_2$)$_2$-), 1.39 (s, 9H, Boc). **^{13}C NMR (CDCl$_3$, 100MHz, ppm)):** δ 168.3, 156.1, 143.2, 122.7, 78.9, 77.3, 77.0, 76.7, 61.8, 54.9, 53.0, 41.5, 31.2, 30.1, 28.1, 23.5; **ES$^-$MS:** $[M^+H]^+$ calculated for $C_{15}H_{27}N_4O_5^+$:343.19*m/z*,found:343.26*m/z*. **HRMS (ESI+):** $[M+H]^+$ calculated for : $C_{15}H_{27}N_4O_5$ *m/z* 343.1981; found *m/z* 343.1970(experimental).

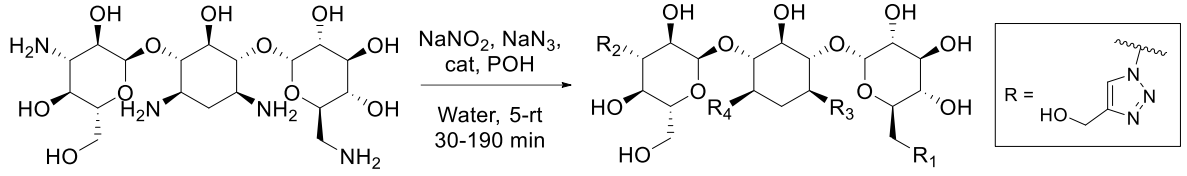


1,N4-bis(3-(4-phenyl-1*H*-1,2,3-triazol-1-yl)propyl)butane-1,4-diamine (3p) :The method adheres to same protocol as mentioned in general procedure by adding *N*, *N*-butane1,4-diylbispropane1,3-diamine (202mg, 1.00mmol) and phenylacetylene (235µl,1.0 mmol). The product was isolated as yellow thick liquid (330mg, 72%); **^{1}*H* NMR (DMSO-d$_6$+CDCl$_3$, 400MHz, ppm):** δ 7.85 (d, *J* = 7.0 Hz, 6H, 2Triazole-**H**, 4-Ar**H**), 7.39 (d, *J* = 6.6 Hz, 6H, 6-Ar**H**), 4.44 (t, *J* = 7.0 Hz, 4H, 2-NC**H**$_2$), 2.96 (t, *J* = 6.9 Hz, 4H, 2NHC**H**$_2$), 2.71 (t, *J* = 7.7 Hz, 4H, 2-NHC**H**$_2$), 2.17 (p, *J* = 6.9 Hz, 4H, NCH$_2$C**H**$_2$CH$_2$NH), 1.62 (t, *J* = 7.5 Hz, 4H, NHCH$_2$(C**H**$_2$)$_2$CH$_2$NH); **^{13}C NMR (DMSO-d$_6$,CDCl$_3$, 100MHz, ppm):** δ 142.9, 129.7, 128.8, 128.7, 124.9, 120.1, 77.3, 77.0, 76.7, 50.4, 48.2, 48.1, 29.1, 28.4; **ES$^-$MS:** $[M^+H]^+$ calculated for $C_{26}H_{35}N_8^+$:459.29*m/z*, found:459.32 *m/z*. **HRMS (ESI+):** $[M+H]^+$ calculated for : $C_{26}H_{35}N_8$ *m/z* 343.1981; found *m/z* 343.1970(experimental).



Procedure for the synthesis of **1,2-bis(4-((2-(2-methoxyethoxy)ethoxy)methyl)-1*H*-1,2,3-triazol-1-yl)cyclohexane (3q):** The method adheres to same protocol as mentioned in general procedure by adding 1,2-diethynylcyclohexane (132mg,1.0mmol) and 2-(2-(2-methoxyethoxy)ethoxy)ethan-1-amine (341 µl,1.0mmol). The product is isolated as yellow thick liquid(435mg, 90%).**^{1}H NMR (DMSO-d$_6$+CDCl$_3$, 400MHz, ppm):** δ 8.05 (s, 2H, triazole-**H**), 5.34 (s, 4H, 2-C**H**$_2$O), 5.13 (dd, *J* = 7.7, 4.6 Hz, 2H, NC**H**), 3.62 (d, *J* = 5.1 Hz, 8H, 2-O(C**H**$_2$)$_2$O), 3.52 (s, 8H, 2-O(CH$_2$)$_2$O(C**H**$_2$)$_2$O), 3.38 (s, 6H, 2-OCH$_3$), 2.77 (m, 2H, 2-NCHC**H**$_{ax}$H$_{eq}$), 2.62 (m, 2H, 2-NCHCH$_{ax}$**H**$_{eq}$), 2.09 (d, *J* = 14.5 Hz, 2H, NCHCH$_2$C**H**$_{ax}$H$_{eq}$), 1.61 – 1.43 (m, 2H, , NCHCH$_2$CH$_{ax}$**H**$_{eq}$); **^{13}C NMR (DMSO-d$_6$+CDCl$_3$, 100MHz, ppm):** δ 145.1, 124.0, 77.3, 77.0, 76.7, 71.6, 70.9, 69.1, 69.2, 68.1, 65.0, 58.8, 24.5; **ES$^-$MS:** [M$^+$*H*]$^+$ calculated for $C_{22}H_{39}N_6O_6^+$:483.29*m/z*, found:483.36*m/z*; **HRMS (ESI+):** [M+H]$^+$ calculated for : $C_{22}H_{39}N_6O_6$ *m/z* 483.2931; found *m/z* 483.2925(experimental). .

Triazolization of Kanamycin



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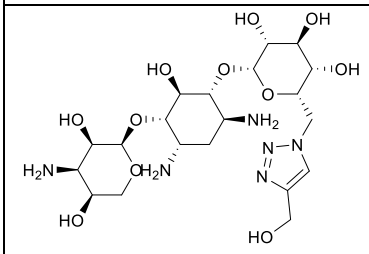
b	0.02:02:02:02	R	R	NH_2	NH_2	65	74
c	0.04:03:03:03	R	R	R/NH_2	R/NH_2	65	65
d	0.05:04:04:04	R	R	R	R	180	82

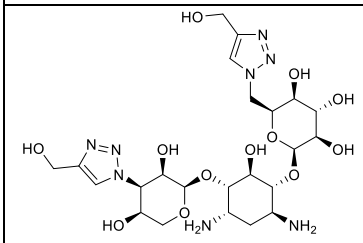
Figure S3. One pot diazotisation-azidation Click based modification of Kanamycin A

In another set of experiment, we applied our optimized reaction conditions to synthetically modified Kanamycin, an antibiotic drug previously reported effective for copper Ullman reaction. [35] Interestingly, using $NaNO_2$ and NaN_3 in ratios of 1:1, 2:2 and 4:4 with 1% w/w of Cu@Amberlyst we predominantly obtained single products **a**, **b** and **c** in moderate to good yields, respectively, however in the case where 3:3 ratio was used as per HPLC and NMR studies revealed the formation of two products in 20:80 ratio.

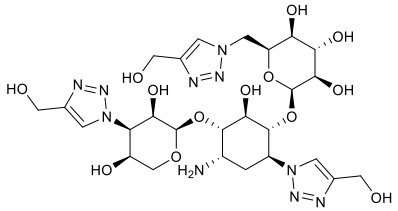


Procedure: Same as mentioned in General procedure for the synthesis of **(2*R*,3*R*,4*S*,5*S*,6*S*)-2-(((1*R*,2*R*,3*S*,4*S*,6*S*)-4,6-diamino-3-(((2*R*,3*R*,4*R*,5*S*)-4-amino -3,5-dihydroxytetrahydro-2*H*-pyran-2-yl) oxy)-2-hydroxycyclohexyl) oxy)-6-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)tetrahydro-2*H*-pyran-3,4,5-triol.** **^{1}H NMR (DMSO-d$_6$, ppm, 400MHz):** δ 7.93 (s,1H, Triazole C***H***), 5.21 (brs,O***H***, exchangeable in D$_2$O shake),5.09 (s, O***H***, brs),4.72 (d, *J* = 3.6 Hz, 2H, C***H***$_2$), 4.57 (dd, *J* = 12.0, 5.4 Hz,3H, C***H***$_2$, C***H***), 4.43 (d, *J* = 5.8 Hz, 1H, C***H***), 4.20-4.13(m, 1H, C***H***), 4.03(s, O***H***, brs), 3.97 – 3.90 (m, 1H, C***H***), 3.76 (d, *J* = 10.7 Hz, 2H, C***H***), 3.67(s, N***H***$_2$, brs), 3.65(d, 2H, C***H***$_2$), 3.53 (d, *J* = 6.4 Hz, 1H, C***H***), 3.37(s, 1H, C***H)***, 3.18(s, 1H,

C***H***), 2.98(s, 1H, C***H***), 2.77 (s, 1H, C***H***), 1.95 (s, 1H, C***H***), 1.77(s, 2H, CH_2); **^{13}C NMR (DMSO-d$_6$, ppm, 100MHz):** δ 143.5, 122.5, 100.6, 100.3, 78.0, 77.9, 76.3, 73.5, 72.9, 71.7, 68.8, 62.2, 62.1, 55.9, 54.9, 52.6, 47.1, 47.2, 36.3.

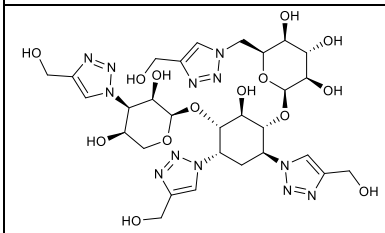


Procedure: Same as mentioned in General procedure for the synthesis of **(2*R*,3*R*,4*S*,5*S*,6*R*)-2-(((1*R*,2*R*,3*S*,4*R*,6*S*)-4,6-diamino-3-(((2*R*,3*R*,4*S*,5*S*)-3,5-dihydroxy-4-(4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)tetrahydro-2*H*-pyran-2-yl)oxy)-2-hydroxycyclohexyl)oxy)-6-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)tetrahydro-2*H*-pyran-3,4,5-triol, ^{1}*H* NMR (DMSO-d$_6$, ppm, 400MHz):** δ 8.16(s,1*H*, Trizole C***H***), 7.93(s,1*H*, Trizole C***H***), 5.21 (brs, O***H***, exchangeable in D2O shake), 5.01 (brs, O***H***, exchangeable in D2O shake) ,4.72 (d, *J* = 3.6 Hz, 2*H*, CH_2), 4.60 – 4.51 (m, 5*H*, CH_2, C***H***), 4.43 (d, *J* = 5.8 Hz, 1*H*, C***H***), 4.16(s, 1*H*, C***H***), 4.03(s, O***H***, brs), 3.93(s, 1*H*, C***H***), 3.76 (d, *J* = 10.7 Hz, 2*H*, C***H***), 3.67(s, NH_2, brs), 3.57 – 3.49 (m, 2*H*, C***H***), 3.39 (t, *J* = 13.9 Hz, 1*H*, C***H***), 3.19 (d, *J* = 6.9 Hz, 1*H*, C***H***), 2.98 (s, 1*H*, C***H***), 1.77(s, 2*H*, CH_2);**^{13}*C* NMR (DMSO-d$_6$, ppm, 100MHz):** δ 145.8, 143.5, 125.5, 122.5, 102.9, 99.0, 79.9, 76.3, 75.5, 75.5, 72.2, 69.4, 64.8, 64.2, 61.8, 55.0, 54.9, 49.8, 36.2.

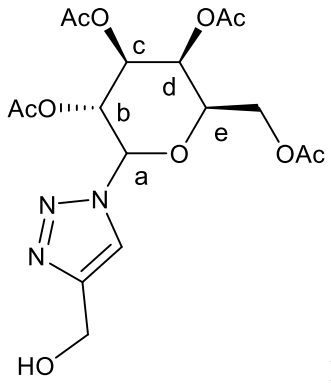


Procedure: Same as mentioned in General procedure using 3 equivalent of propargylalcohol and $NaNO_2$ and NaN_3 to obtain **(2*R*,3*R*,4*S*,5*S*,6*R*)-2-(((1*R*,2*R*,3*S*,4*R*,6*S*)-4-amino-3-(((2*R*,3*R*,4*R*,5*S*)-3,5-dihydroxy-4-(4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)tetrahydro-2*H*-pyran-2-yl)oxy)-2-hydroxy-6-(4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)cyclohexyl)oxy)-6-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)tetrahydro-2*H*-pyran-3,4,5-triol**

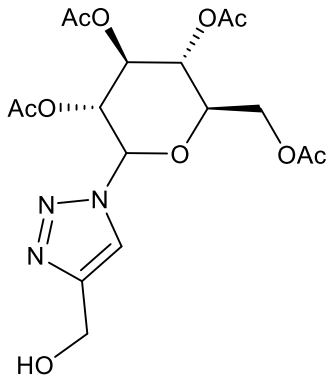
^{1}*H* NMR (DMSO-d$_6$, ppm, 400MHz): δ 8.16 (s, 2*H*, Trizole C***H***),7.93 (s, 1*H*, Trizole C***H***), 5.21 (brs, O***H***, exchangeable in D2O shake), 5.01 (brs, O***H***, exchangeable in D2O shake) , 4.72 (d, *J* = 4.7 Hz, 2*H*, CH_2), 4.55 (d, *J* = 5.4 Hz, 8*H*, CH_2), 4.43 (d, *J* = 5.8 Hz, 1*H*, C***H***), 4.16 (s, 1*H*, C***H***), 4.05 (s, O***H***, brs), 3.94(s,1*H*,C***H***), 3.80 (d, *J* = 10.2 Hz, 2*H*, C***H***), 3.67 (s, NH_2, brs), 3.65 (s, 2*H*, CH_2),3.53 (t, *J* = 6.7, 6.7 Hz, 2*H*, C***H***), 3.37 (s, 1*H*, C***H***), 3.19(d, *J* = 6.9 Hz, 1*H*, C***H***), 2.98 (s, 1*H*, C***H***), 1.77 (s, 2*H*, CH_2); **^{13}*C* NMR (DMSO-d$_6$, ppm, 100MHz):**δ 145.8, 143.5, 125.5, 122.5, 102.9, 99.0, 79.9, 75.5, 71.8, 69.4, 64.7, 64.1, 61.8, 55.0, 54.9, 49.8, 36.2.



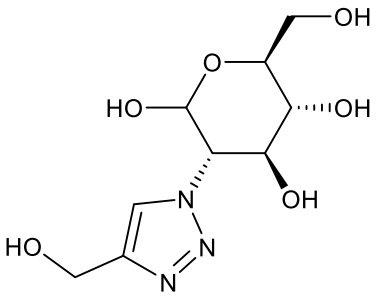
Procedure: Same as mentioned in General procedure using 4 equivalent of propargylalcohol and $NaNO_2$ and NaN_3 to obtain **(2*R*,3*R*,4*S*,5*S*,6*R*)-2-(((1*R*,2*R*,3*S*,4*R*,6*S*)-3-(((2*R*,3*R*,4*S*,5*S*)-3,5-dihydroxy-4-(4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)tetrahydro-2*H*-pyran-2-yl)oxy)-2-hydroxy-4,6-bis(4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)cyclohexyl)oxy)-6-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)tetrahydro-2*H*-pyran-3,4,5-triol: ^{1}*H* NMR (DMSO-d$_6$, ppm, 400MHz):**δ 8.16(s, 3*H*, Trizole C***H***), 7.93(s, 1*H*, Trizole C***H***), 5.17(brs, ***OH***, exchangeable in D_2O shake), 5.01 (brs, O***H***, exchangeable in D_2O shake), 4.72 (d, *J* = 3.6 Hz, 2*H*, CH_2), 4.60(s, 1*H*, C***H***), 4.55 (d, *J* = 5.4 Hz, 8*H*, CH_2), 4.43 (d, *J* = 5.8 Hz, 1*H*, C***H***), 4.16 (s, 1*H*, C***H***), 4.05 (s, O***H***, brs), 3.94 (s, 1*H*, C***H***), 3.80 (d, *J* = 8.4 Hz, 1*H*, C***H***), 3.65 (s, 2*H*, CH_2), 3.59 – 3.48 (m, 1*H*, C***H***), 3.42 – 3.31 (m, 1*H*, C***H***), 3.18 (s, 1*H*, C***H***), 2.98 (s, 1*H*, C***H***), 1.77 (t, *J* = 6.1, 6.1 Hz, 2*H*, CH_2); **^{13}*C* NMR (DMSO-d$_6$, ppm, 100MHz):** δ 145.8, 143.5, 125.5, 122.7, 122.5, 101.3, 99.0, 78.3, 78.1, 77.6, 76.3, 73.5, 71.3, 70.9, 68.8, 64.8, 64.4, 64.2, 63.6, 55.0, 54.9, 52.6.



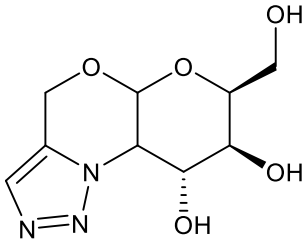
P**rocedure** for the synthesis of **(2R,3S,4S,5R)-2-(acetoxymethyl)-6-(4-(hydroxymethyl)-1H-1,2,3-triazol-1-yl)tetrahydro-2H-pyran-3,4,5-triyl triacetate (4a): ^{1}H NMR (400 MHz, CDCl$_3$, ppm)** δ 8.00 (s, 1H, Triazole-**H**), 5.94 (t, *J* = 9.4 Hz, 1H, C$_b$**H**), 5.70 (d, *J* = 8.8 Hz, 1H, C$_a$**H**), 5.47 – 5.31 (m, 1Hm C$_c$**H**), 5.24 (m, 1H, C$_d$**H**), 4.74 (s, 2H, C**H**$_2$OH), 4.24 (dd, *J* = 11.4, 3.9 Hz, 1H, C**H**HOAc), 4.10 (dd, *J* = 11.4, 8.6 Hz, 1H, C$_e$**H**), 3.97 (dd, *J* = 8.7, 4.0 Hz, 1H, CH**H**OAc), 2.11 (s, 3H, OAc), 2.09 (s, 3H, OAc), 2.07 (s, 3H, OAc), 2.05 (s, 3H, OAc). **13C NMR (CDCl$_3$, 100MHz, ppm):** δ 170.2, 169.6, 168.6, 168.2, 147.5, 124.3, 89.6, 73.4, 72.5, 72.0, 66.0, 61.2, 53.8, 20.9, 20.7, 20.7, 20.5;



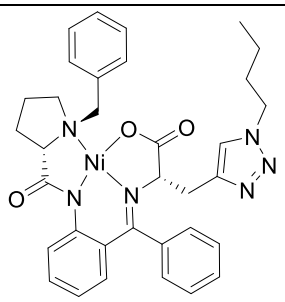
Procedure for the synthesis of (2R,3R,4S,5R)-2-(acetoxymethyl)-6-(4-(hydroxymethyl)-1H-1,2,3-triazol-1-yl)tetrahydro-2H-pyran-3,4,5-triyl triacetate (4b): ^{1}H NMR (400 MHz, CDCl3, ppm) δ 8.00 (s, 1H, Triazole-**H**), 5.94 (t, *J* = 9.0 Hz, 1H, C$_b$**H**), 5.70 (d, *J* = 9.3 Hz, 1H, C$_a$**H**), 5.38 (t, *J* = 9.4 Hz, 1H, C$_c$**H**), 5.24 (t, *J* = 9.6 Hz, 1H, C$_d$**H**), 4.74 (s, 2H, C**H**$_2$OH), 4.24 (dd, *J* = 11.8, 2.3 Hz, 1H, C**H**HOAc), 4.10 (dd, *J* = 12.0, 7.2 Hz, 1H, C$_e$**H**), 4.03 – 3.88 (m, 1H, CH**H**OAc), 2.07 (s, 3H, OAc), 2.05 (s, 3H, OAc), 2.02 (s, 3H, OAc), 2.00 (s, 3H, OAc). **^{13}C NMR (CDCl3, 100MHz, ppm):** δ 170.2, 169.4, 168.8, 168.2, 147.5, 124.3, 89.6, 75.2, 72.0, 70.3, 67.4, 62.3, 53.8, 20.5, 20.5.



Procedure for the synthesis of (3S,4S,5R,6S)-6-(hydroxymethyl)-3-(4-(hydroxymethyl)-1H-1,2,3-triazol-1-yl)tetrahydro-2H-pyran-2,4,5-triol (4c) and (7*S*,8*S*,9*R*)-7-(hydroxymethyl)-5a,8,9,9a-tetrahydro-4*H*,7*H*-pyrano[2,3-b][1,2,3]triazolo[1,5-d][1,4]oxazine-8,9-diol (4d)was accomplished using glucosamine (54 mg, as amine and was reacted with propargylacohol (1.1 eq) in presence of $NaNO_2$ (1.1 eq) and NaN_3 (1.1 eq) under optimised reaction condition after the completeion of reaction the product 4c and 4d was isolated using column chromatogrphy**:^{1}H NMR (400 MHz, DMSO-d_6+$CDCl_3$, 100MHz, ppm)** δ 8.03 (s, 1H, triazole-H), 5.40 (t, *J* = 6.9 Hz, 1H, C_b**H**), 4.72 (d, *J* = 7.2 Hz, 2H, C**H**$_2$OH), 4.26 – 4.09 (m, 2H, C_a**H**,C_c**H**), 4.08 – 3.95 (m, 1H, C_d**H**), 3.81 (dd, *J* = 12.0, 5.4 Hz, 1H), 3.79 – 3.63 (m, 2H). **^{13}C NMR (DMSO-d_6+$CDCl_3$, 100MHz, ppm):** δ 142.9, 122.9, 97.5, 74.7, 73.7, 72.4, 65.8, 65.5, 55.2.

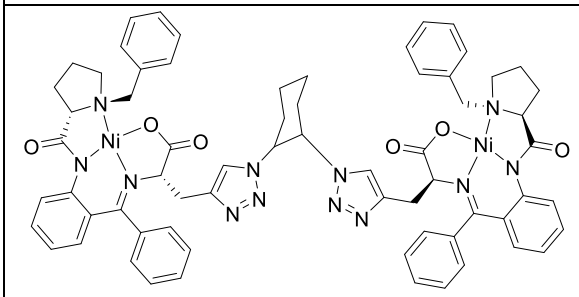


(7*S*,8*S*,9*R*)-7-(hydroxymethyl)-5a,8,9,9a-tetrahydro-4*H*,7*H*-pyrano[2,3-b][1,2,3]triazolo[1,5-d][1,4]oxazine-8,9-diol (4d): ^{1}H NMR (**400 MHz, $CDCl_3$+DMSO-d_6, ppm**) δ 7.96 (s, 1H), 5.33 (d, *J* = 6.2 Hz, 1H), 5.18 – 4.88 (m, 2H), 4.51 (t, *J* = 6.7 Hz, 1H), 4.23 – 4.05 (m, 2H), 3.91 – 3.79 (m, 1H), 3.79 – 3.68 (m, 2H). **^{13}C NMR (100MHz, $CDCl_3$+DMSO-d_6, ppm):** δ 137.2, 128.6, 95.7, 73.4, 72.1, 71.4, 62.6, 61.7, 61.1**.**

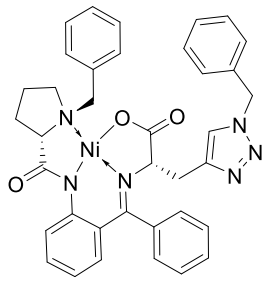


Procedure: P1 (0.052 mg) as alkyne partner was reacted with *n*-$BuNH_2$ (1.1 eq), $NaNO_2$ (1.2 eq) and NaN_3 (1.1 eq) using the our catalsyst under condition mentioned in the general procedure to obtain **(*S*)-2-(((*E*)-(2-((*S*)-1-benzylpyrrolidine-2-carboxamido)phenyl)(phenyl)methylene)amino)-3-(1-butyl-1H-1,2,3-triazol-4-yl)propanoate Nickel(II)complex (5a) : ^{1}*H* NMR (DMSO-d_6, 400MHz, ppm):**δ 7.93 (d, *J* = 4.2 Hz, 1H, ArH), 7.87 (d, *J* = 5.8 Hz, 1H, ArH), 7.71 – 7.56 (m, 3H, 2ArH, Triazole-H), 7.56 – 7.35 (m, 8H, ArH), 7.30 (t, *J* = 5.4 Hz, 2H, ArH), 6.91 (d, *J* = 5.8 Hz, 1H, ArH), 6.69 (d, *J* = 5.3 Hz, 1H, ArH), 4.66 (d, *J* = 8.8 Hz, 2H, CO-CH), 4.40 (d, *J* = 9.8 Hz, 1H, =N-CH), 4.14 (t, *J* = 5.4 Hz, N-CH_2), 3.75 (m, 3H), 3.13(m, 1H) 2.90 (d, *J* = 4.7 Hz, 2H, ArCH_2), 2.28 – 2.14 (t, *J* =3.2 Hz, CH_2), 1.99 (t, *J* = 5.6 Hz, 2H, CH_2), 1.87 (m, 2H, CH_2), 1.66 – 1.47 (m, 1H, CHH), 1.39 (q, *J* = 5.6 Hz, 2H, CH_2CH_3), 0.97 (t, *J* = 5.4 Hz, 3H, CH_3); **^{13}C NMR (DMSO-d_6, 100MHz, ppm)):** δ 181.8, 164.6, 161.4, 134.8, 133.6, 131.9, 131.0, 130.7, 130.6, 130.3, 129.9, 129.1,

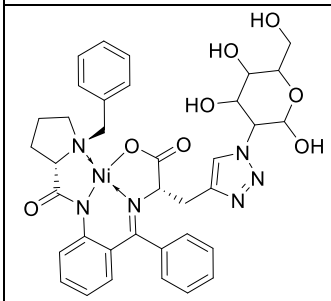
128.8, 128.6, 128.2, 128.0, 127.7, 127.6, 126.8, 124.7, 114.6, 111.9, 58.3, 52.0, 51.6, 48.3, 47.9, 30.9, 30.2, 25.9, 22.0, 19.2, 13.7.



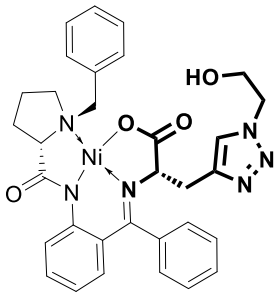
Procedure: P1 (0.052 mg) as alkyne partner was reacted with 1,2diaminocyclohexane (0.55 eq), NaNO2 (1.2 eq) and NaN3 (1.1 eq) using the our catalsyst under condition mentioned in the general procedure to obtain **(2*S*,2'*S*)-3,3'-(((1*S*)-cyclohexane-1,2-diyl)*bis*(1H-1,2,3-triazole-1,4-diyl))bis(2-(((*E*)-(2-((*S*)-1-benzylpyrrolidine-2-carboxamido)phenyl)(phenyl)methylene)amino)propanoate Nickel (II)) complex (5b): ^{1}H NMR (400MHz , DMSO-d_6, ppm):**δ 7.94 (d, *J* = 4.5 Hz, 3H), 7.87 (d, *J* = 5.6 Hz, 2H), 7.69 – 7.56 (m, 5H), 7.55 – 7.36 (m, 13H), 7.30 (dt, *J* = 8.0, 3.1 Hz, 2H), 6.91 (d, *J* = 5.5 Hz, 2H), 6.69 (t, *J* = 4.7 Hz, 2H), 4.66 (d, *J* = 8.4 Hz, 4H), 4.47 – 4.30 (m, 2H), 3.75 (s, 4H), 3.29 (d, *J* = 4.8 Hz, 2H), 3.14 (s, 2H), 2.89 (d, *J* = 5.8 Hz, 4H), 2.21 (p, *J* = 5.8 Hz, 4H), 1.94 – 1.75 (m, 5H), 1.66 (s, 2H), 1.49 (dd, *J* = 10.9, 5.7 Hz, 2H), 1.26 (s, 2H); **^{13}C NMR (100 MHz, DMSO-d_6, ppm):** δ 181.8, 164.6, 161.4, 134.8, 133.6, 131.9, 131.0, 130.7, 130.6, 130.3, 129.1, 128.2, 128.0, 127.6, 126.8, 126.6, 124.7, 114.6, 70.2, 6.30, 51.6, 48.3, 47.5, 36.3, 30.1, 26.0, 25.8, 22.0.



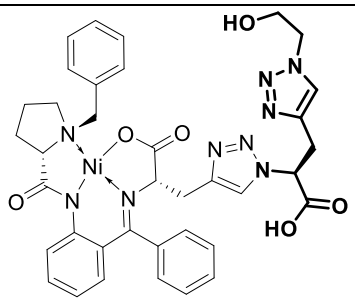
Procedure: P1 (0.052 mg) as alkyne partner was reacted with 1,2diaminocyclohexane (0.55 eq), NaNO2 (1.2 eq) and NaN3 (1.1 eq) using the our catalsyst under condition mentioned in the general procedure to obtain **(*S*)-3-(1-benzyl-1H-1,2,3-triazol-4-yl)-2-(((*E*)-(2-((*S*)-1-benzylpyrrolidine-2-carboxamido)phenyl)(phenyl)methylene)amino)propanoate Nickel(II) complex (5c) : ^{1}H NMR (400MHz, DMSO-d_6, ppm):**δ 7.92 (d, *J* = 3.9 Hz, 2H, 13), 7.87 (d, *J* = 5.6 Hz, 1H), 7.64 (d, *J* = 5.0 Hz, 2H), 7.59 (s, 1H), 7.33 – 7.25 (m, 1H), 6.91 (d, *J* = 5.6 Hz, 1H), 6.67 (d, *J* = 5.3 Hz, 1H), 5.53 (s, 2H), 4.66 (d, *J* = 8.7 Hz, 2H), 4.40 (d, *J* = 9.8 Hz, 1H), 3.75 (s, 4H), 3.13 (s, 1H), 2.90 (d, *J* = 4.7 Hz, 2H), 2.21 (t, *J* = 5.7 Hz, 2H), 1.87 (dd, *J* = 10.6, 5.6 Hz, 1H), 1.49 (t, *J* = 8.4 Hz, 1H); **^{13}C NMR (100MHz, DMSO-d_6, ppm):** δ 181.8, 165.2, 161.4, 135.5, 134.8, 133.6, 131.9, 131.0, 130.7, 130.6, 130.3, 129.9, 129.1, 128.8, 128.7, 128.6, 128.4, 128.2, 128.0, 127.94, 127.89, 127.6, 126.8, 124.7, 114.6, 112.7, 58.3, 55.6, 51.6, 48.3, 46.9, 29.5, 260, 22.0.



Procedure: P1 (0.052 mg) as alkyne partner was reacted with glucosamine (0.55 eq), $NaNO_2$ (1.2 eq) and NaN_3 (1.1 eq) using the our catalsyst under condition mentioned in the general procedure to obtain **(2*S*)-2-(((*E*)-(2-((*S*)-1-benzylpyrrolidine-2-carboxamido)phenyl)(phenyl)methylene)amino)-3-(1-(2,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2*H*-pyran-3-yl)-1*H*-1,2,3-triazol-4-yl)propanoate Nickel(II) complex (5d): . ^{1}H NMR (400MHz, DMSO-d_6, ppm):δ** 7.93 (d, *J* = 4.2 Hz, 2H), 7.87 (d, *J* = 5.7 Hz, 1H), 7.68 – 7.56 (m, 3H), 7.52 – 7.35 (m, 7H), 7.30 (t, *J* = 5.8 Hz, 2H), 6.91 (d, *J* = 5.8 Hz, 1H), 6.70 (d, *J* = 5.6 Hz, 1H), 5.46 (d, *J* = 5.7 Hz, 1H), 4.78 – 4.57 (m, 2H), 4.45 (d, *J* = 9.9 Hz, 2H), 3.89 (t, *J* = 7.5 Hz, 3H), 3.84 – 3.66 (m, 7H), 3.61 (d, *J* = 6.2 Hz, 2H), 3.49 (t, *J* = 7.0 Hz, 2H), 3.10 (s, 1H), 2.90 (s, 2H), 2.32 – 2.15 (m, 2H), 1.87 (d, *J* = 11.1 Hz, 1H), 1.51 (d, *J* = 8.1 Hz, 1H); **^{13}C NMR (100MHz, DMSO-d_6, ppm):** δ 181.8, 164.6, 161.4, 134.8, 133.6, 131.9, 131.0, 130.6, 130.1, 129.9, 129.4, 129.1, 128.8, 128.6, 128.2, 128.0, 127.6, 126.8, 126.5, 124.7, 114.6, 107.6, 94.0, 75.4, 71.9, 70.9, 67.4, 61.6, 58.3, 51.6, 48.2, 47.8, 27.1, 25.9, 22.0.



Procedure: P1 (0.052 mg) as alkyne partner was reacted with 2-aminoethanol (0.55 eq), $NaNO_2$ (1.2 eq) and NaN_3 (1.1 eq) using the our catalsyst under condition mentioned in the general procedure to obtain **(*S*)-2-(((*E*)-(2-((*S*)-1-benzylpyrrolidine-2-carboxamido)phenyl)(phenyl)methylene)amino)-3-(1-(2-hydroxyethyl)-1*H*-1,2,3-triazol-4-yl)propanoate Nickel(II) complex (5e):** . **^{1}*H* NMR (400MHz, DMSO-d_6, ppm):** δ 7.92 (d, *J* = 4.0 Hz, 2H), 7.87 (d, *J* = 5.7 Hz, 1H), 7.68 – 7.54 (m, 3H), 7.51 – 7.34 (m, 7H), 7.30 (t, *J* = 5.7 Hz, 2H), 6.91 (d, *J* = 5.9 Hz, 1H), 6.67 (d, *J* = 4.6 Hz, 1H), 4.79 – 4.56 (m, 2H), 4.45 (d, *J* = 10.0 Hz, 1H), 4.12 (t, *J* = 4.1 Hz, 3H), 3.88 (d, *J* = 4.3 Hz, 4H), 3.76 (s, 3H), 3.10 (s, 1H), 2.90 (s, 2H), 2.29 – 2.09 (m, 2H), 1.94 – 1.76 (m, 1H), 1.51 (d, *J* = 7.9 Hz, 1H); **^{13}*C* NMR (100MHz, DMSO-d_6, ppm)):** δ 181.8, 164.4, 161.4, 134.8, 133.6, 131.9, 131.0, 130.6, 130.1, 129.9, 129.4, 129.1, 128.8, 128.6, 128.2, 128.0, 127.6, 127.2, 126.8, 124.7, 114.6, 109.7, 59.2, 58.3, 51.6, 51.4, 48.2, 47.3, 26.0, 22.0.



Procedure: P1 (0.052 mg) as alkyne partner was reacted with (*S*)-2-amino-3-(1-(2-hydroxyethyl)-1*H*-1,2,3-triazol-4-yl)propanoic acid (0.55 eq obtain from the hydrolysis of **5e**), $NaNO_2$ (1.2 eq) and NaN_3 (1.1 eq) using the our catalsyst under condition mentioned in the general procedure to obtain **(*S*)-2-(((*E*)-(2-((*S*)-1-benzylpyrrolidine-2-carboxamido)phenyl)(phenyl)methylene)amino)-3-(1-((*S*)-1-carboxy-2-(1-(2-hydroxyethyl)-1*H*-1,2,3-triazol-4-yl)ethyl)-1*H*-1,2,3-triazol-4-yl)propanoate Nickel(II) complex (5f): ^{1}*H* NMR (400MHz, DMSO-d_6, ppm):** δ 7.93 (d, *J* = 3.8 Hz, 2H), 7.87 (d, *J* = 5.7 Hz, 1H), 7.61 (dd, *J* = 8.1, 3.4 Hz, 4H), 7.45 (td, *J* = 12.3, 5.5 Hz, 8H), 7.34 – 7.22 (m, 2H), 6.91 (d, *J* = 5.9 Hz, 1H), 6.71 (t, *J* = 4.8 Hz, 1H), 4.74 – 4.58 (m, 2H), 4.45 (d, *J* = 10.2 Hz, 1H), 4.12 (t, *J* = 4.7 Hz, 3H), 3.87 (t, *J* = 4.1 Hz, 3H), 3.76 (s, 3H), 3.32 – 3.19 (m, 1H), 3.17 – 2.97 (m, 2H), 2.90 (d, *J* = 4.7 Hz, 2H), 2.21 (t, *J* = 5.6 Hz, 2H), 1.87 (q, *J* = 5.6 Hz, 1H), 1.48 (d, *J* = 9.6 Hz, 1H); **^{13}*C* NMR (100MHz, DMSO-d_6, ppm)):** δ 181.8, 168.9, 165.6, 161.4, 134.8, 133.6, 131.9, 131.8, 131.0, 130.6, 130.1, 129.9, 129.4, 129.1, 128.8, 128.6, 128.6, 128.2, 127.9, 127.6, 126.8, 124.7, 117.9, 114.6, 109.5, 59.2, 58.6, 58.3, 51.6, 50.2, 48.2, 47.2, 30.69, 25.9, 25.9, 22.0.

General Procedure for PPTP, PPTC and IMTC: To aminol (5 mmol, 1 equiv) and alkyne (1 equiv) substrates, Cu@Amberlyst (5% w/w), $NaNO_2$ (1.05 eq), NaN_3 (1.05 eq) and water (5 mL) were added at 0°C. After addition the reaction was stirred and allowed to come to room temerature after naibtaining 0°C for at least 5 min, After the completion of the rection as the TLC, DCM (5 mL) and water (1 mL) were added, and the aqueous layer was extracted with dichloromethane (3 × 15 mL). The combined organic layers dried over anhydrous magnesium sulfate and concentrated under reduced pressure to yield the product. The product could be purified by hydrochloride precipitation to obtain **2-{4-[(Piperidin-1-yl)methyl]-1*H*-1,2,3-triazol-1-yl}cyclopentan-1-ol (PPTP); ^{1}*H* NMR (DMSO-d_6, 400MHz, ppm):** δ 8.03 (s, CH, 1H), 5.40 (s, CH, 1H), 4.49 (d, *J* = 1.3 Hz, CH_2, 2H), 4.38 (brs, OH), 4.00 – 3.90 (m, CH, 1H), 2.57 (d, *J* = 4.5 Hz, CH_2, 4H), 2.22 – 1.88 (m, CH_2, 4H), 1.74 – 1.23 (m, CH_2, 8H); **^{13}*C* NMR (DMSO-d_6, 100MHz, ppm)):** δ 133.6, 119.1, 75.0, 63.0, 53.4, 52.3, 31.4, 27.0, 25.6, 23.2, 23.0.

Procedure: 2-{4-[(Piperidin-1-yl)methyl]-1*H*-1,2,3-triazol-1-yl}cyclohexan-1-ol (PPTC) was prepared using the procedure mentioned for PPTP**; ^{1}*H* NMR (DMSO-d_6, 400MHz, ppm):** δ 8.03 (s, CH, 1H), 4.49 (d, *J* = 1.3 Hz, CH_2, 2H), 3.80 – 3.69 (m, 2H, CH), 3.33 (brs, OH), 2.57(m, CH_2, 4H), 2.11 – 0.85 (m,CH_2,13H); **^{13}*C* NMR (DMSO-d_6, 100MHz, ppm)):** δ 133.0, 118.8, 68.5, 60.1, 53.4, 52.3, 32.9, 31.6, 26.5, 25.6, 23.0, 20.0.

Procedure: 2-{4-[(1*H*-Imidiazol-1-yl)methyl]-1*H*-1,2,3-triazol-1-yl}cyclohaxan-1-ol (IMTC) was prepared using the procedure mentioned for the PPTC. **^{1}*H* NMR (DMSO-d_6, 400MHz, ppm):** δ 8.03 (s, CH, 1H), 7.53 (s, CH, 1H),

7.19 (d, *J* = 2.2 Hz, CH_2, 2H), 6.96 (d, *J* = 2.0 Hz, CH_2, 2H), 5.54 (s, CH_2, 2H), 4.42 (brs,OH), 3.83 – 3.70 (m, CH, 2H), 1.96 – 1.13 (m, CH_2, 8H); **^{13}*C* NMR (DMSO$^-$d$_6$, 100MHz, ppm)):** δ 135.7, 135.5, 126.2, 119.2, 118.2, 68.5, 59.2, 42.2, 32.9, 31.6, 26.5, 20.0.

Procedure: Rufinamide; ^{1}*H* NMR (DMSO$^-$d$_6$, 400MHz, ppm): δ 8.40 (s, CH, 1H), 7.28 (brs, NH_2, 2H), 7.15 (t, *J* = 6.0 Hz, ArH, 1H), 7.03 – 6.97 (m, ArH, 2H), 5.52 (s, CH_2, 2H); **^{13}*C* NMR (DMSO$^-$d$_6$, 100MHz, ppm)):** δ 163.8, 163.5, 163.4, 160.8, 142.2, 131.4, 131.4, 131.3, 129.7, 113.9, 113.7, 113.6, 113.5.

General Procedure for the preparation of THETA and THPTA: To a RB (20 mL) charged with 0.01g of Cu@Amberlyst in 0.5 mL of TDW to this was added 2-aminoethanol (0.18g, 0.0023 mol, 1 equiv) and stirred the reaction mixture for 10 min at 5oC followed by addition of tripropargylamine (0.081 mL, 0.000575 mol, 0.25 equiv). After completion of the reaction the resulting mixture was treated with MeOH (3 mL) filtered the resulting solution to seperated the catalyst. The aqueous MeOH was evaporated under vacuo to obtain 0.258 g of dark green viscous oil, this was later crystallized in methanol (3 mL) overnight in 2–8 °C decanted yielding 0.7 g of a dark green precipitate, which was further purified using column chromatography (MeOH/DCM, 1/3 v/v, as eluent), yielding 0.21 g of THETA as slightly yellow crystal **{Tris[1-(2-hydroxyethyl)-1*H*-1,2,3-triazol-4-yl]methyl}amine (THETA); ^{1}*H* NMR (DMSO$^-$d$_6$, 400MHz, ppm):** δ 8.03 (s, CH, 1H), 4.91 (brs, OH), 4.49 (s, CH_2, 6H), 4.15 (t, *J* =4.1 Hz, CH_2, 6H),), 3.64 (q, *J* = 4.1 Hz); **^{13}*C* NMR (DMSO$^-$d$_6$, 100MHz, ppm)):** δ 128.2, 118.3, 59.5, 49.3, 48.1.

Procedure: {Tris[1-(3-hydroxypropyl)-1*H*-1,2,3-triazol-4-yl]methyl}amine (THPTA) was prepared using the procedure mentioned for the preparation of **THETA; ^{1}*H* NMR (DMSO$^-$d$_6$, 400MHz, ppm):** δ 8.03(s, CH, 1H), 4.61 (t, *J* = 4.7 Hz, CH_2, 6H), 4.49 (s, 6H, CH_2), 4.21 (q, *J* = 4.8 Hz, CH_2, 6H), 3.75 (brs, OH), 1.88 (p, *J* = 5.0 Hz, CH_2, 6H); **^{13}*C* NMR (DMSO$^-$d$_6$, 100MHz, ppm)):** δ 128.2, 120.7, 57.2, 48.8, 48.6, 31.6;

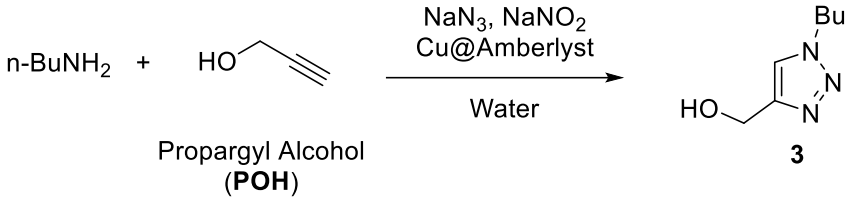
Green metrics formulas

$$E_{factor} = \frac{\sum reagents + \sum solvents - product}{product}$$

$$RME = \frac{product}{\sum reagents}$$

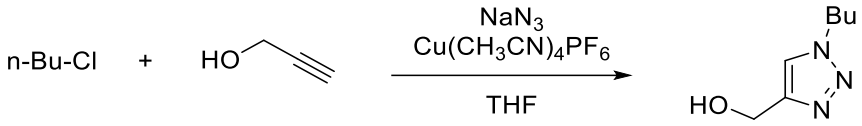
$$gRME = \frac{product}{\sum reagents + \sum solvents}$$

Table S5. *GCM calculation of preparation of (1-butyl-1H-1,2,3-triazol-4-yl)methanol (**3**) using our optimised reaction conditions*



Reagents	Amount (in mg)	Mw	***Catalyst Loss Consideration***
			0.03
Reagents and catalyst			$\frac{\sum(Amberlyst + CuSO4 + nBuNH2 + NaNO2 + NaN3 + POH) + \sum(H2O + EtOAc) - (triazole)}{(triazole)}$
Amberlyst	200	>1000	$= \frac{(200+50+730+680+650+560)+(8000+19000)-1440)}{1440}$
$CuSO_4$	50	159	**e-factor** = 19.74305556
n-$BuNH_2$	730	93	$\boldsymbol{RME} = \frac{product}{\sum reagents}$
$NaNO_2$	680	68	$= \frac{1440}{(200+50+730+680+650+560)}$
NaN_3	650	65	**RME** = 0.50174216
Propargyl Alcohol (POH)	560	56	$gRME = \frac{product}{\sum reagents + \sum solvents}$
Solvent			$\frac{1440}{(200+50+730+680+650+560)+(8000+19000)}$
H_2O	8000	18	**gRME** = 0.048208905
EtOAc	19000	88.11	
Product			***After Catalyst loss consideration*** $gRME = \frac{product}{\sum reagents + \sum solvents + \%loss\ of\ catalyst * (\sum catalyst)}$ $= \frac{1440}{(200+50+730+680+650+560)+(8000+19000)+(0.03)x(200+50)}$
Triazole (**3**)	1440	155.2	**gRME** = 0.048196804

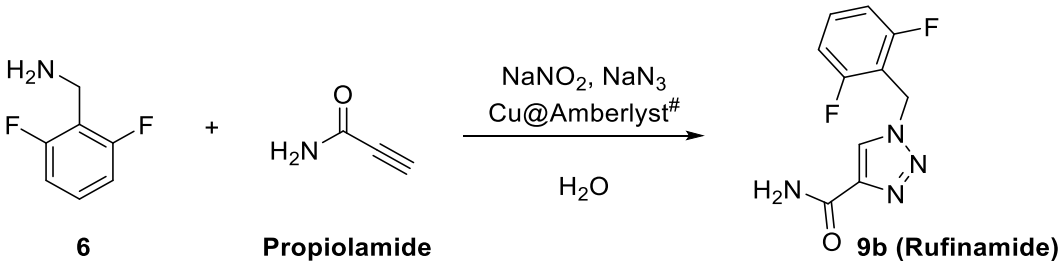
Table S6. GCM calculation of preparation of (1-butyl-1H-1,2,3-triazol-4-yl)methanol (**3**) using n-BuCl as strating material conditions



POH **3**

Reagents	**Amount(in mg)**	**Mw**	**Catalyst Loss consideration**		
Amberlyst	200	>1000	**0.03**		
$Cu(CH_3CN)_4$	100	159	**e-factor**	18.80714286	
n-BuCl	920	93	**RME**	0.574948665	
$NaNO_2$	na	68	**gRME**	0.050477736	0.050461361
NaN_3	650	65			
POH	560	56			
Solvent					
H_2O	4300	18			
EtOAc	20000	88.11			
DMF	1000				
Product					
Triazole (**3**)	1400	155.2			

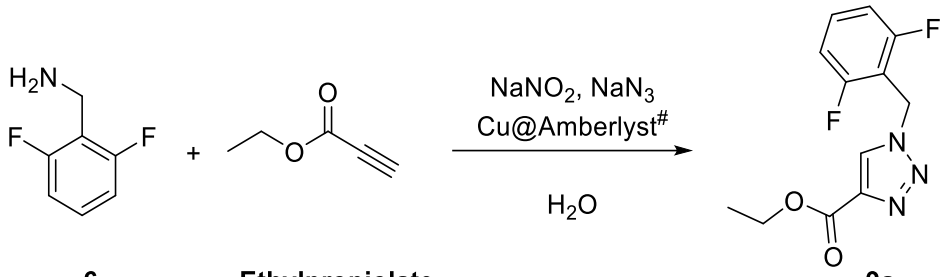
Table S7. GCM calculation of preparation of Rufinamide (**9b**) using our optimised reaction conditions



6 **Propiolamide** **9b (Rufinamide)**

Reagents	**Amount(in mg)**	**Mw**	**Catalyst Loss consideration**		
Amberlyst	200	>1000	**0.03**		
$CuSO_4$	50	159	**e-factor**	15.70148415	
2,6-difluorobenzylamine	1430	134.13	**RME**	0.51354902	
$NaNO_2$	680	68	**gRME**	0.059874918	0.059860256
NaN_3	650	65			
propiolamide	560	69.06			
Solvent					
H_2O	250	18			
EtOAc	26800	88.11			
Product					
Rufinamide (**9b**)	1833.37	238.19			

Table S8. GCM calculation of preparation of **9a** using our optimised reaction conditions



6 **Ethylpropiolate** **9a**

Reagents	**Amount(in mg)**	**Mw**	**Catalyst Loss consideration**		
Amberlyst	200	>1000	**0.03**		
$CuSO_4$	50	159	**e-factor**	10.90650407	
2,6-difluorobenzylamine	1430	134.13	**RME**	0.616541353	
$NaNO_2$	680	68	**gRME**	0.083987709	0.083966209
NaN_3	650	65			
Ethylpropiolate	980	98.03			
Solvent					
H_2O	300	18			
EtOAc	25000	88.11			
Product					
Rufinamide precursor (**9a**)	2460	267			

HPLC studies performed for the assessment of the prepared rufinamide sample with the pure sample of the same: Chromatographic separation was achieved by using a Shimadzu Model HPLC system, equipped with an SPD M20A prominence photodiode array detector (250 mm×4.6 mm, 5 µm particle size) maintained at 25 °C. Isocratic elution was performed using acetonitrile and water (60:40, v/v) with flow rate 0.8 mL/min. 20 µL of sample was injected into the HPLC system. Rufinamide stock solution (1000 µg/mL) was prepared by accurately weighing 25 mg of Rufinamide in a 25 mL amber volumetric flask and making up to volume with mobile phase. Working solutions for HPLC injections were prepared on a daily basis from the stock solution in a solvent mixture of acetonitrile and water (60:40, v/v) (mobile phase). Solutions were filtered through a 0.45 µm membrane filter prior to injection.

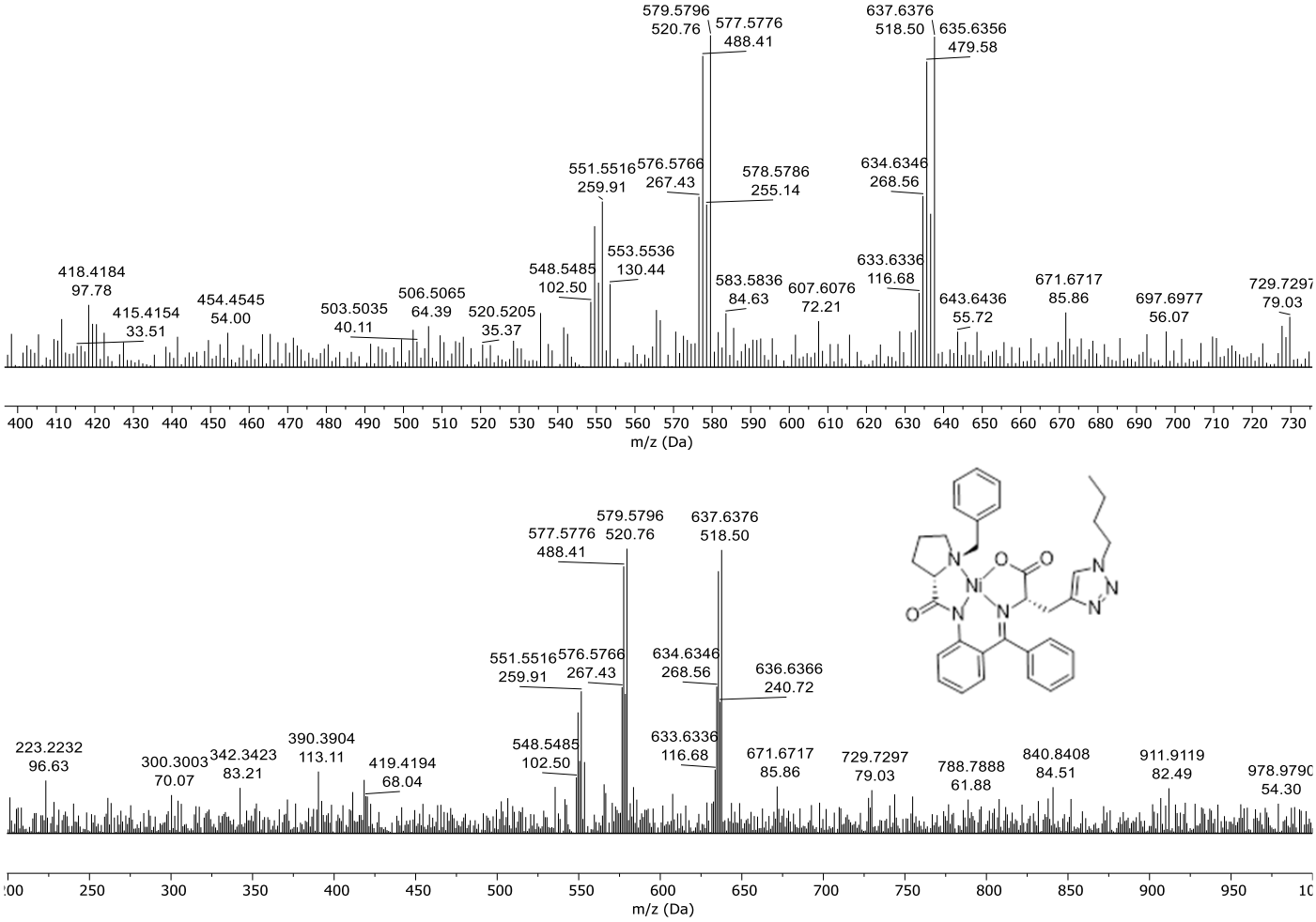


Figure S4.: HRMS **s**pectra of compound 5a

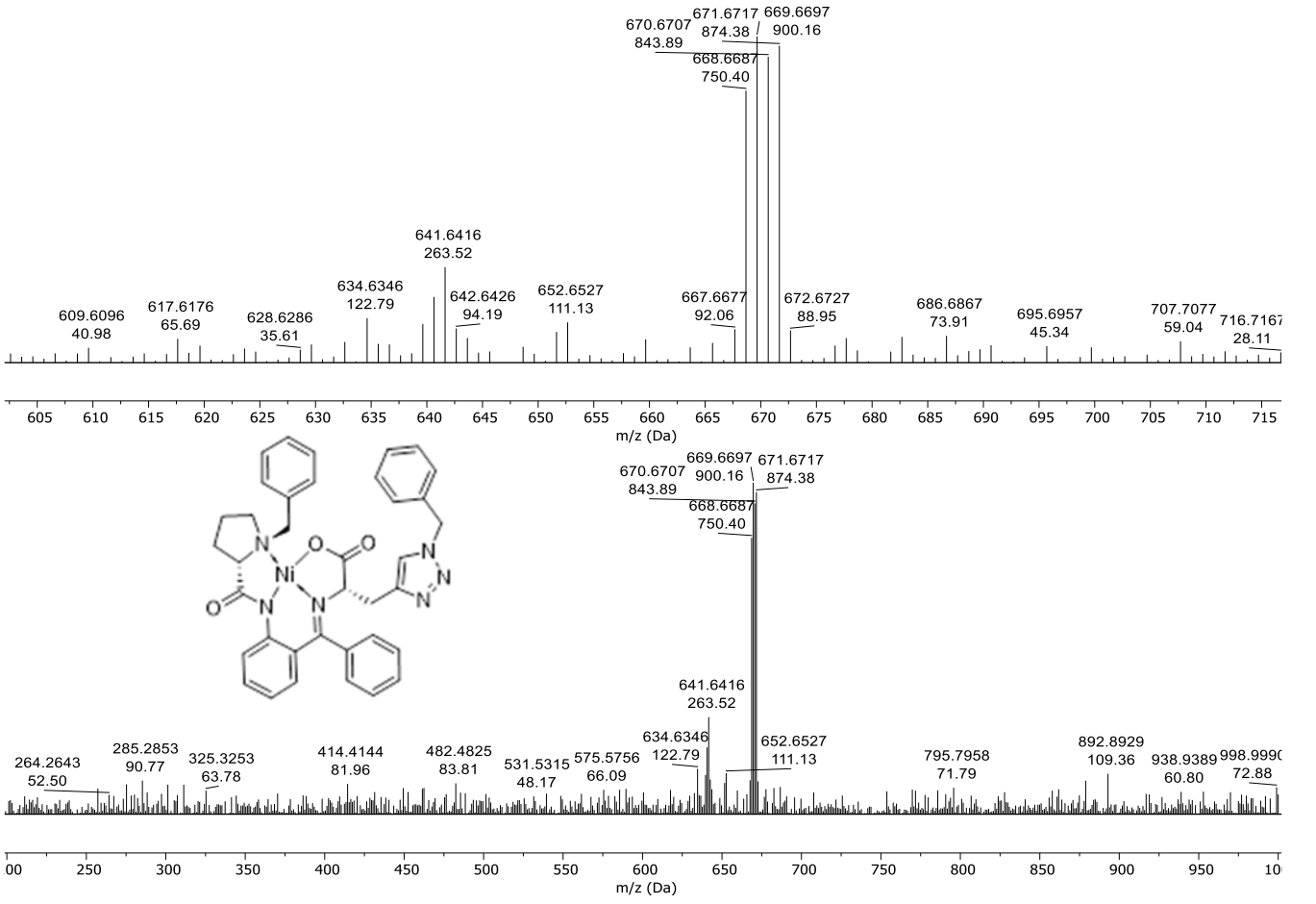


Figure S5: HRMS **s**pectra of compound 5c

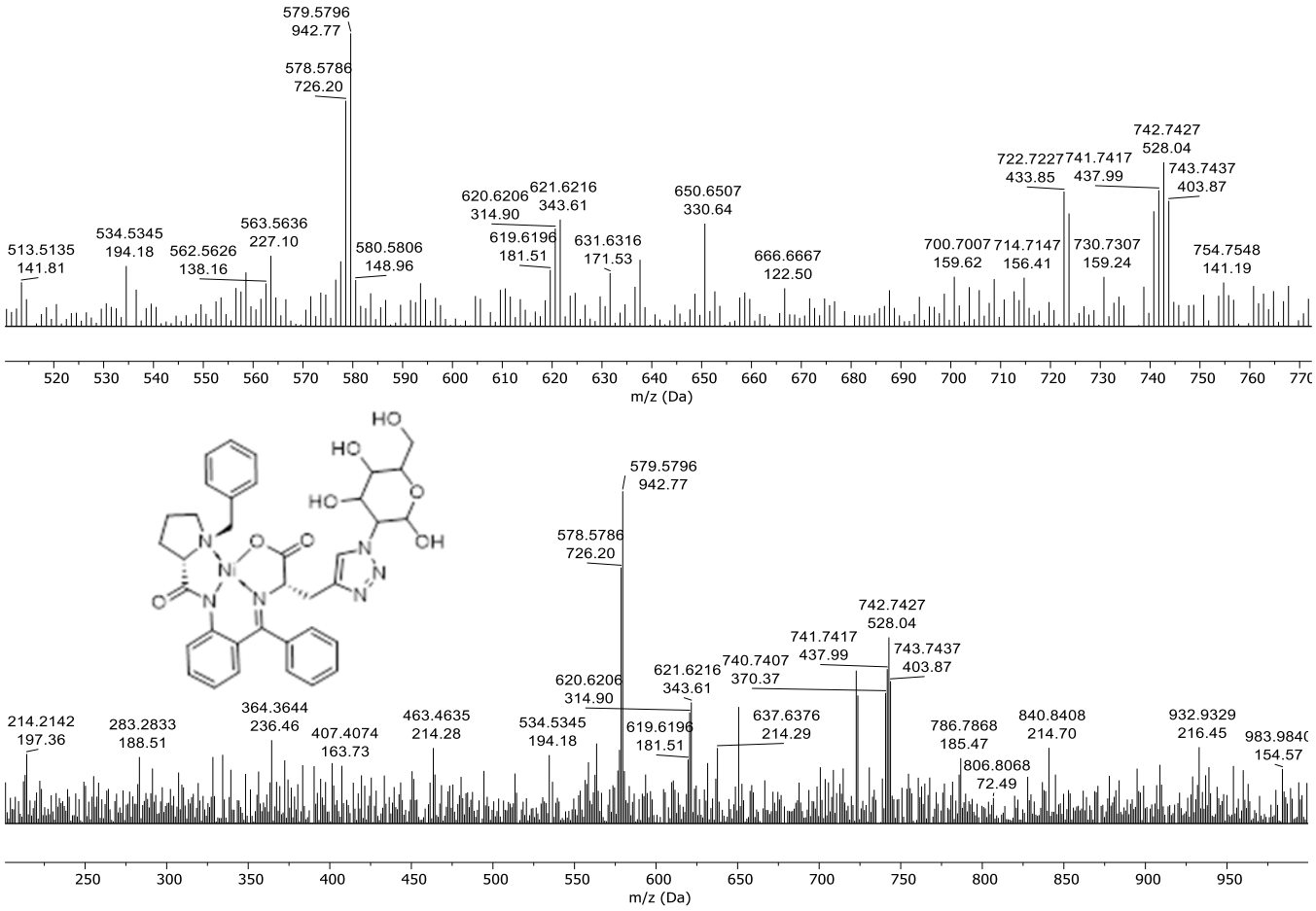


Figure S6: HRMS spectra of compound **5d**

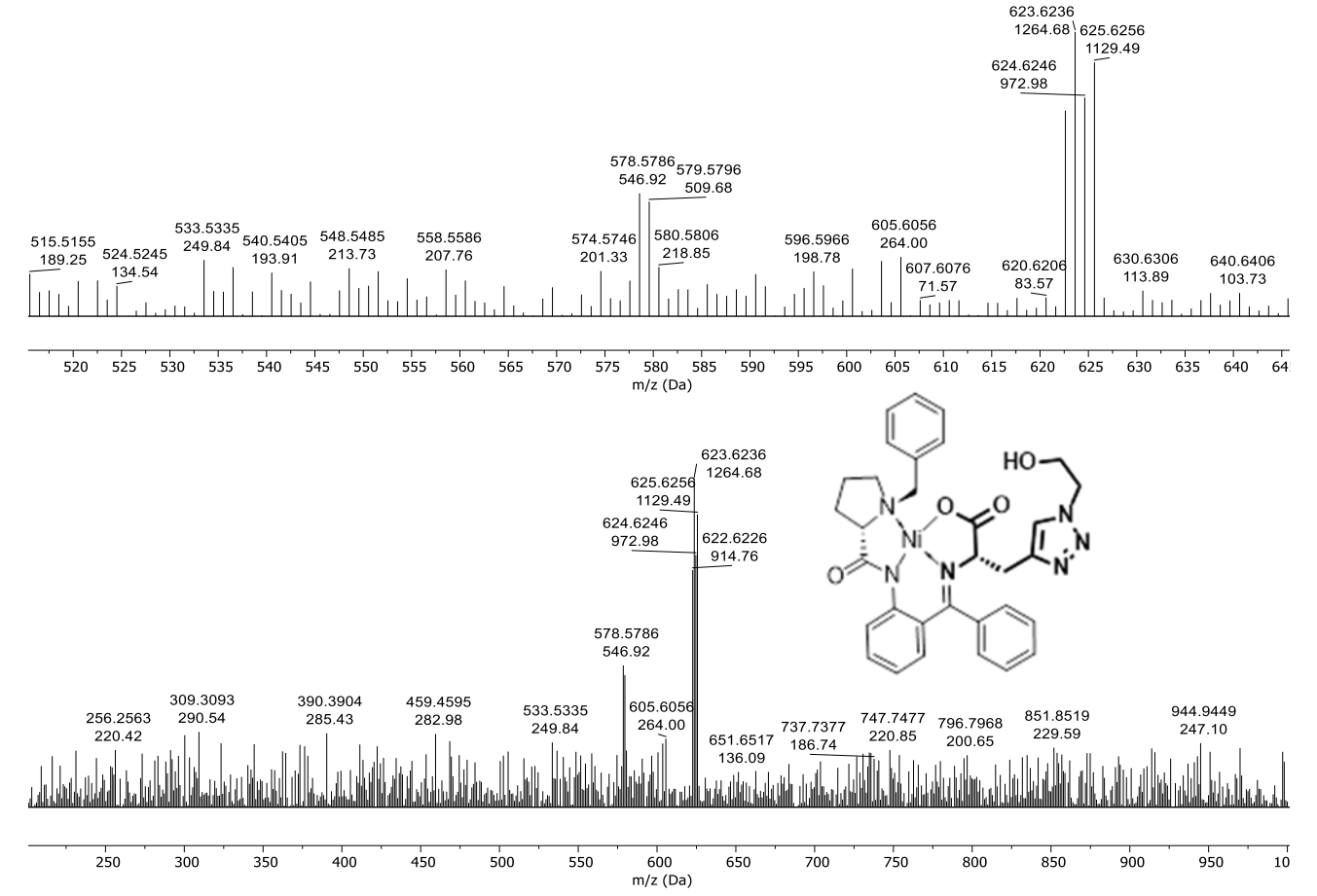


Figure S7: HRMS spectra of compound **5e**

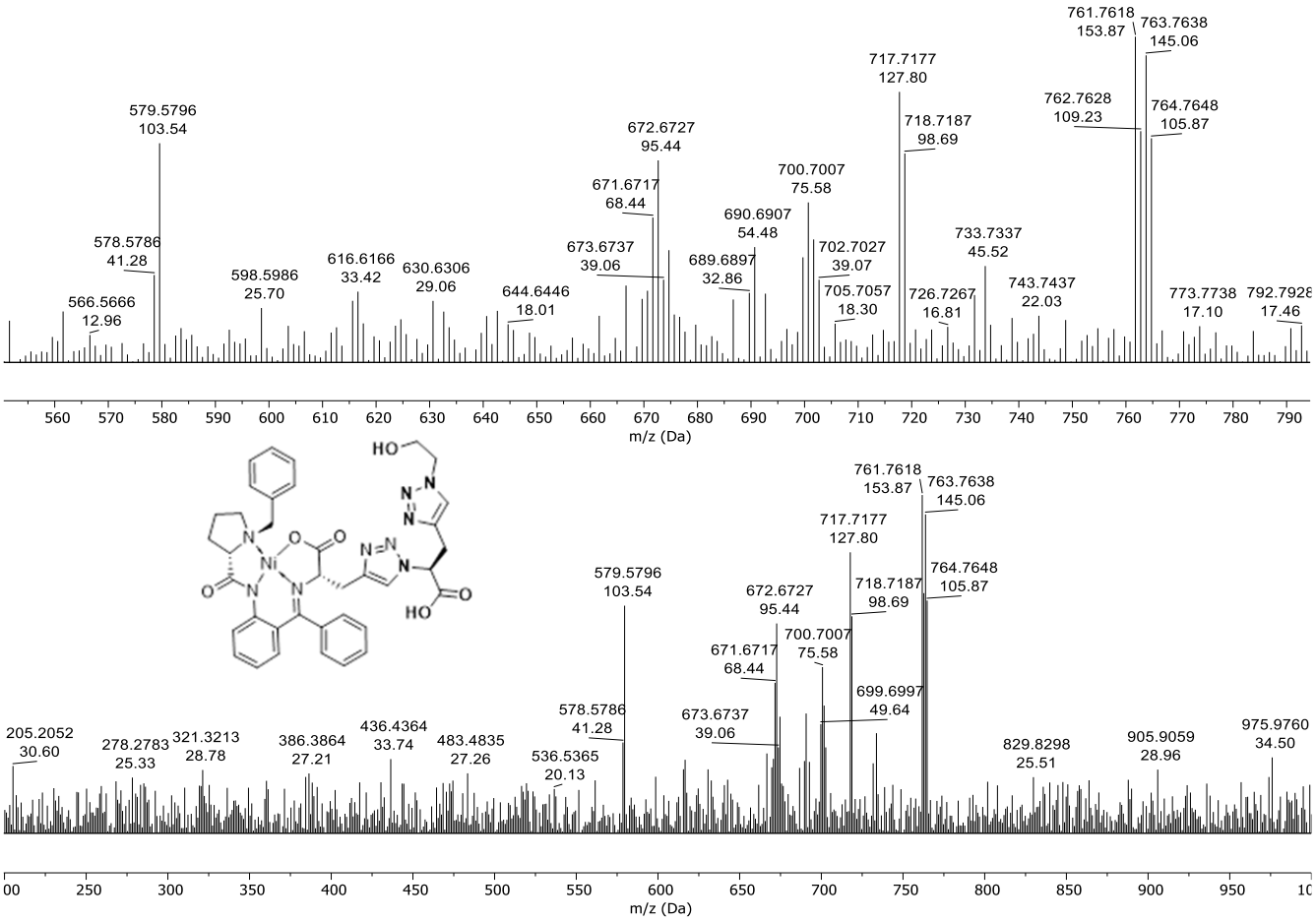


Figure S8: HRMS **s**pectra of compound **5f**

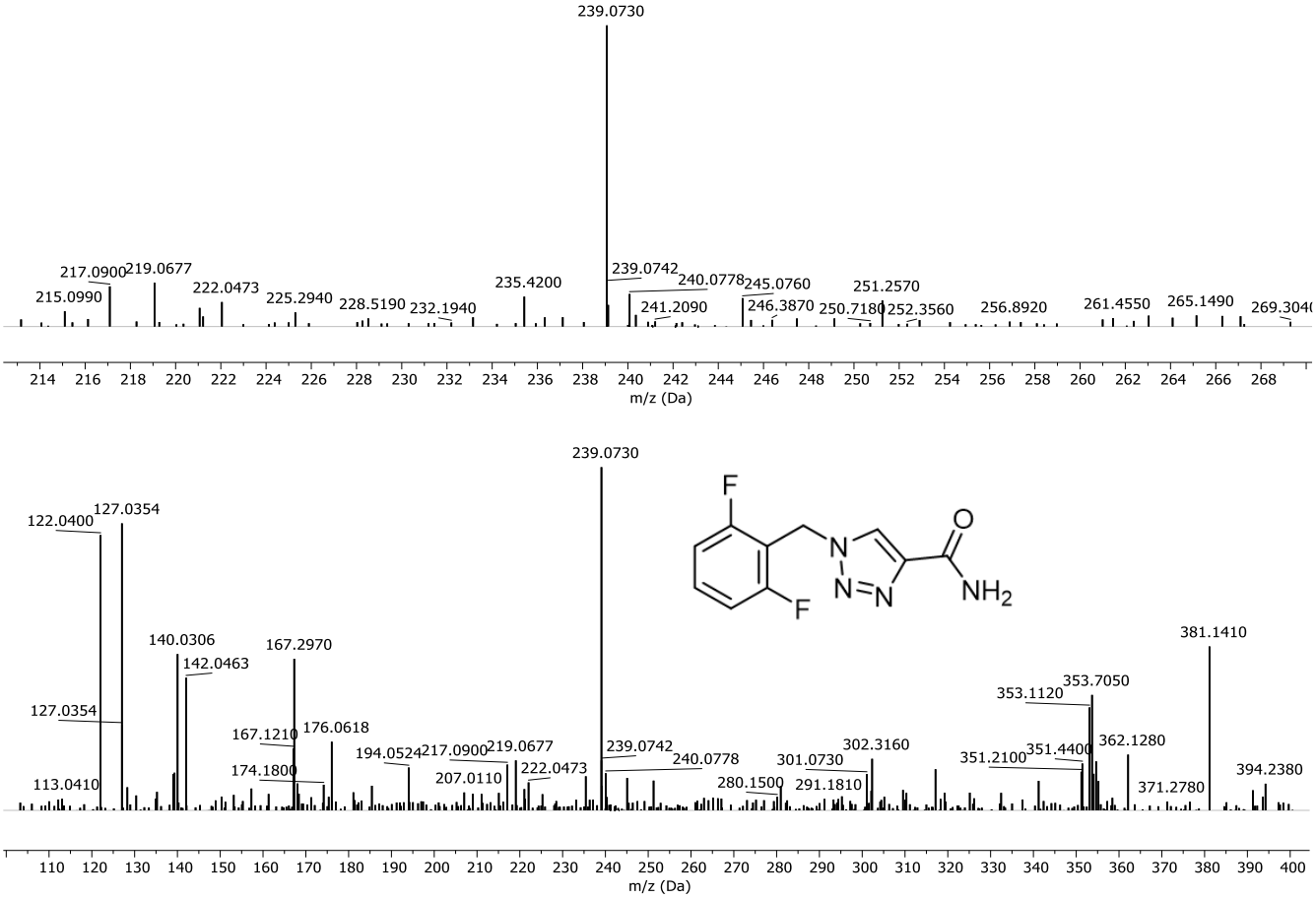


Figure S9: HRMS spectra of compound Rufinamide

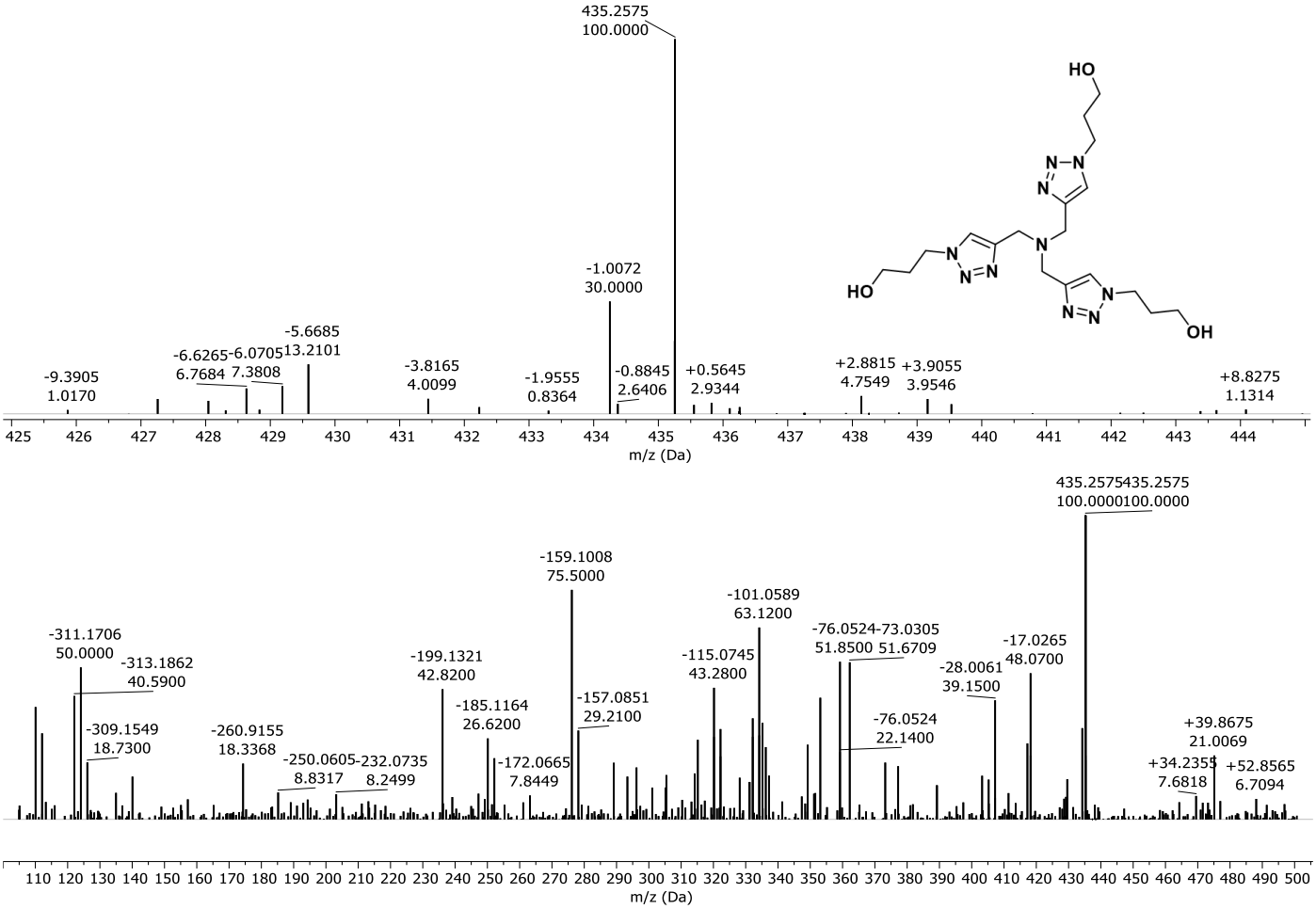


Figure S10: HRMS spectra of compound THPTA

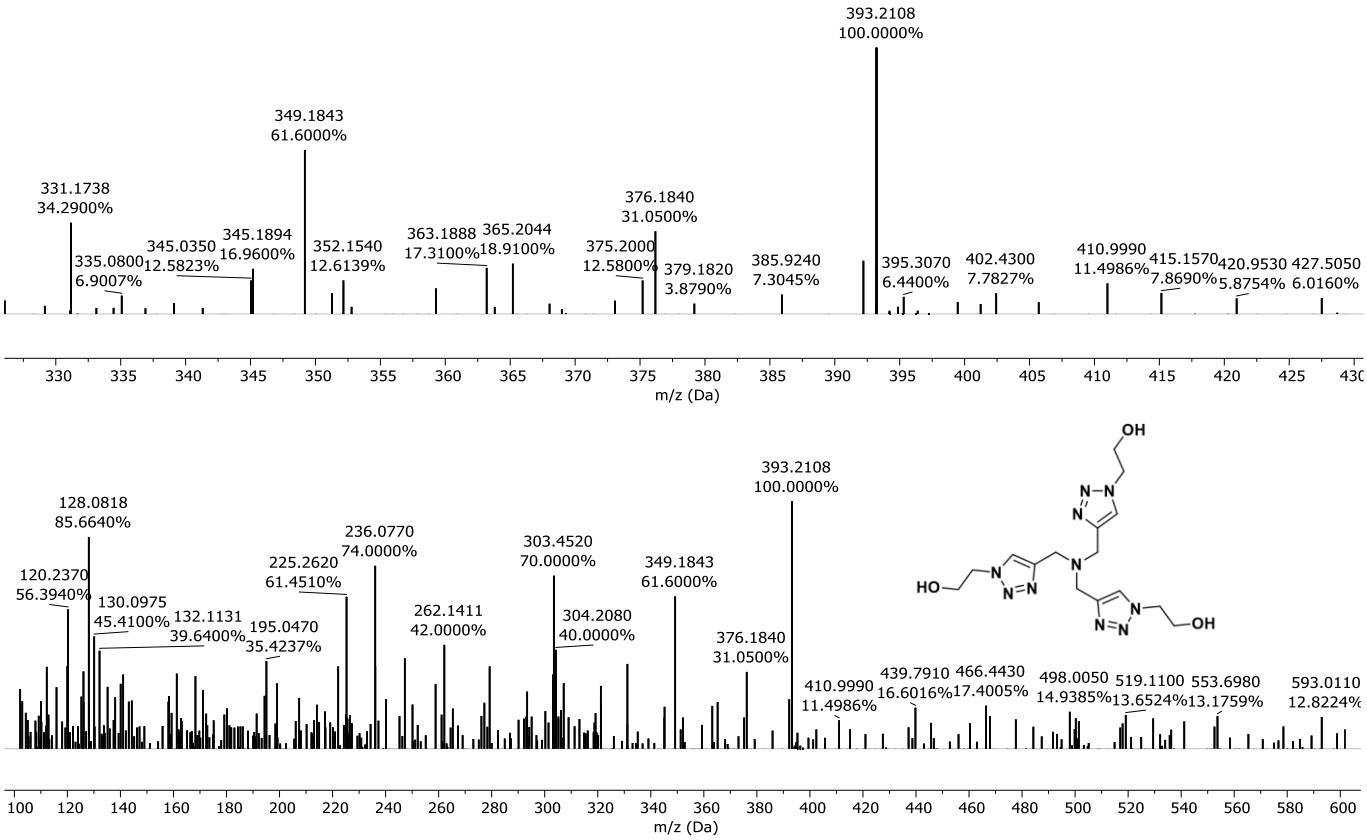


Figure S11: HRMS spectra of compound THETA

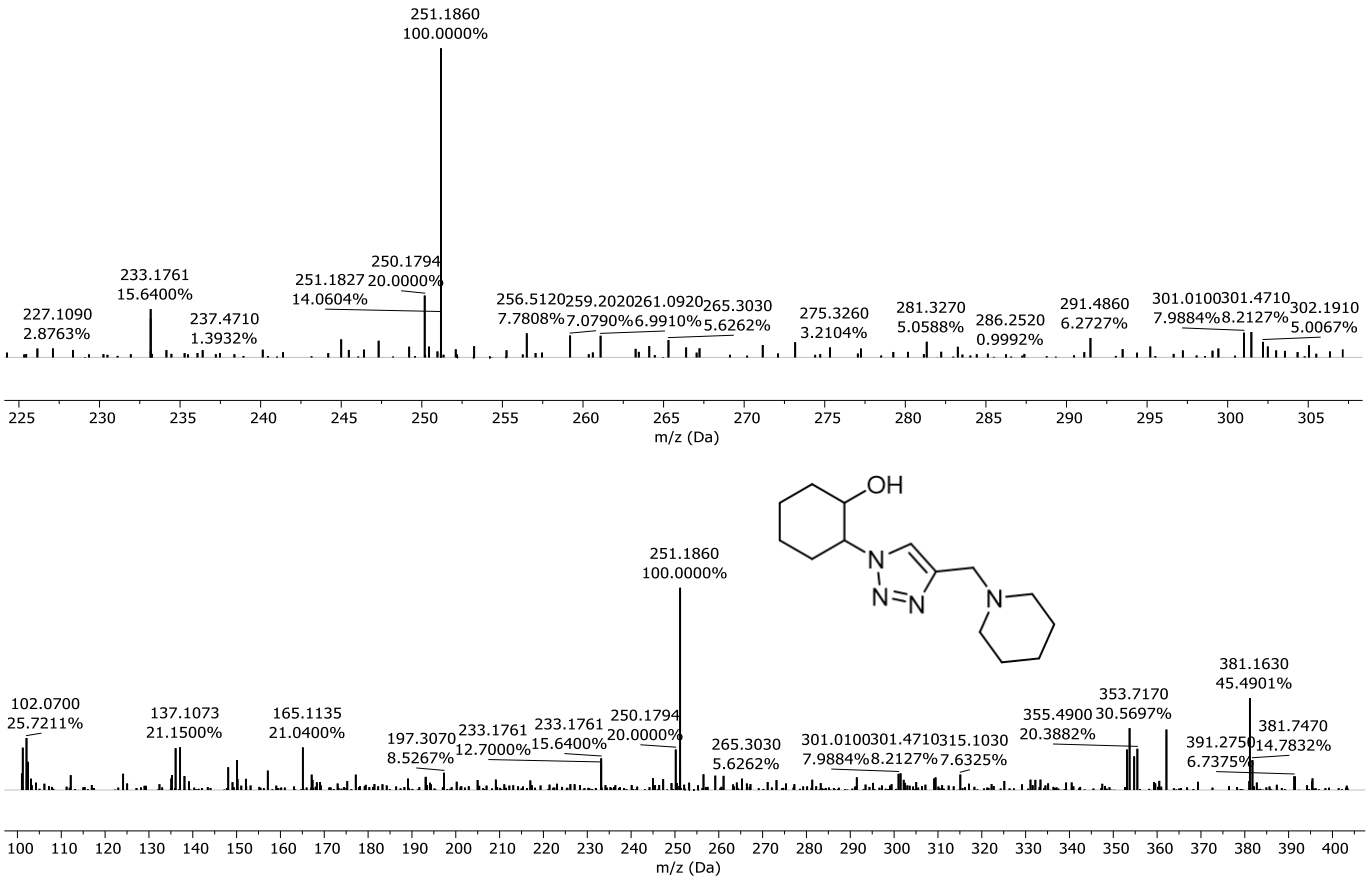


Figure S12: HRMS spectra of compound PPTP

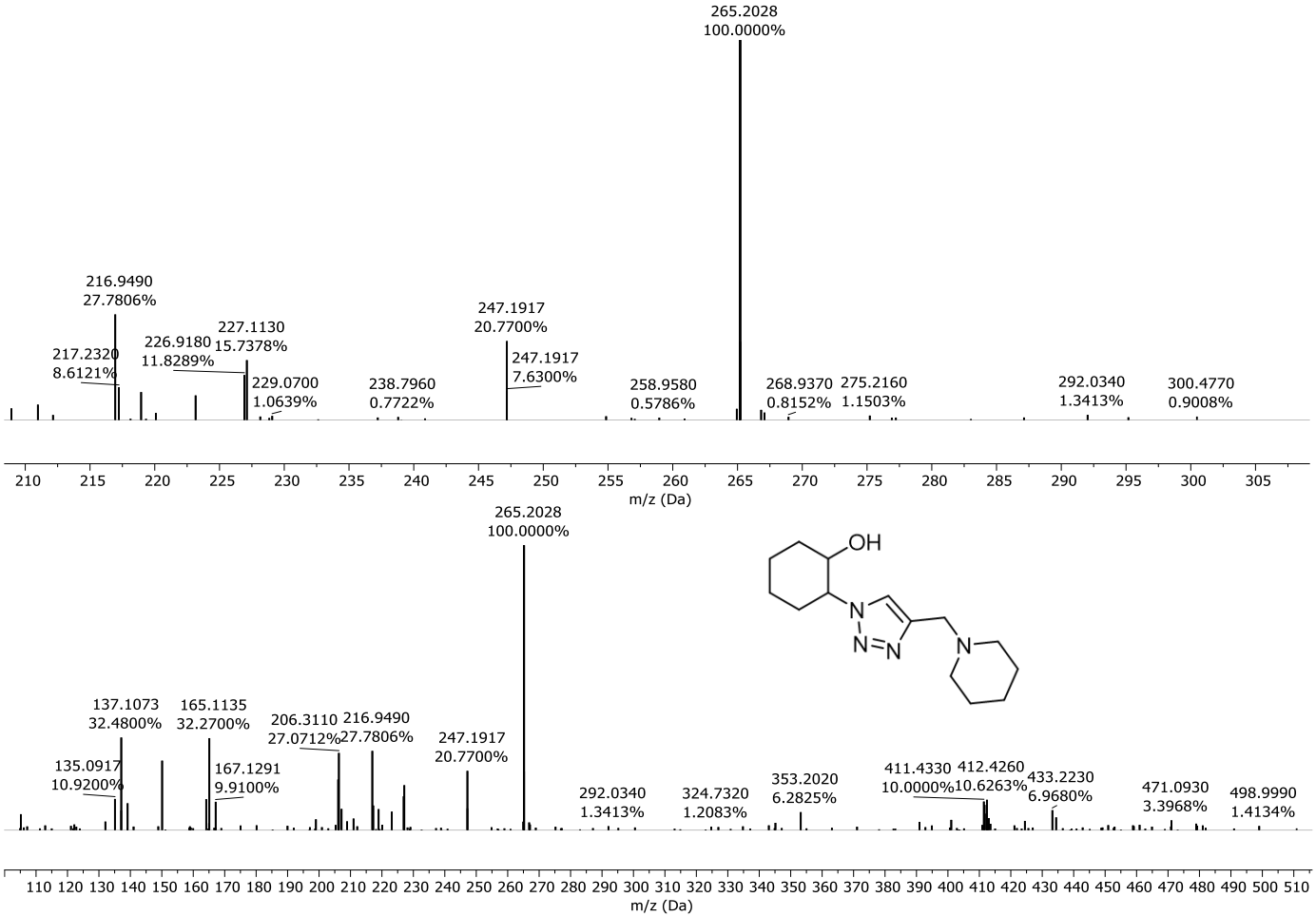


Figure S13: HRMS spectra of compound PPTC

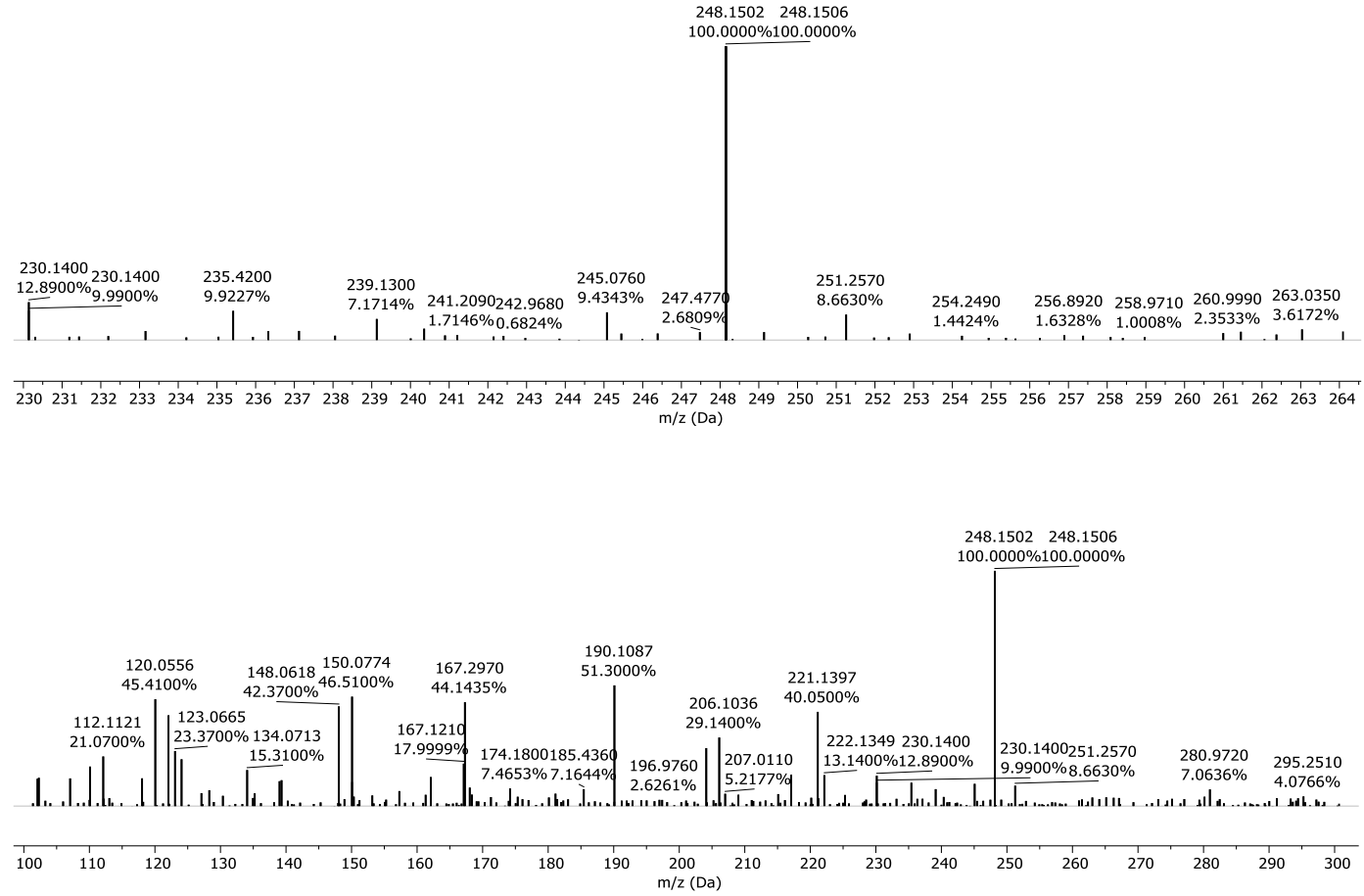


Figure S14: HRMS spectra of compound IMTC

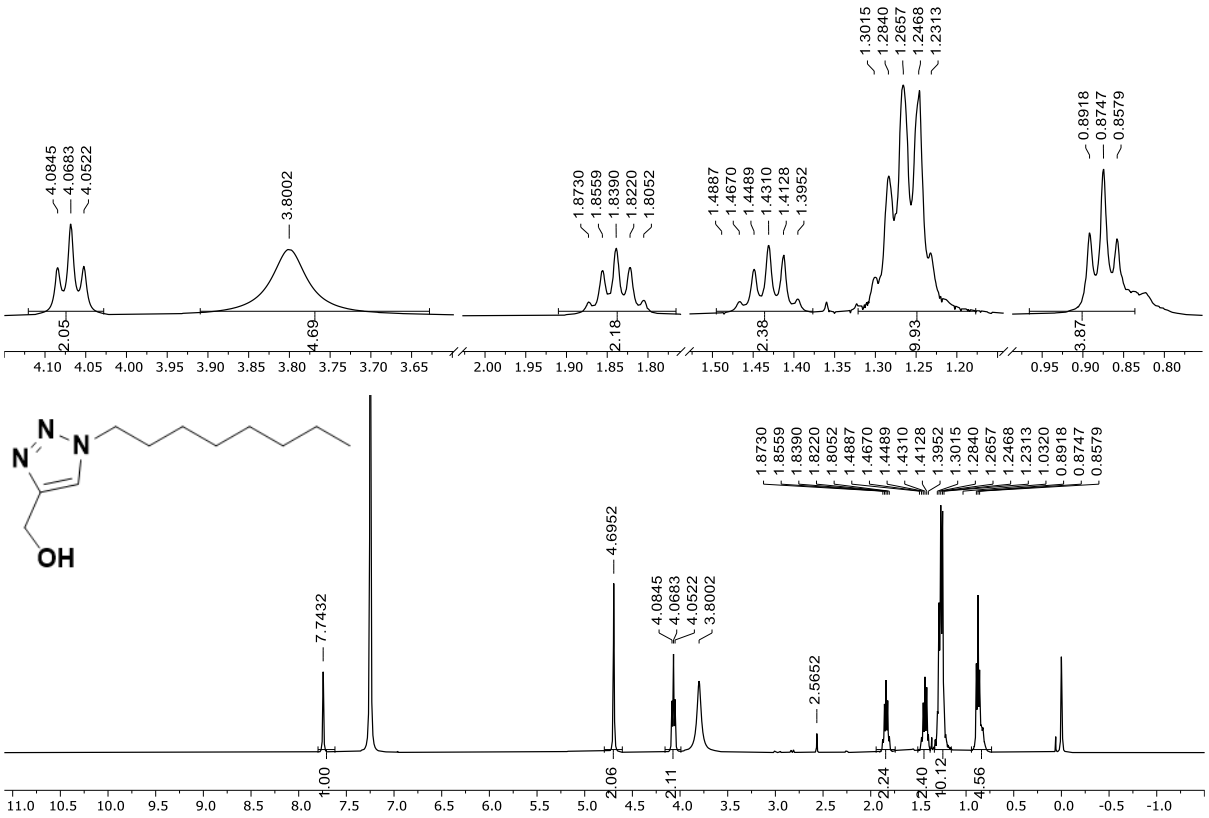


Figure S15. ^{1}H NMR of (1-octyl-1*H*-1,2,3-triazol-4-yl)methanol (**3a**) in $CDCl_3$ at 400MHz

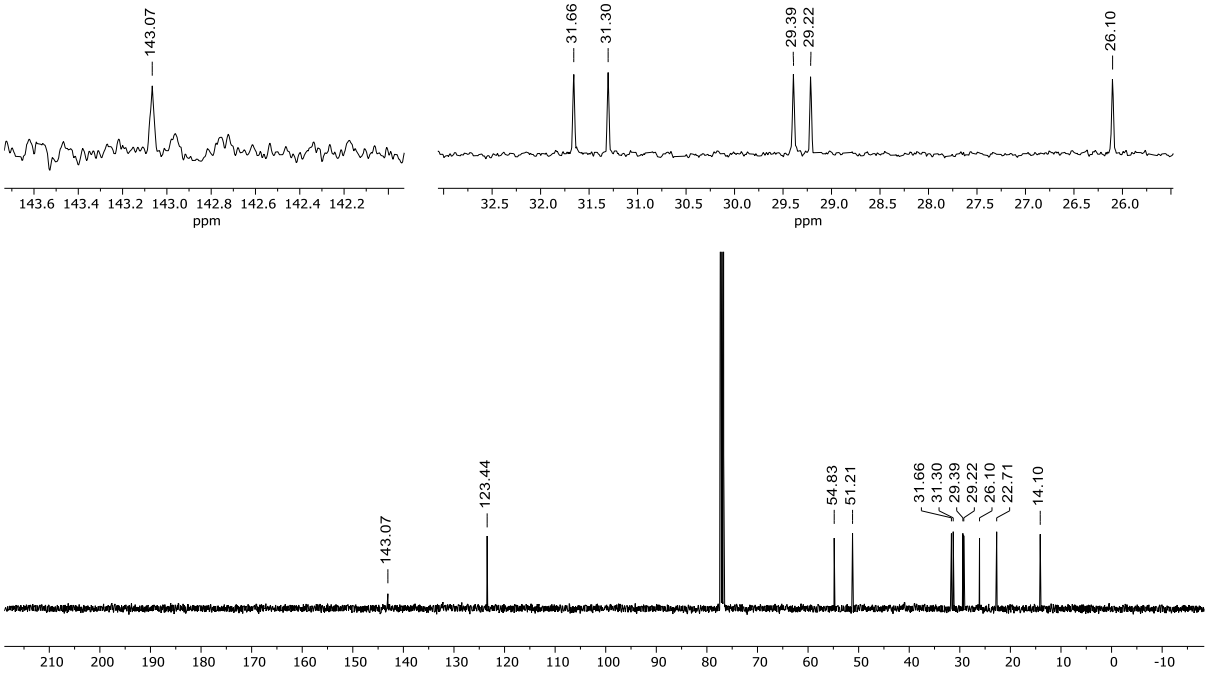


Figure S16. ^{13}C NMR of (1-octyl-1*H*-1,2,3-triazol-4-yl)methanol (**3a**) in $CDCl_3$ at 100MHz

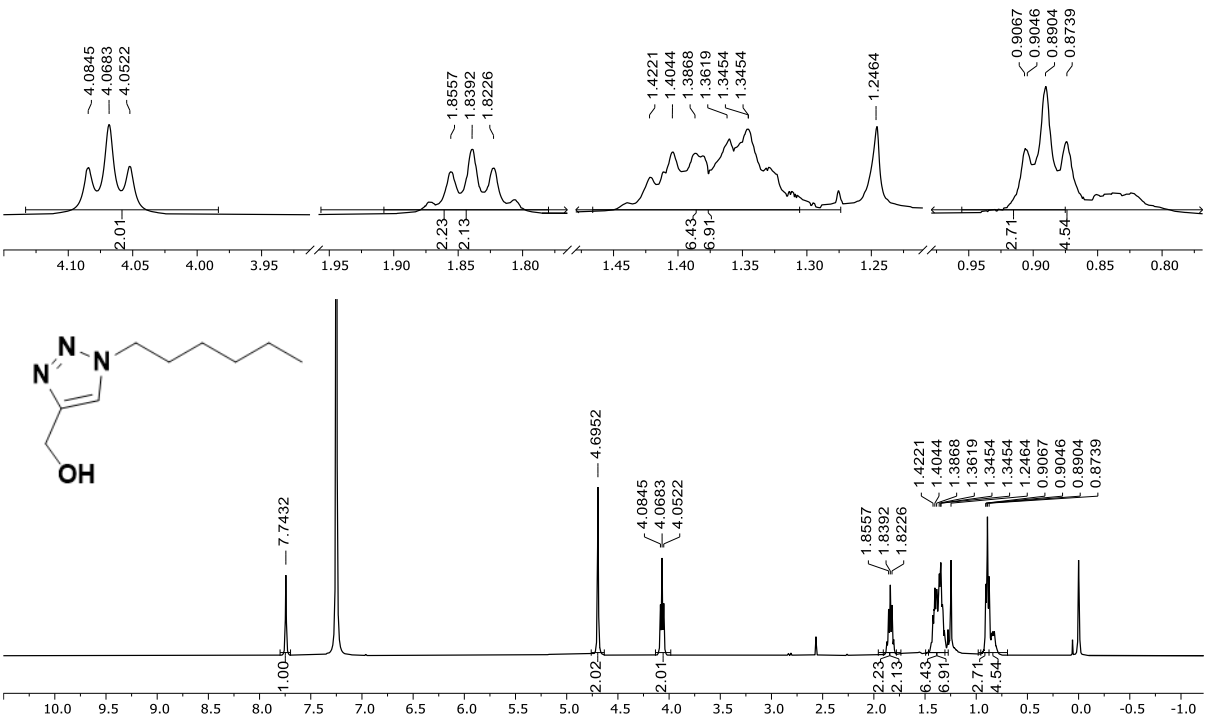


Figure S17. ^{1}H NMR of (1-hexyl-1*H*-1,2,3-triazol-4-yl)methanol (**3b**) in $CDCl_3$ at 400MHz

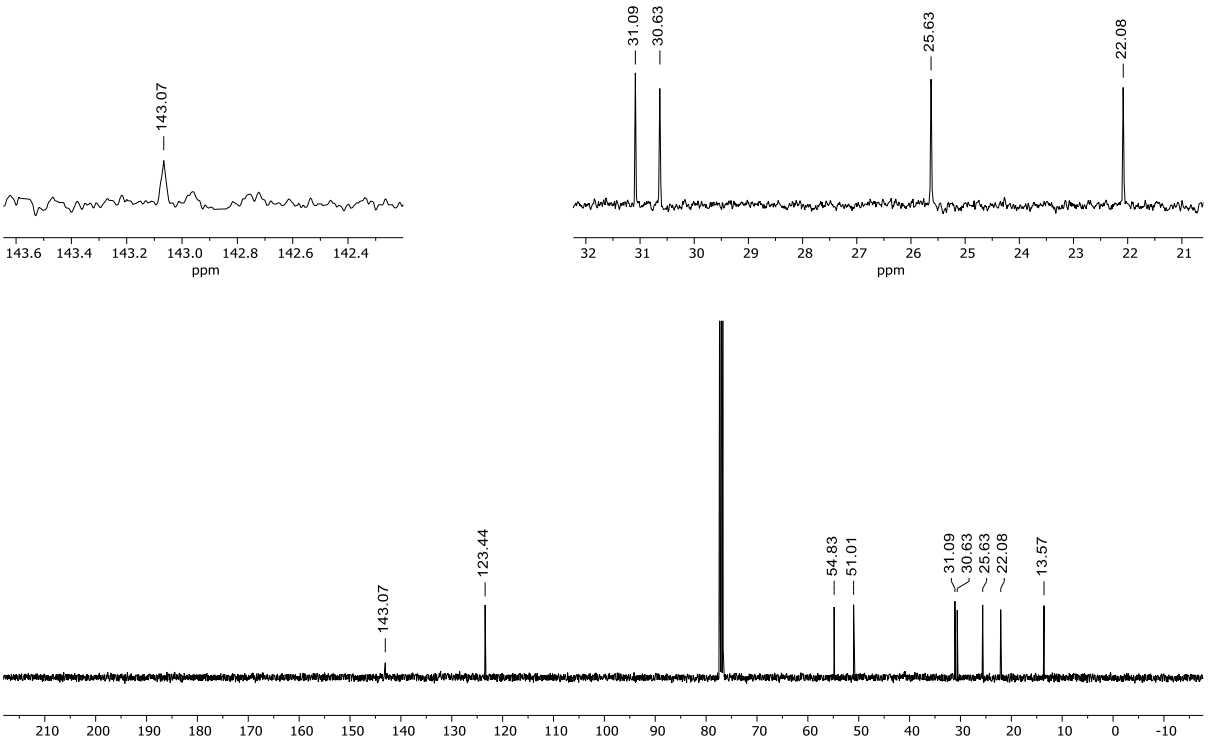


Figure S18. ^{13}C NMR of (1-hexyl-1*H*-1,2,3-triazol-4-yl)methanol (**3b**) in $CDCl_3$ at 100MHz

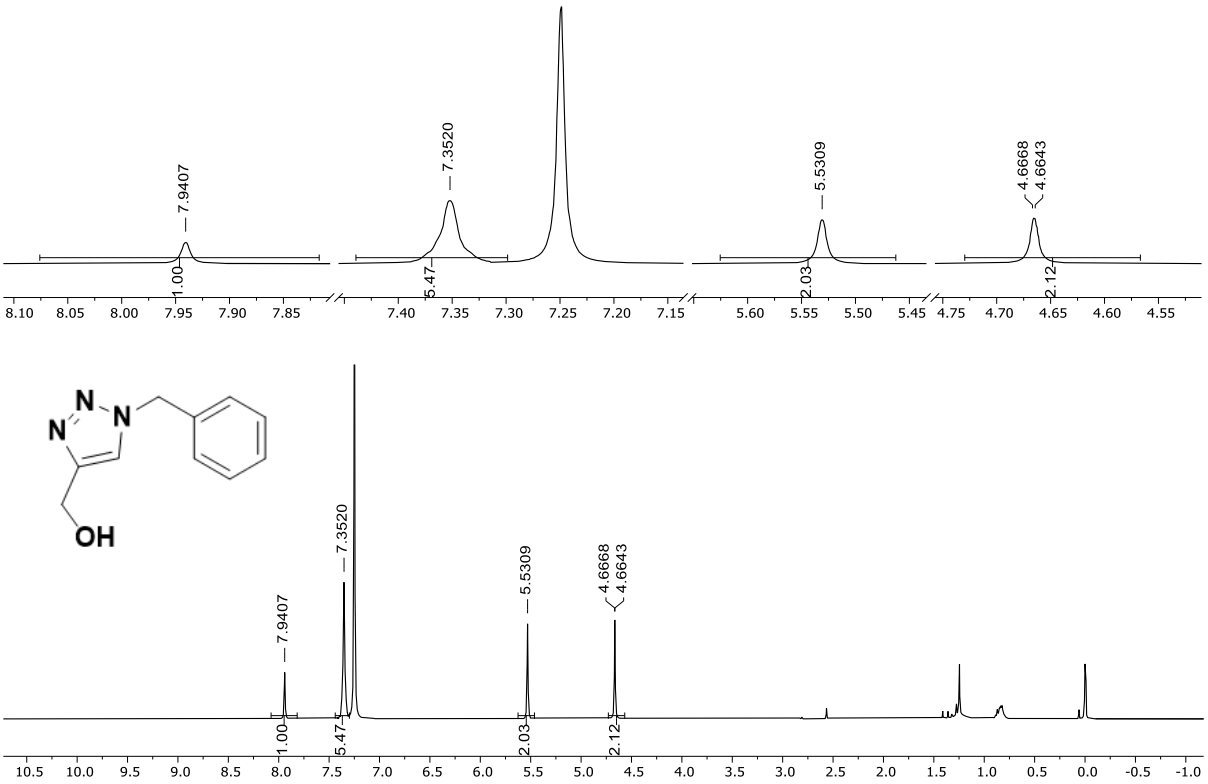


Figure S19. ^{1}H NMR of (1-benzyl-1*H*-1,2,3-triazol-4-yl)methanol (**3c**) in $CDCl_3$ at 400MHz

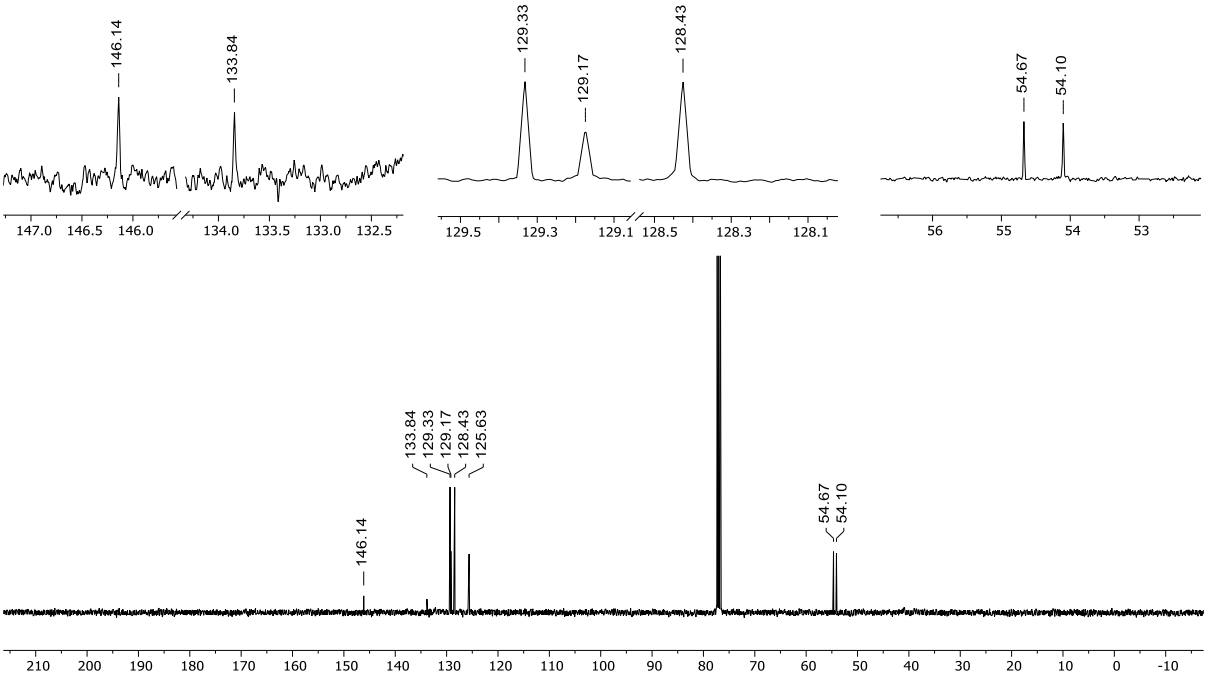


Figure S20. ^{13}C NMR of (1-benzyl-1*H*-1,2,3-triazol-4-yl)methanol (**3c**) in $CDCl_3$ at 100MHz

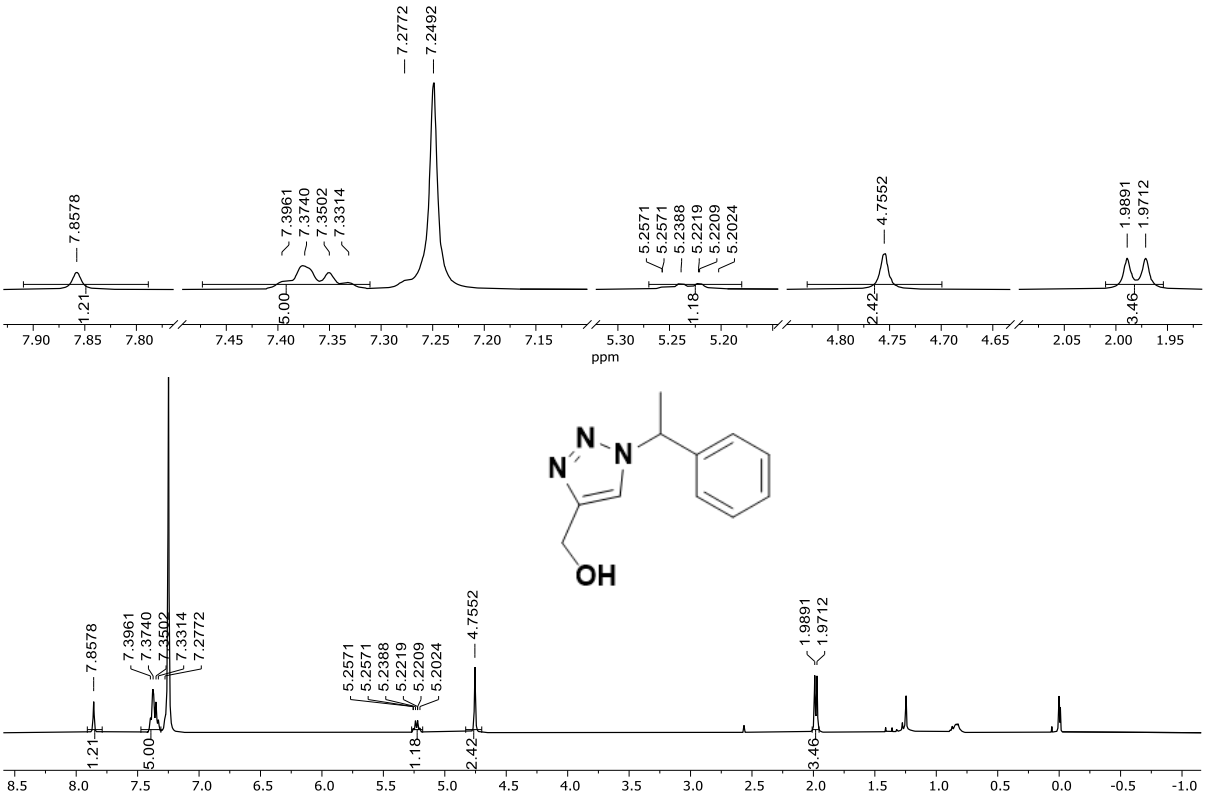


Figure S21. ^{1}H NMR of (1-(1-phenylethyl)-1*H*-1,2,3-triazol-4-yl)methanol (**3d**) in $CDCl_3$ at 400MHz

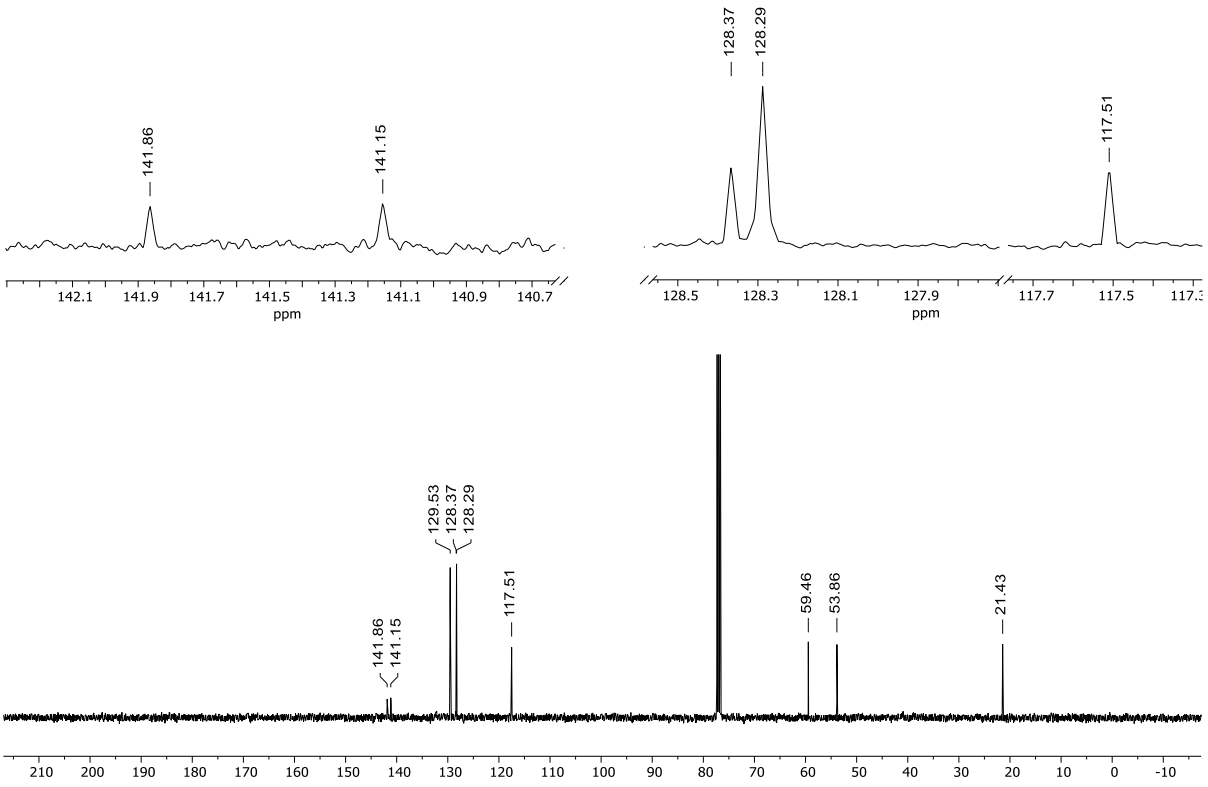


Figure S22. ^{13}C NMR of (1-(1-phenylethyl)-1*H*-1,2,3-triazol-4-yl)methanol (**3d**) in $CDCl_3$ at 100 MHz

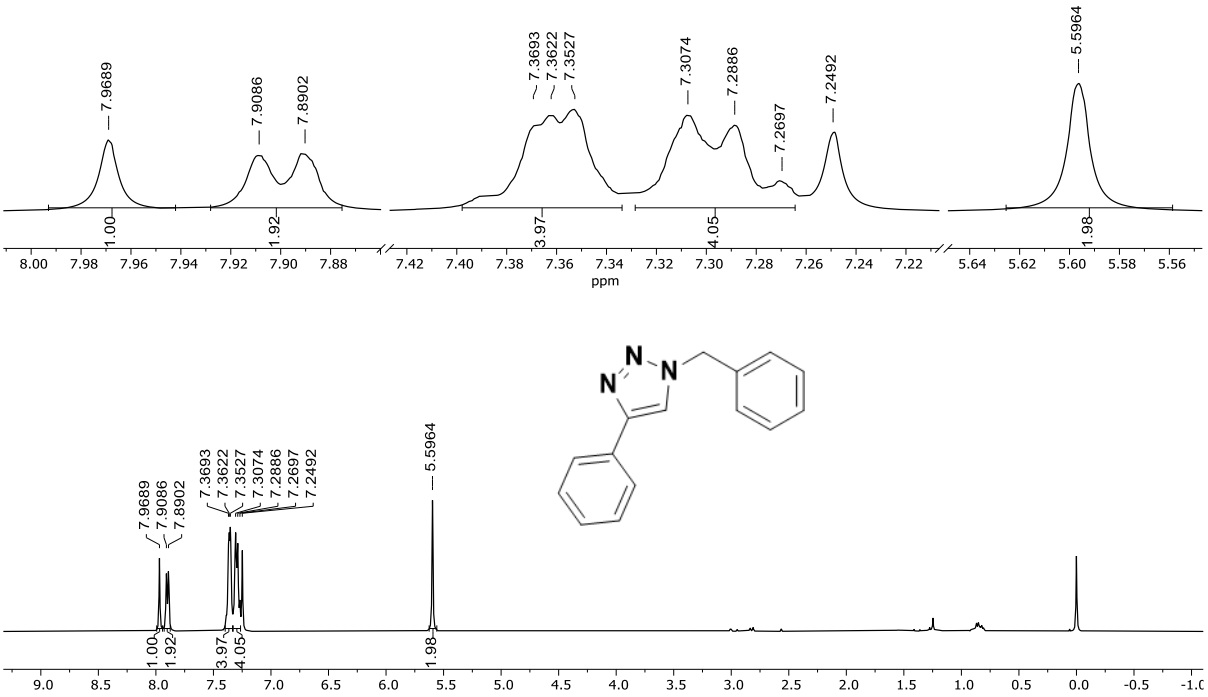


Figure S23. ^{1}H NMR of 1-benzyl-4-phenyl-1*H*-1,2,3-triazole (**3e**) in $CDCl_3$ at 400 MHz

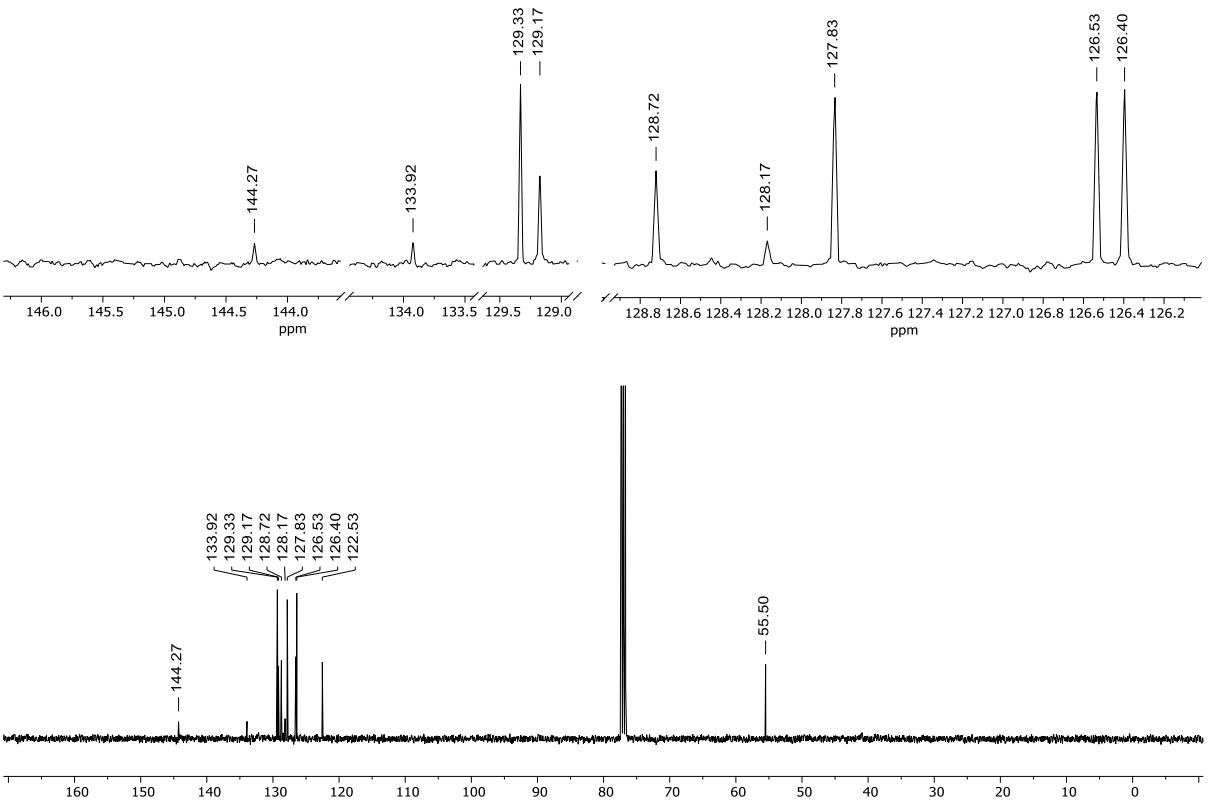


Figure S24. ^{13}C NMR of 1-benzyl-4-phenyl-1*H*-1,2,3-triazole (**3e**) in $CDCl_3$ at 100MHz

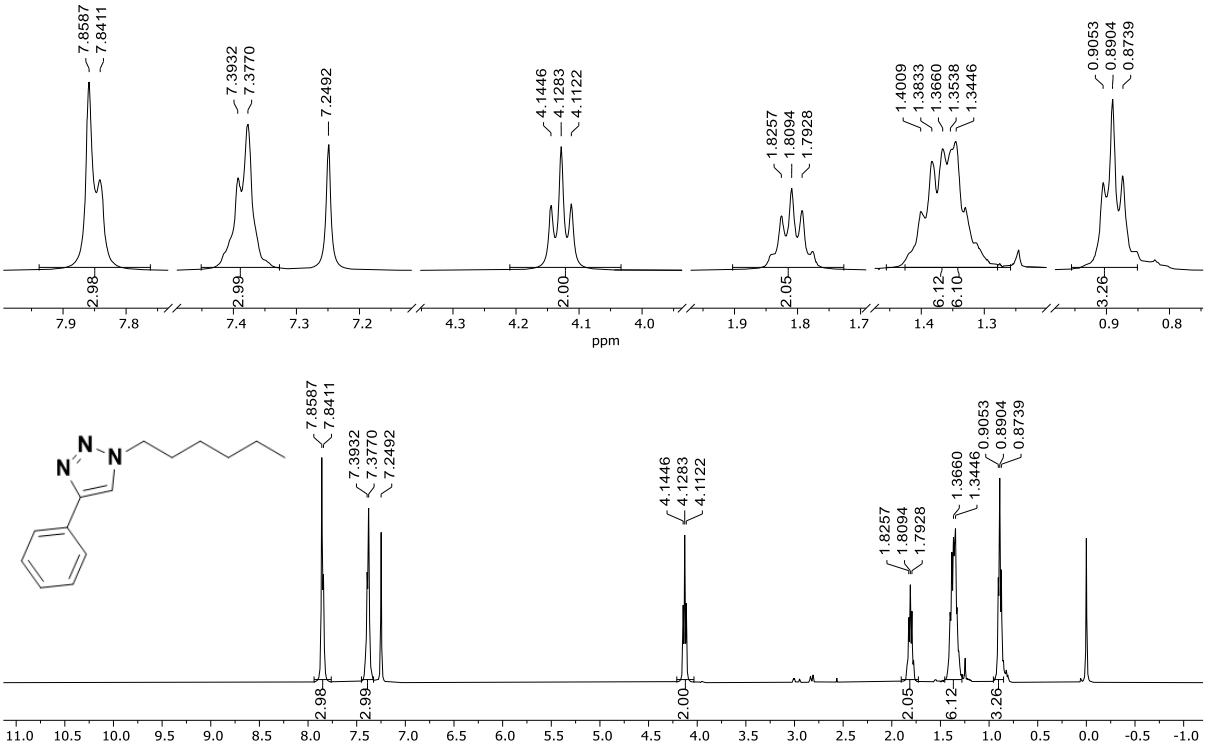


Figure S25. ^{1}H NMR of 1-hexyl-4-phenyl-1*H*-1,2,3-triazole (**3f**) in $CDCl_3$ at 400MHz

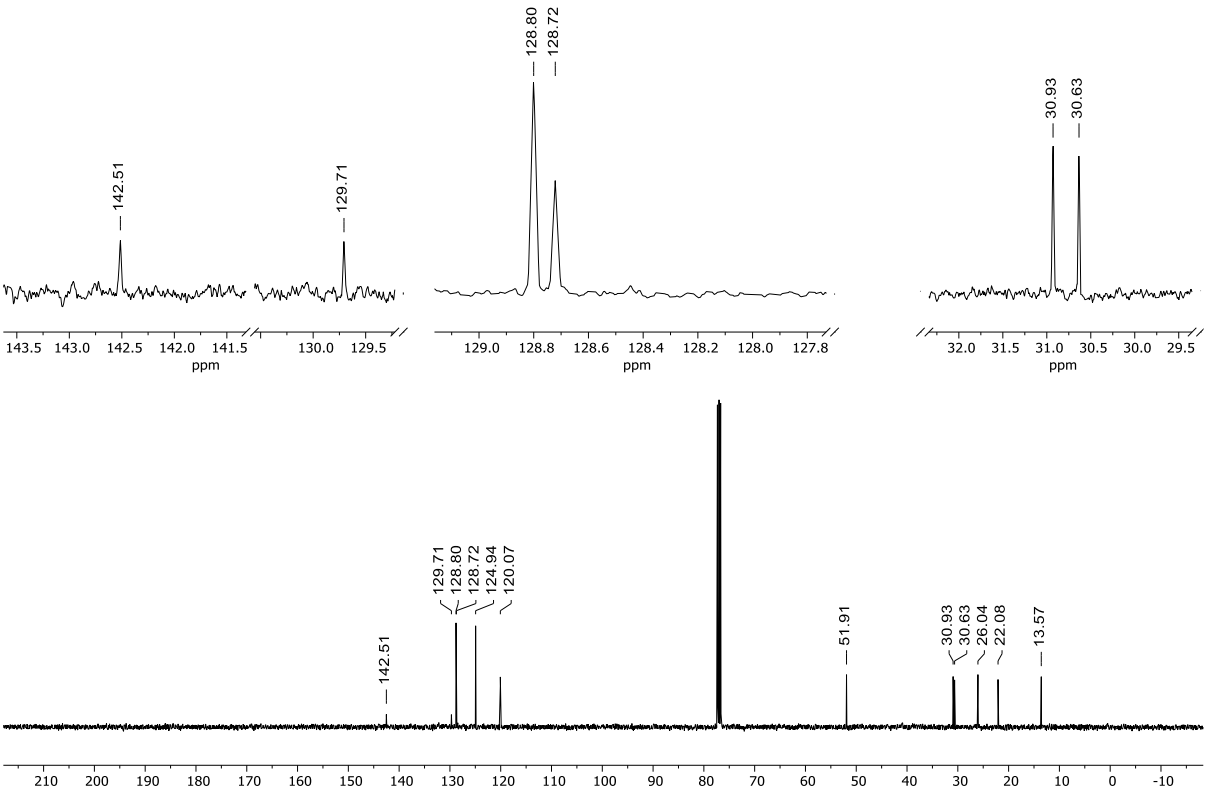


Figure S26. ^{13}C NMR of 1-hexyl-4-phenyl-1*H*-1,2,3-triazole (**3f**) in $CDCl_3$ at 100MHz

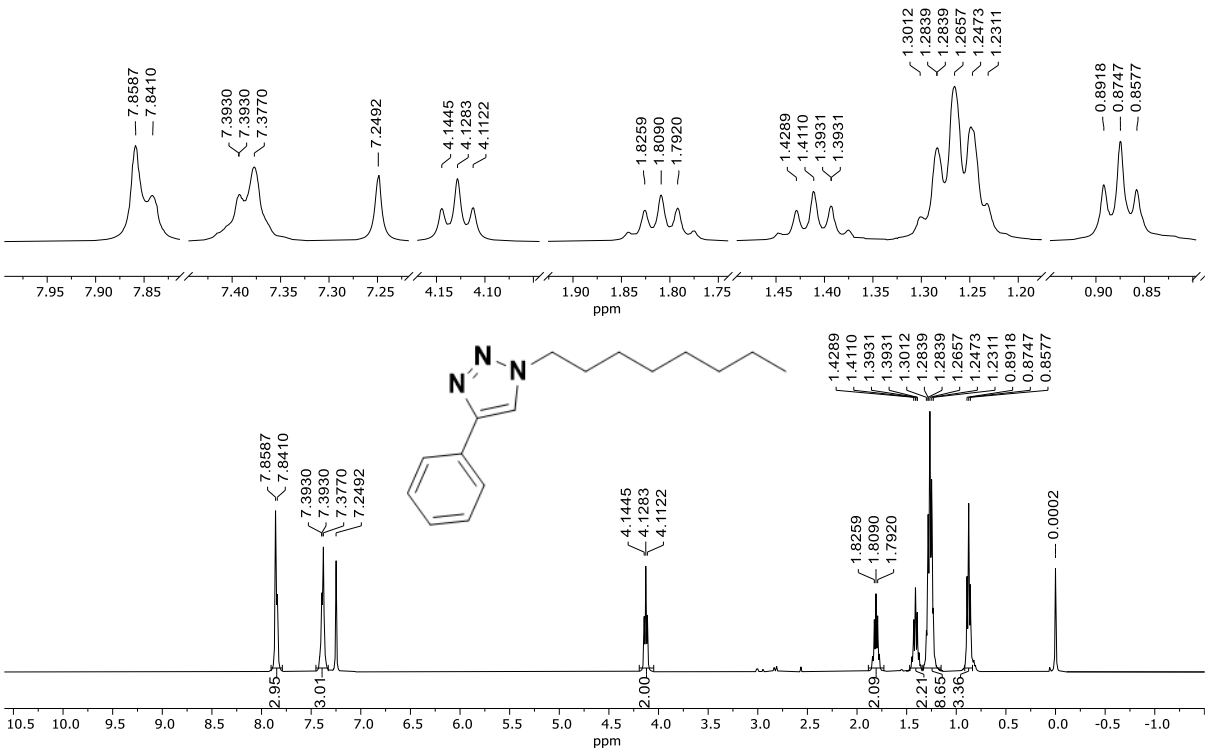


Figure S27. ^{1}H NMR of 1-octyl-4-phenyl-1*H*-1,2,3-triazole (**3g**) in $CDCl_3$ at 400MHz

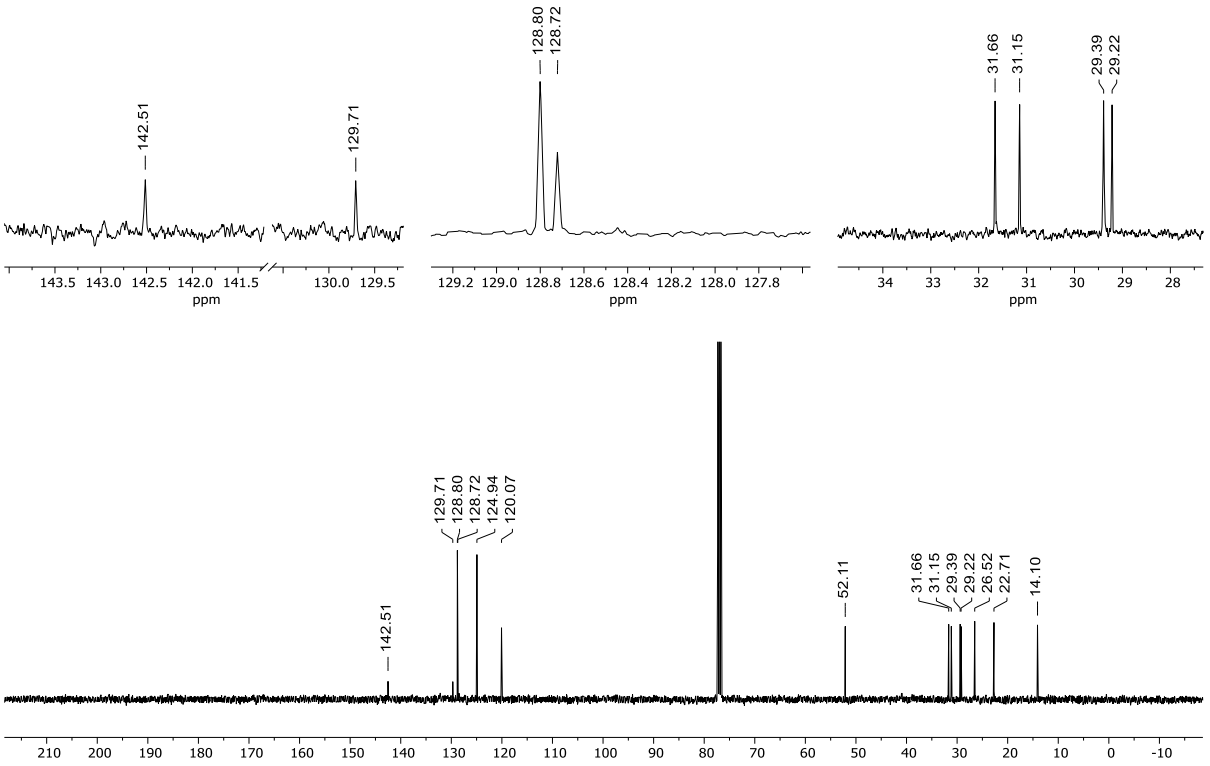


Figure S28. ^{13}C NMR of 1-octyl-4-phenyl-1*H*-1,2,3-triazole (**3g**) in $CDCl_3$ at 100MHz

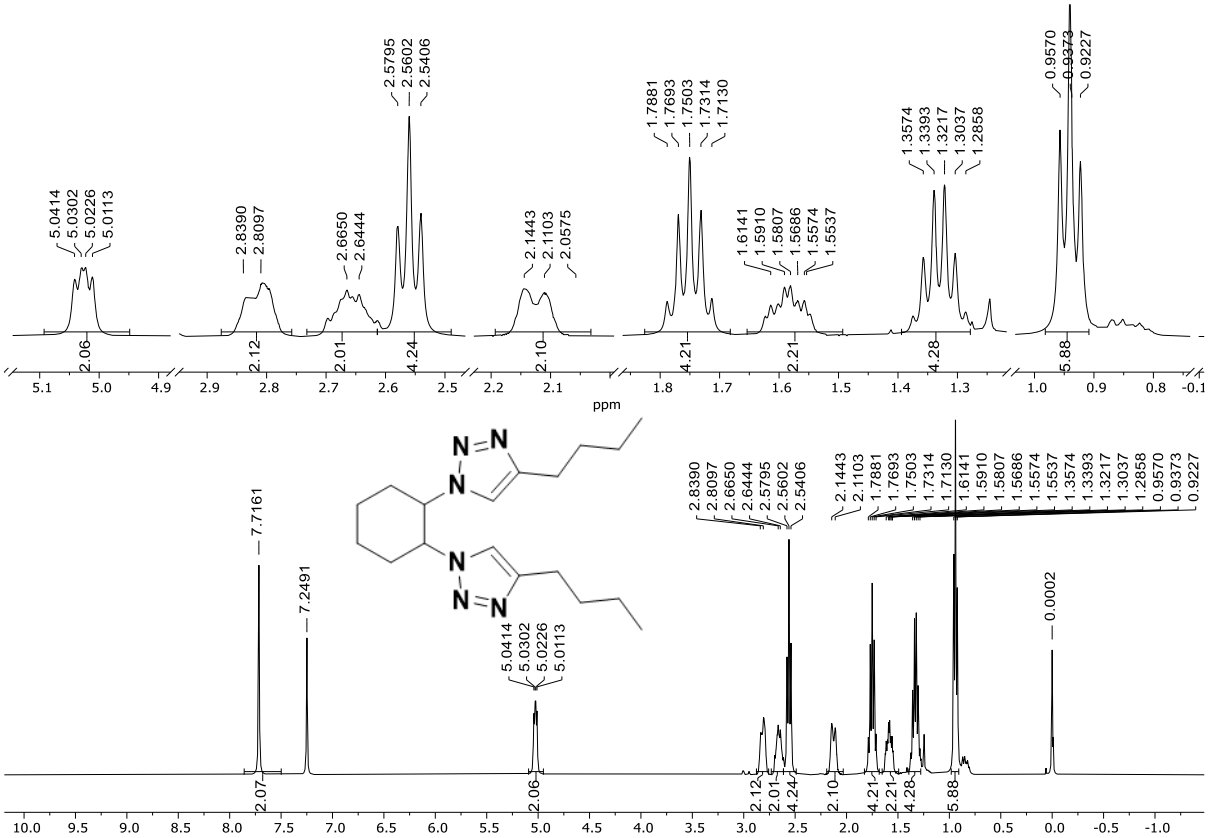


Figure S29. ^{1}H NMR of 1,2-bis(4-butyl-1*H*-1,2,3-triazol-1-yl)cyclohexane (**3h**) in $CDCl_3$ at 400MHz

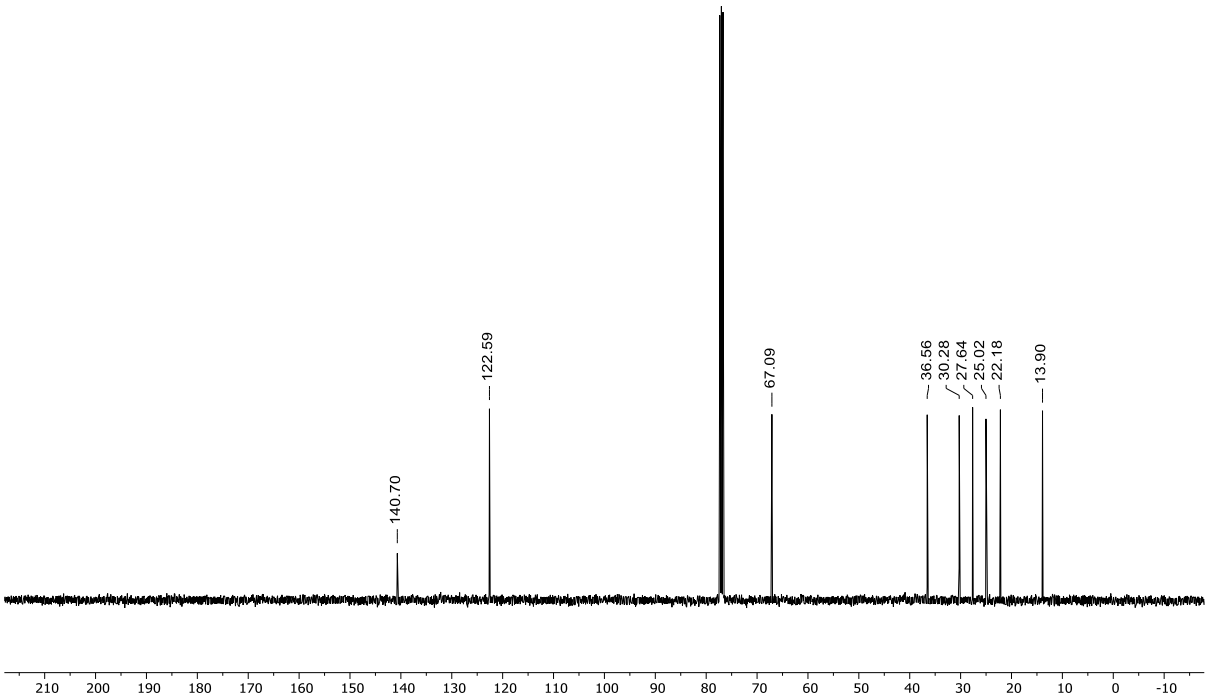


Figure S30. ^{13}C NMR of 1,2-bis(4-butyl-1*H*-1,2,3-triazol-1-yl)cyclohexane (**3h**) in $CDCl_3$ at 100MHz

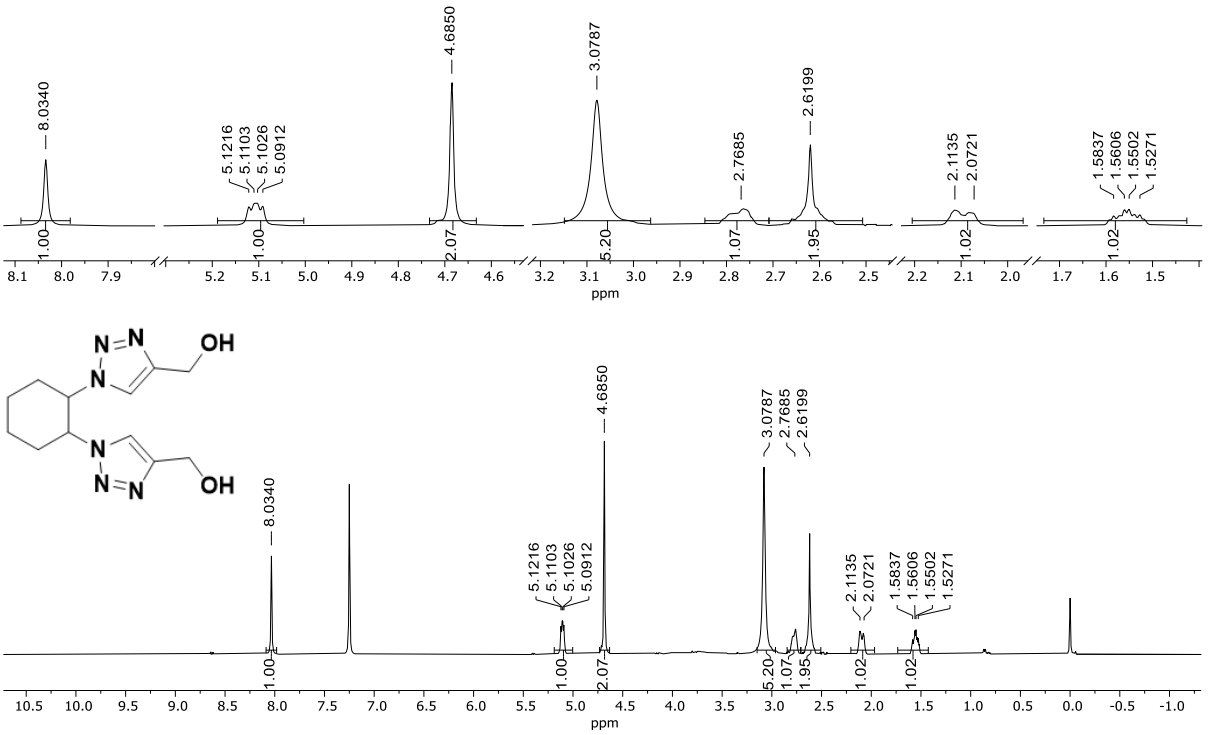


Figure S31. ^{1}H NMR of (cyclohexane-1,2-diylbis(1*H*-1,2,3-triazole-1,4-diyl))dimethanol (**3i**) in $CDCl_3$ at 400MHz

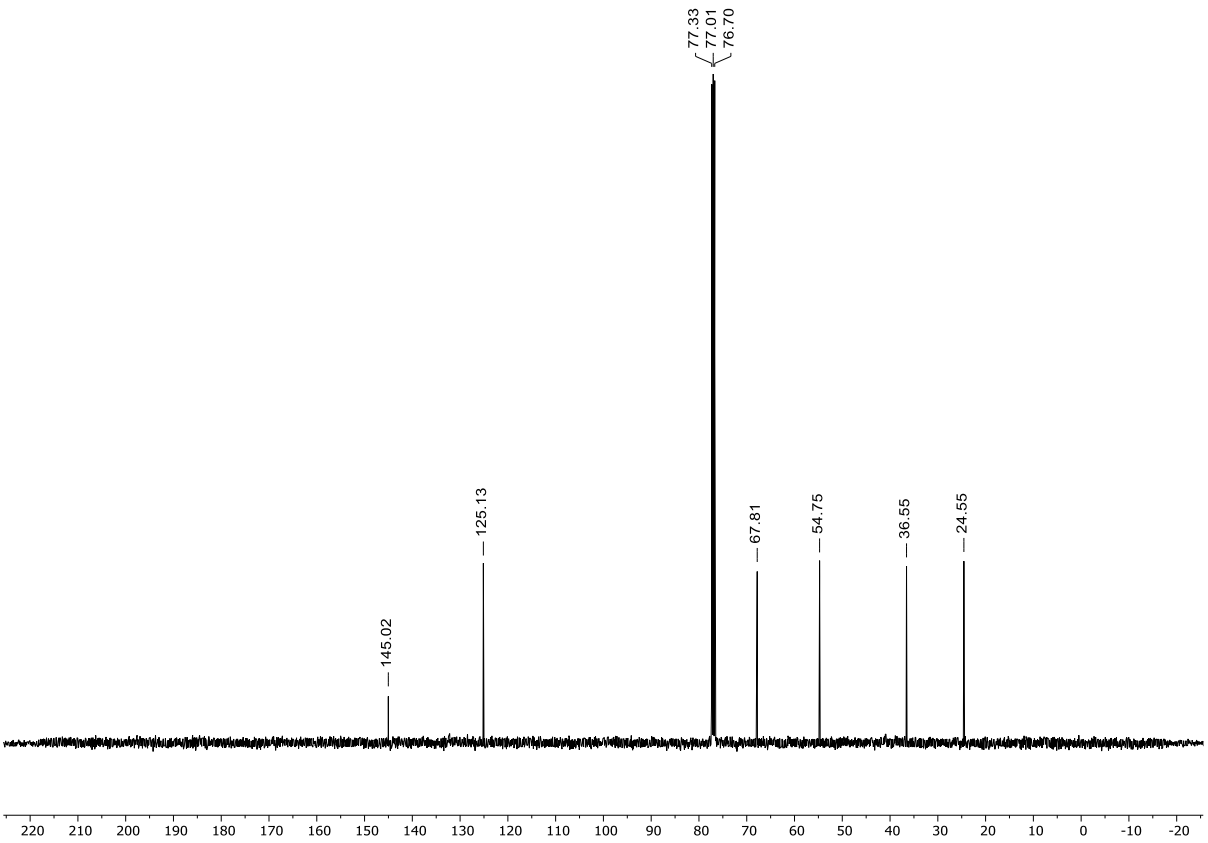


Figure S32. ^{13}C NMR of (cyclohexane-1,2-diylbis(1*H*-1,2,3-triazole-1,4-diyl))dimethanol (**3i**) in $CDCl_3$ at 100MHz

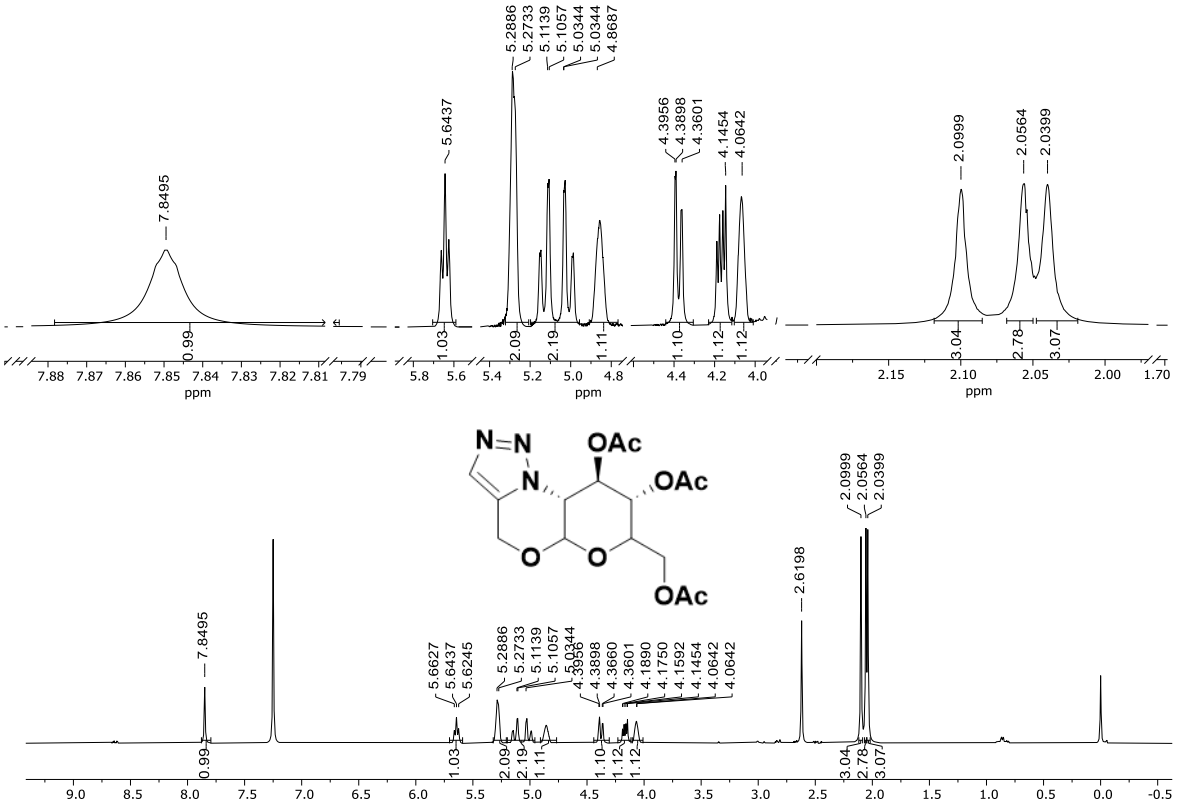


Figure S33. ^{1}H NMR of (8*S*,9*R*,9aR)-7-(acetoxymethyl)-5a,8,9,9a-tetrahydro-4*H*,7*H*-pyrano[2,3-b][1,2,3]triazolo[1,5-d][1,4]oxazine-8,9-diyl diacetate (**3j**) in $CDCl_3$ at 400 MHz

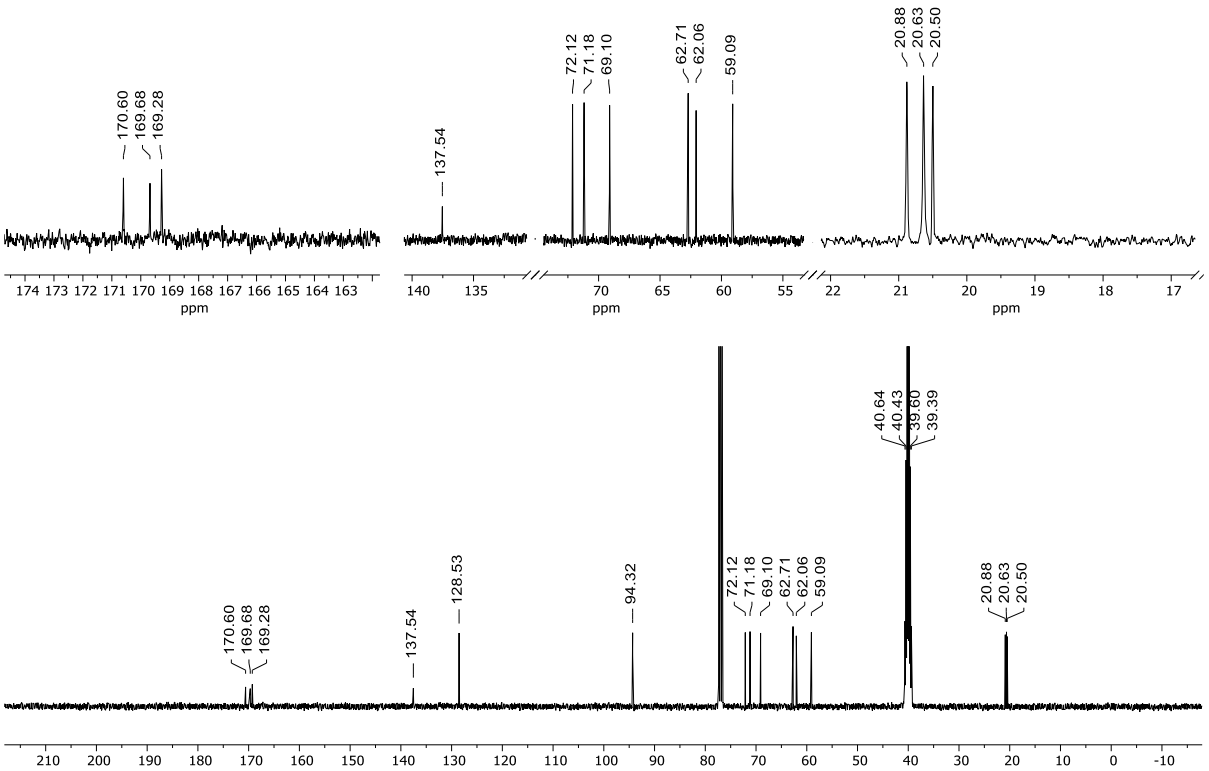


Figure S34. ^{13}C NMR of (8*S*,9*R*,9aR)-7-(acetoxymethyl)-5a,8,9,9a-tetrahydro-4*H*,7*H*-pyrano[2,3-b][1,2,3]triazolo[1,5-d][1,4]oxazine-8,9-diyl diacetate (**3j**) in $CDCl_3$ at 100MHz

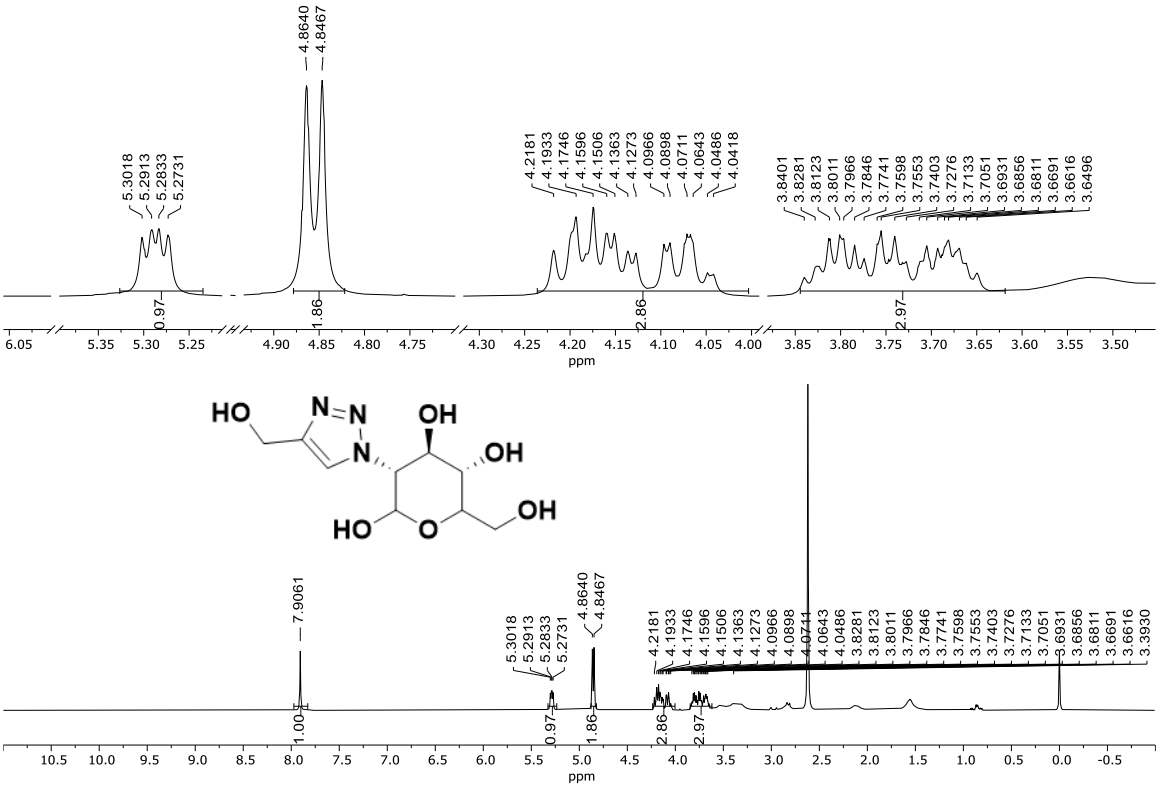


Figure S35. ^{1}H NMR of (3*R*,4*R*,5*S*)-6-(hydroxymethyl)-3-(4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)tetrahydro-2*H*-pyran-2,4,5-triol (**3k**) in DMSO-d_6 at 400MHz

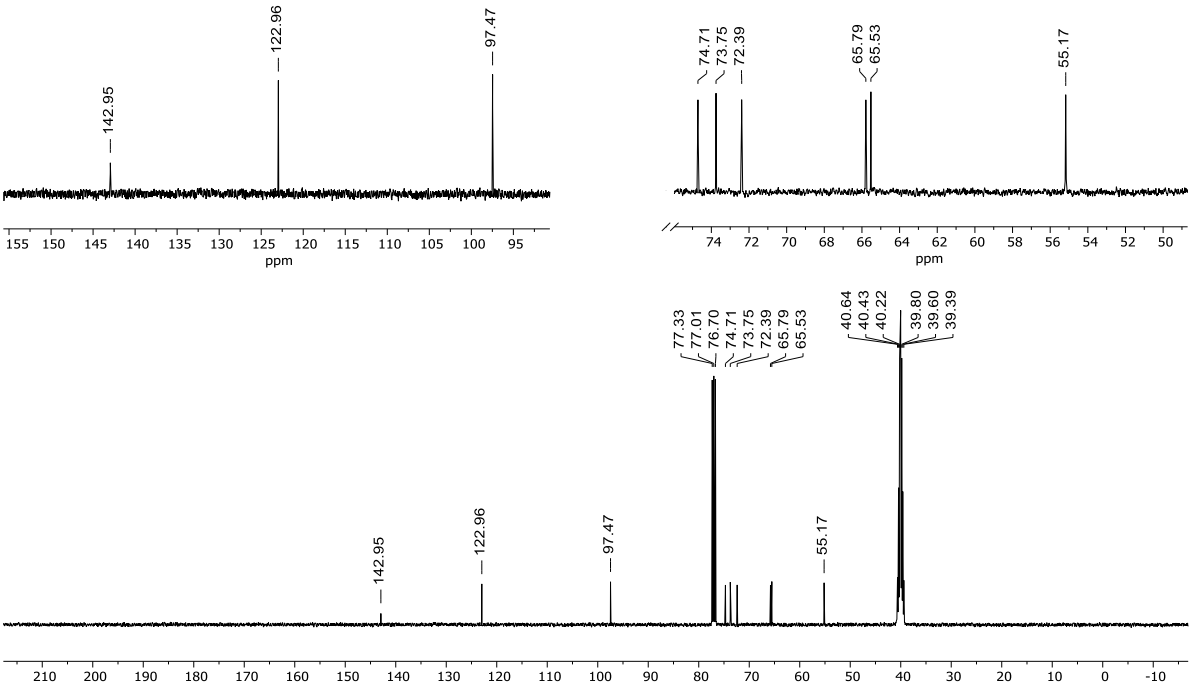


Figure S36. ^{13}C NMR of (3*R*,4*R*,5*S*)-6-(hydroxymethyl)-3-(4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)tetrahydro-2*H*-pyran-2,4,5-triol (**3k**) in $CDCl_3$+DMSO-d_6 at 100MHz

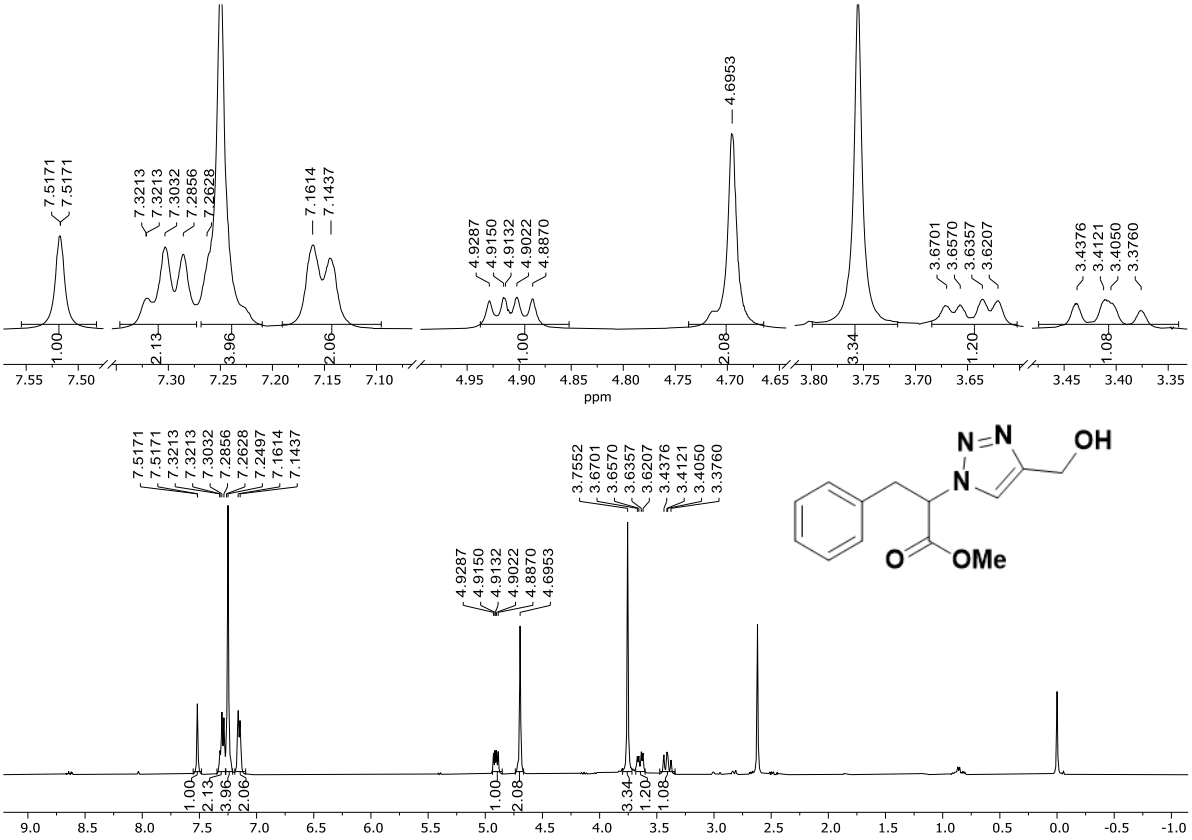


Figure S37. ^{1}H NMR of methyl 2-(4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)-3-phenylpropanoate (**3l**) in DMSO-d_6 +$CDCl_3$ at 400MHz

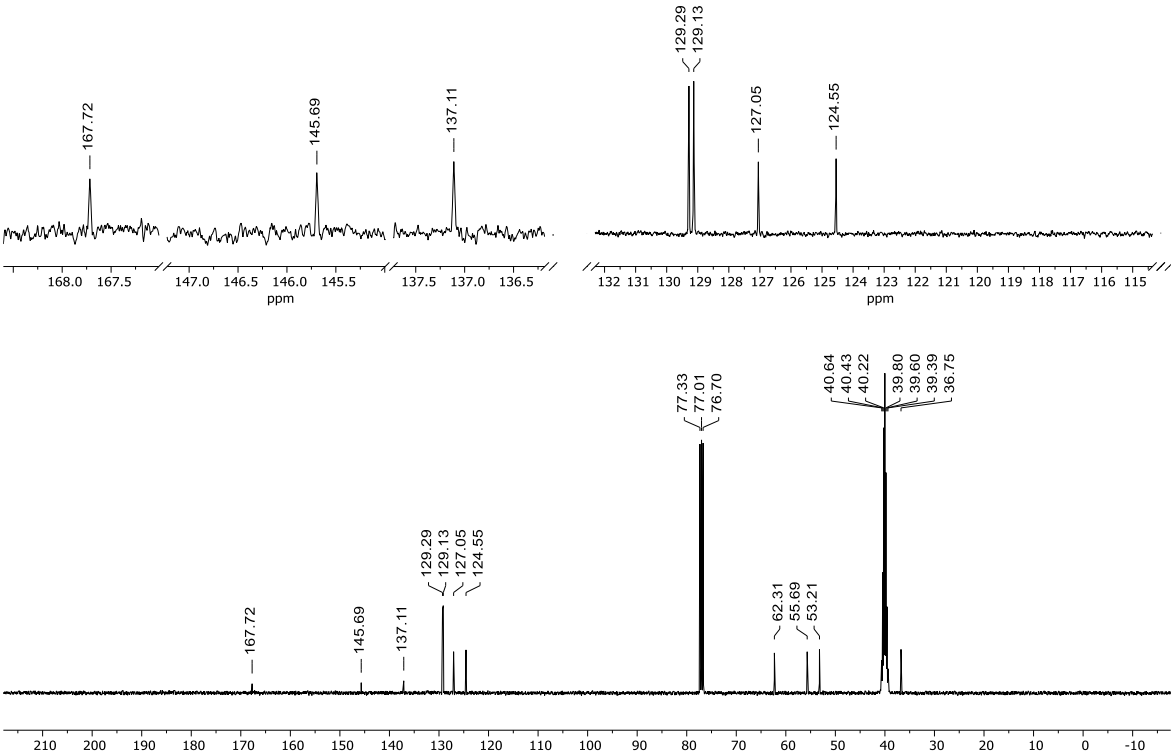


Figure S38.^{13}C NMR of methyl 2-(4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)-3-phenylpropanoate (**3l**) in DMSO-d_6 +$CDCl_3$ at 100MHz

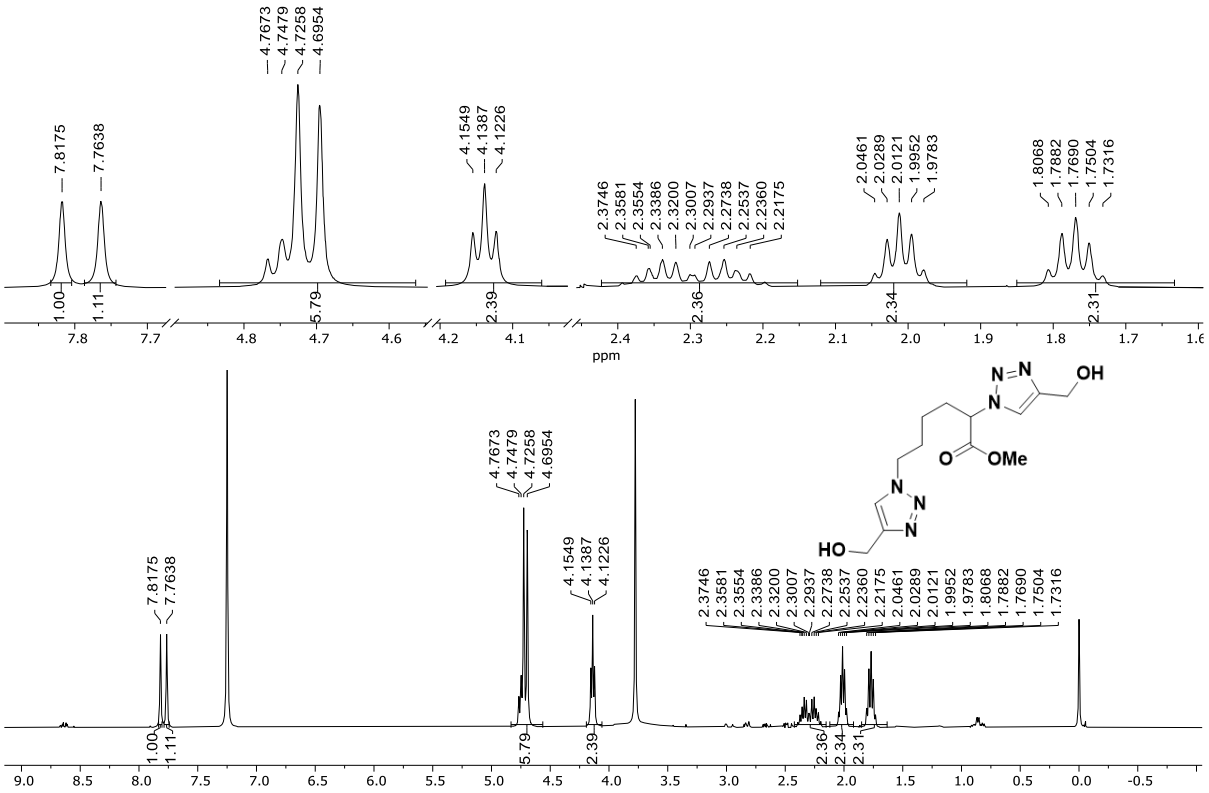


Figure S39. ^{1}H NMR of methyl 2,6-bis(4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)hexanoate (**3m**) in $CDCl_3$ at 400MHz

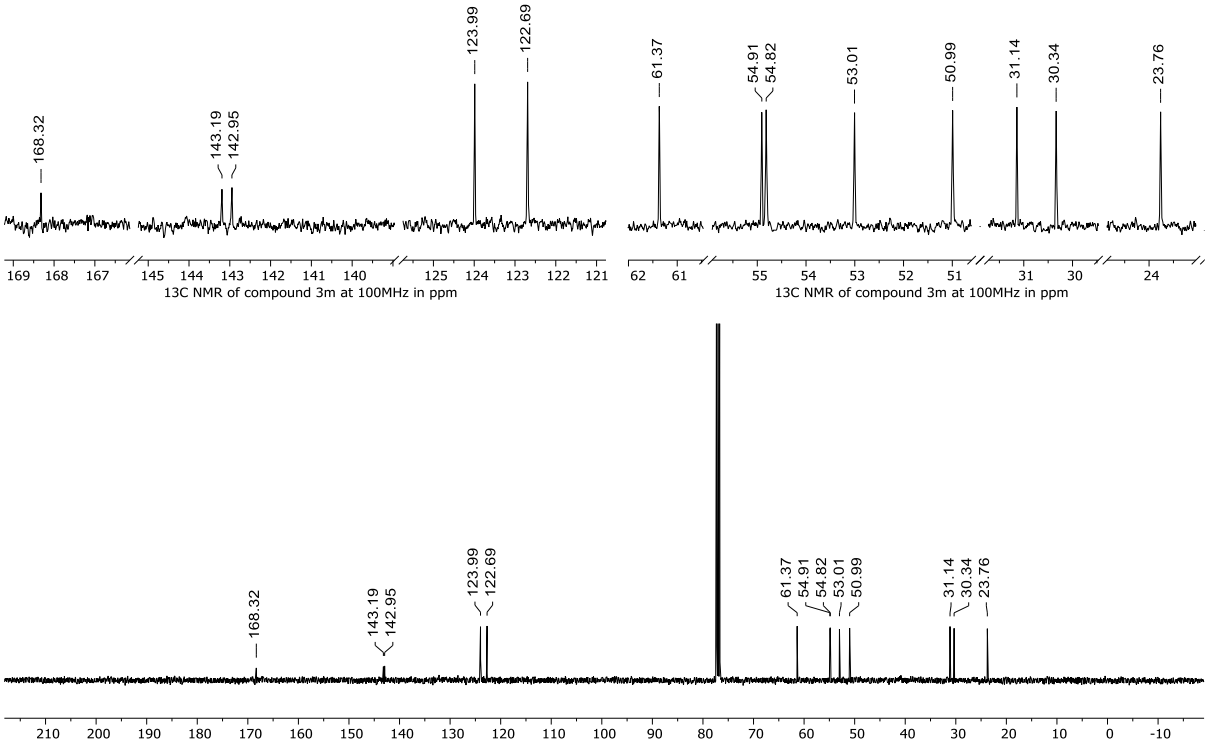


Figure S40. ^{13}C NMR of methyl 2,6-bis(4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)hexanoate (**3m**) in $CDCl_3$ at 100 MHz

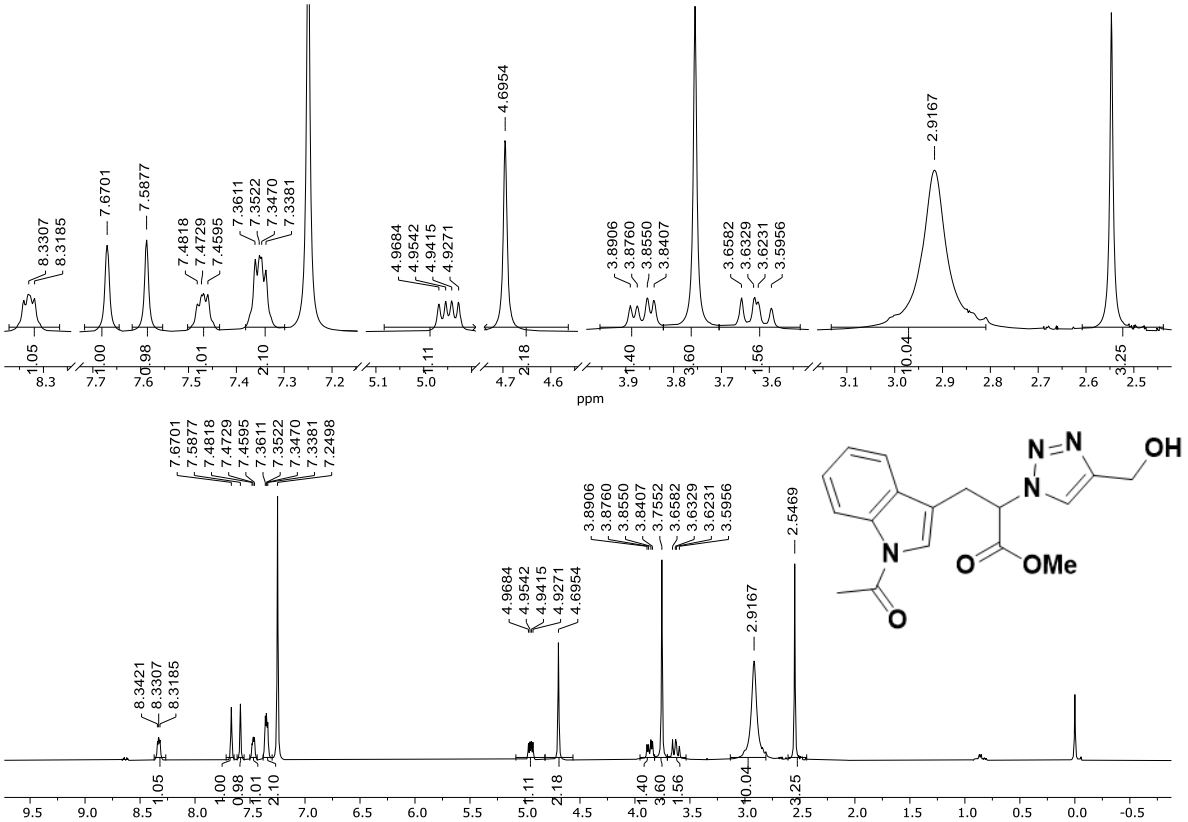


Figure S41. ^{1}H NMR of methyl 3-(1-acetyl-1*H*-indol-3-yl)-2-(4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)propanoate (**3n**) in $CDCl_3$ at 400 MHz

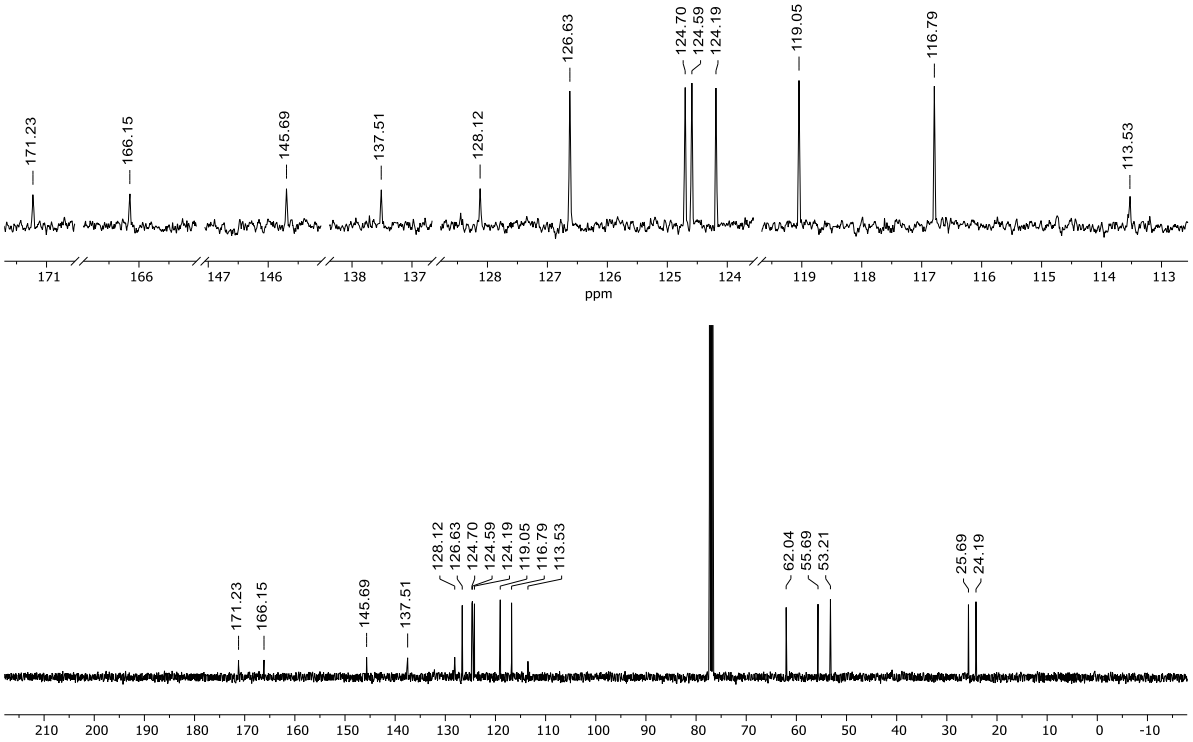


Figure S42. ^{13}C NMR of methyl 3-(1-acetyl-1*H*-indol-3-yl)-2-(4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)propanoate (**3n**) in CDCl3 at 100MHz

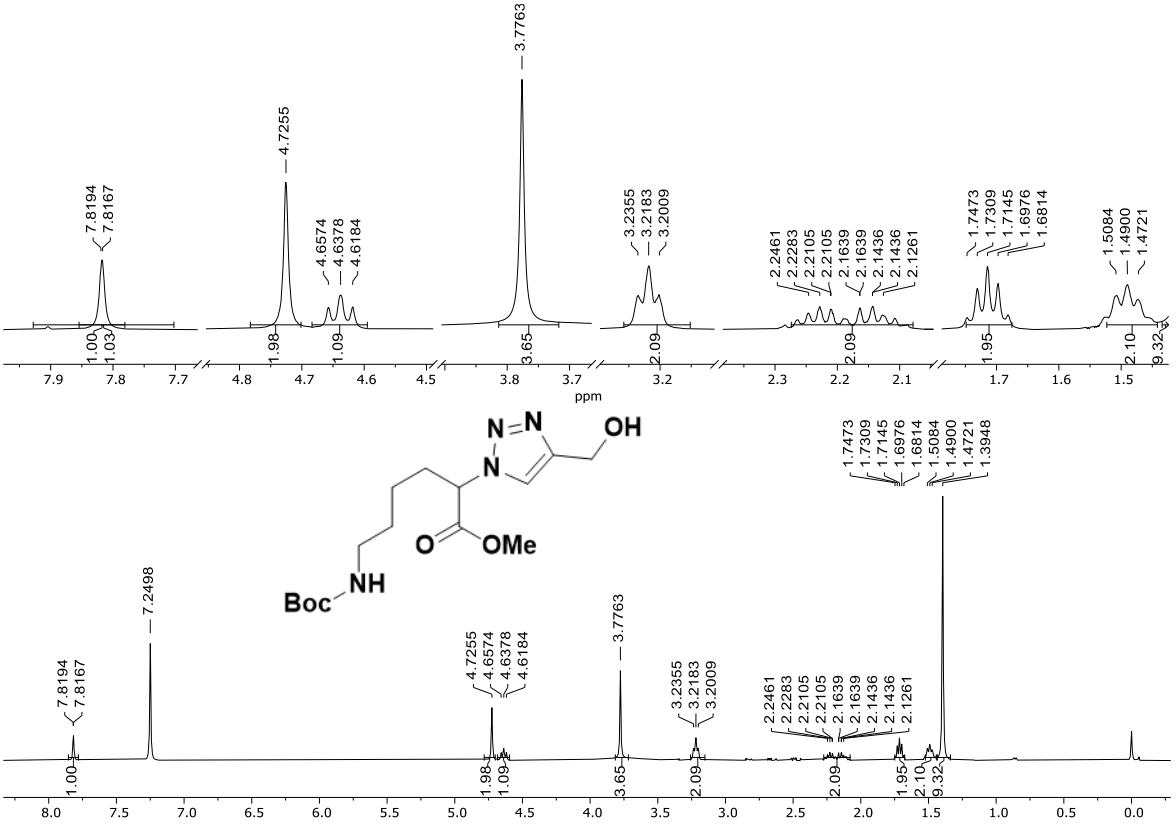


Figure S43. ^{1}H NMR of methyl 6-((*tert*-butoxycarbonyl)amino)-2-(4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)hexanoate (**3o**) in $CDCl_3$ at 400MHz

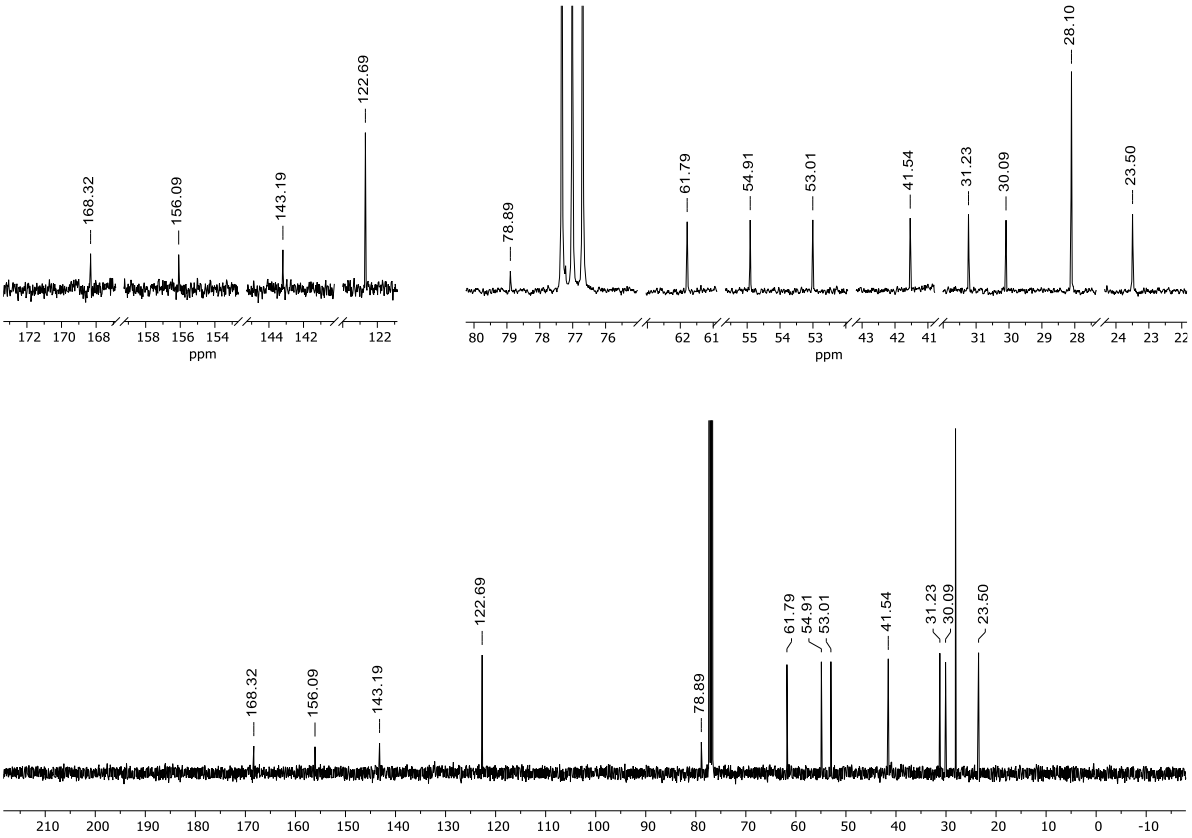


Figure S44. ^{13}C NMR of methyl 6-((*tert*-butoxycarbonyl)amino)-2-(4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)hexanoate (**3o**) in $CDCl_3$ at 100MHz

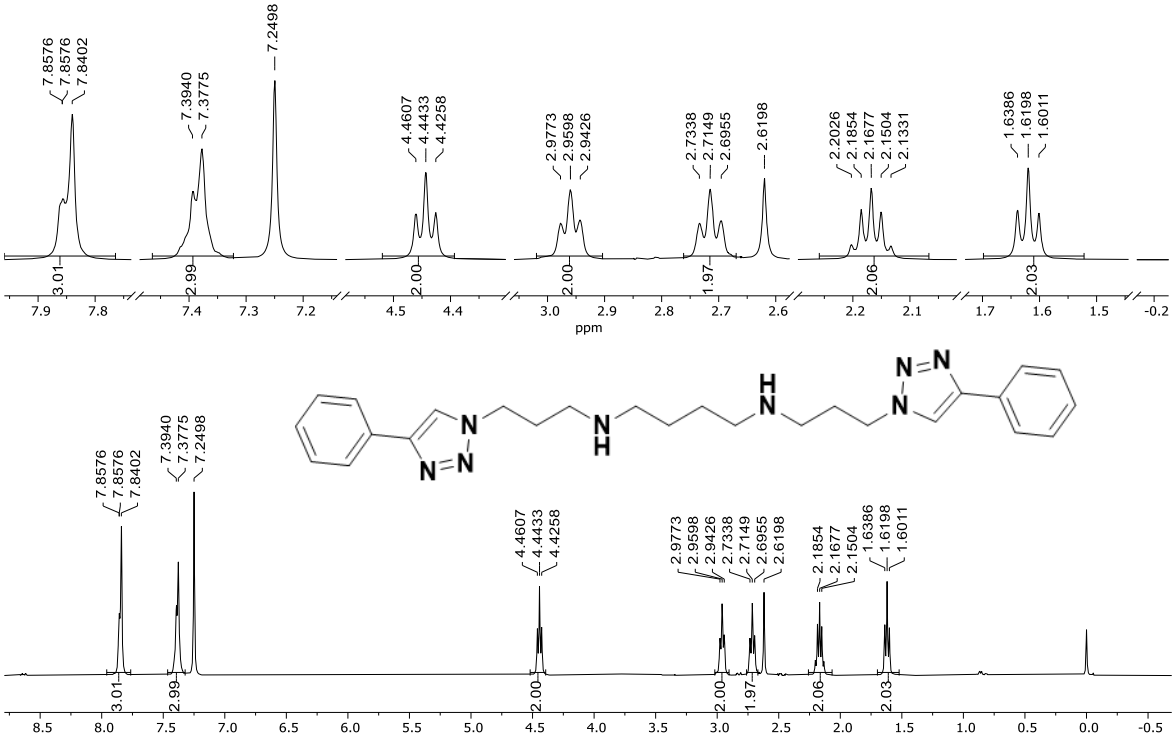


Figure S45. ^{1}H NMR of N1, N4-bis(3-(4-phenyl-1*H*-1,2,3-triazol-1-yl)propyl)butane-1,4-diamine (**3p**) in $CDCl_3$+DMSO-d_6 at 400MHz

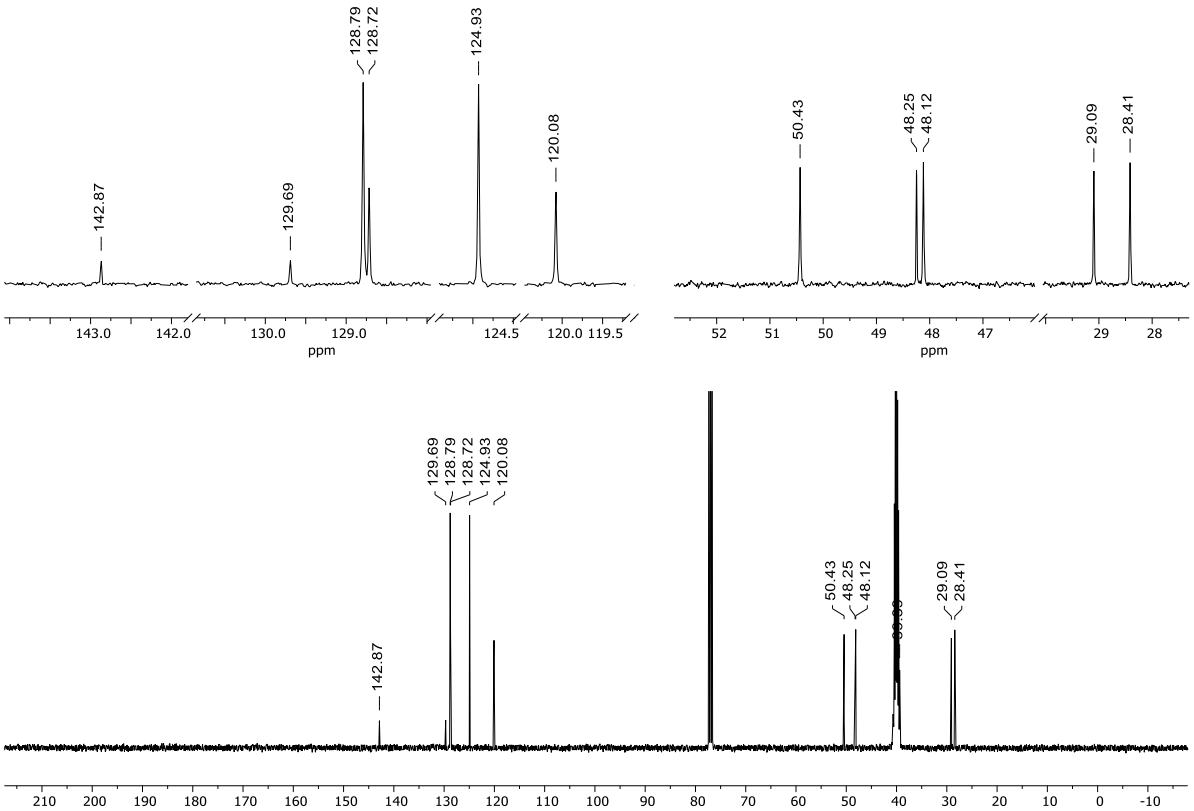


Figure S46. ^{13}C NMR of N1, N4-bis(3-(4-phenyl-1*H*-1,2,3-triazol-1-yl)propyl)butane-1,4-diamine (3p) in $CDCl_3$ + DMSO-d_6 at 100 MHz

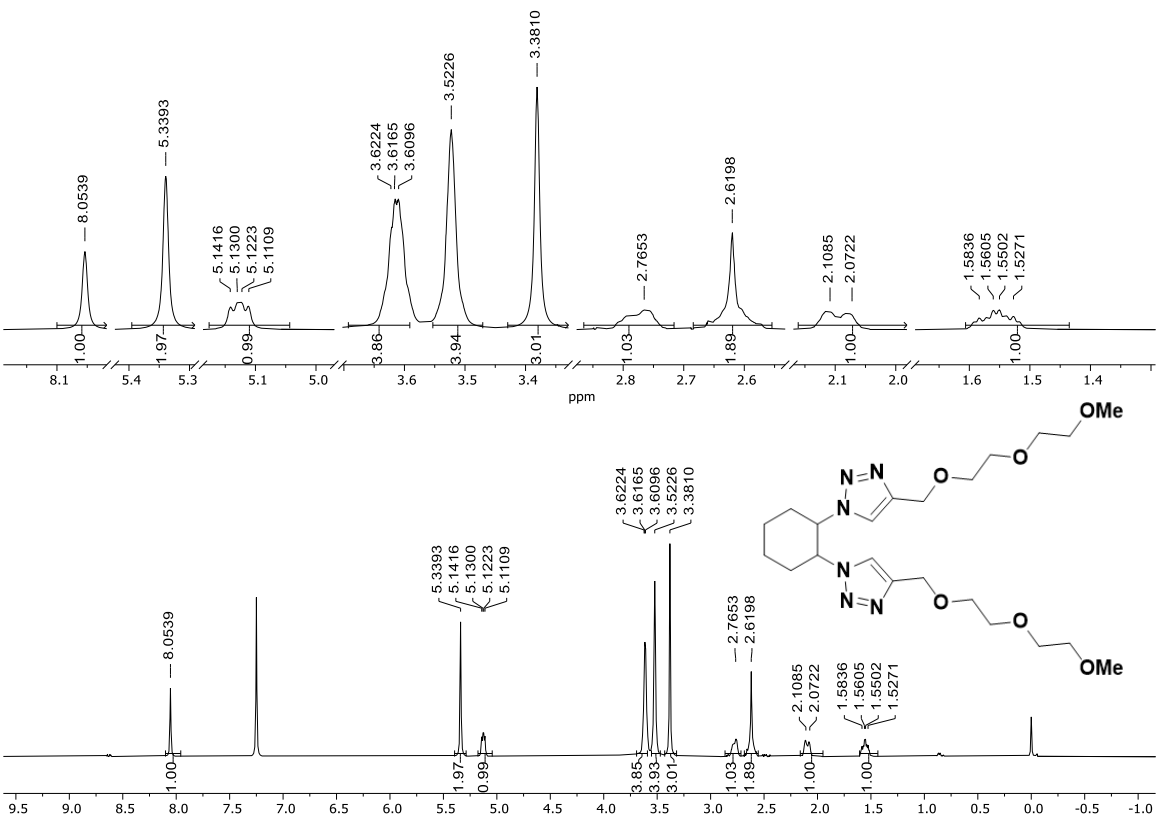


Figure S47. 1H NMR of 1,2-bis(4-((2-(2-methoxyethoxy)ethoxy)methyl)-1*H*-1,2,3-triazol-1-yl)cyclohexane (**3q**) in DMSO-d_6 + $CDCl_3$ at 400MHz

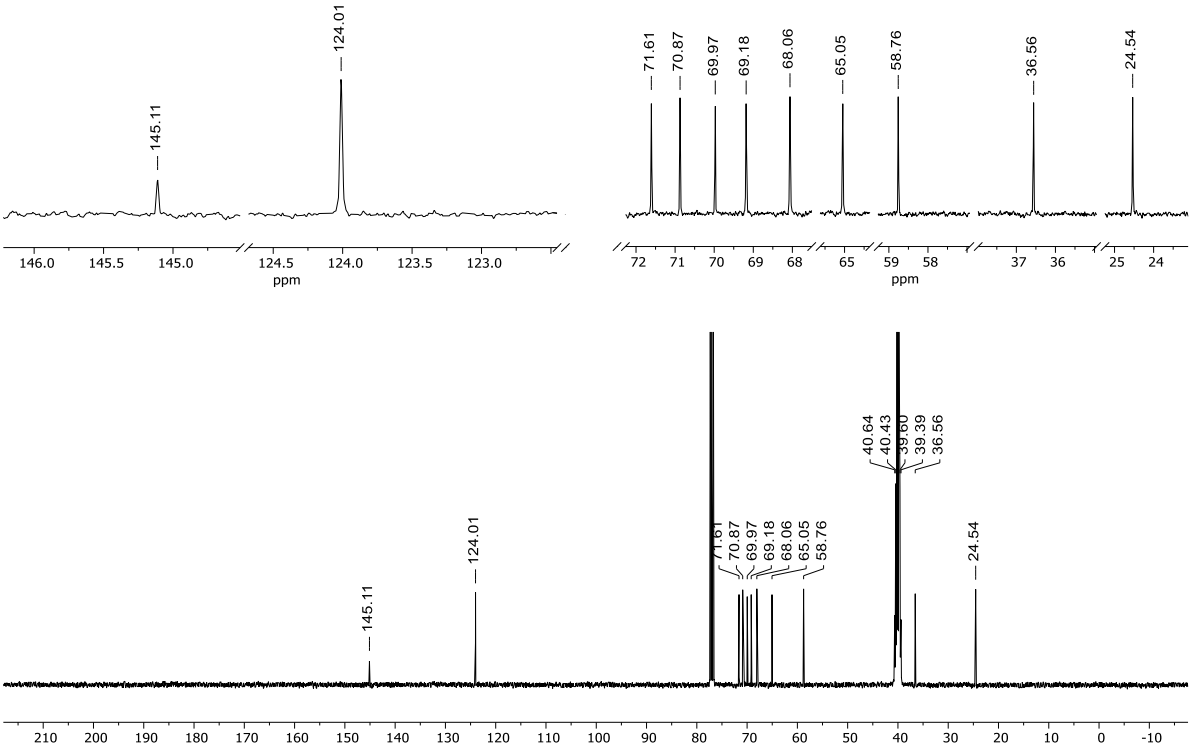


Figure S48. ^{13}C NMR of 1,2-bis(4-((2-(2-methoxyethoxy)ethoxy)methyl)-1*H*-1,2,3-triazol-1-yl)cyclohexane (**3q**) in DMSO-d_6 + $CDCl_3$ at 100 MHz

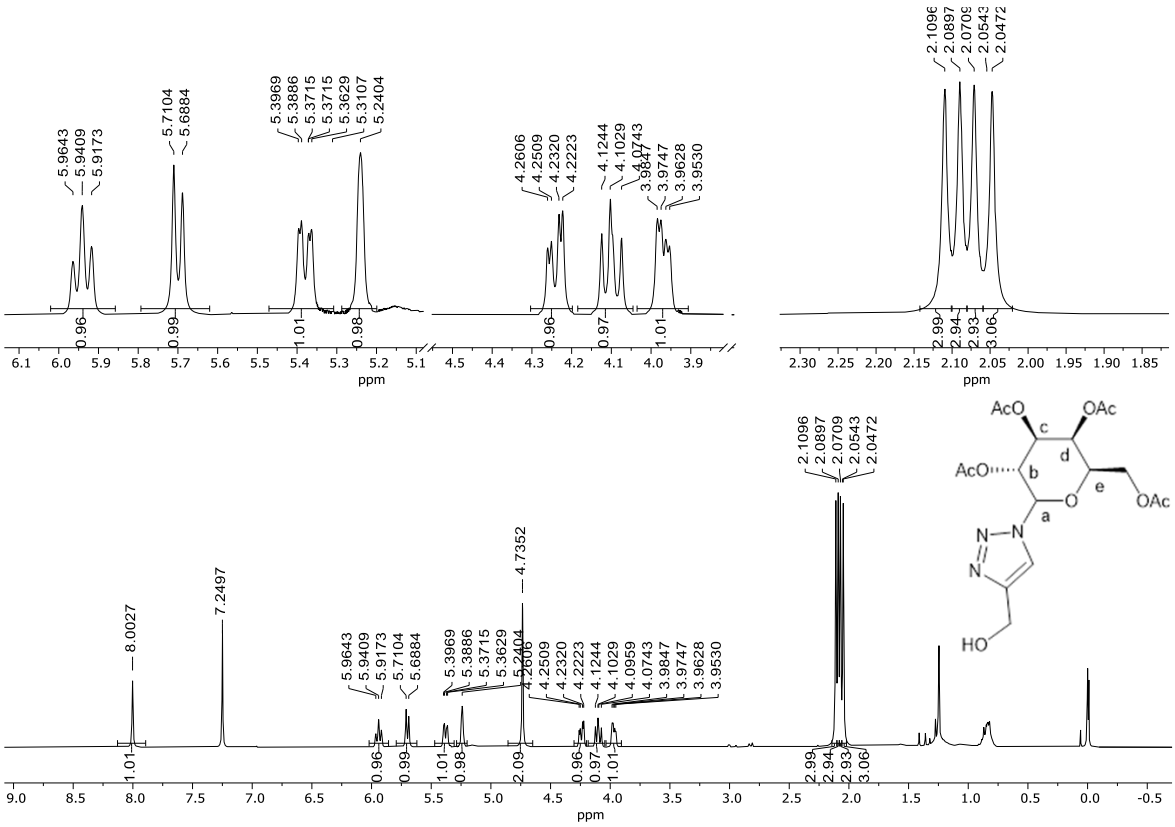


Figure S49. ^{1}H NMR of (2*R*,3*S*,4*S*,5*R*)-2-(acetoxymethyl)-6-(4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)tetrahydro-2*H*-pyran-3,4,5-triyl triacetate (**4a**) in $CDCl_3$ at 400MHz

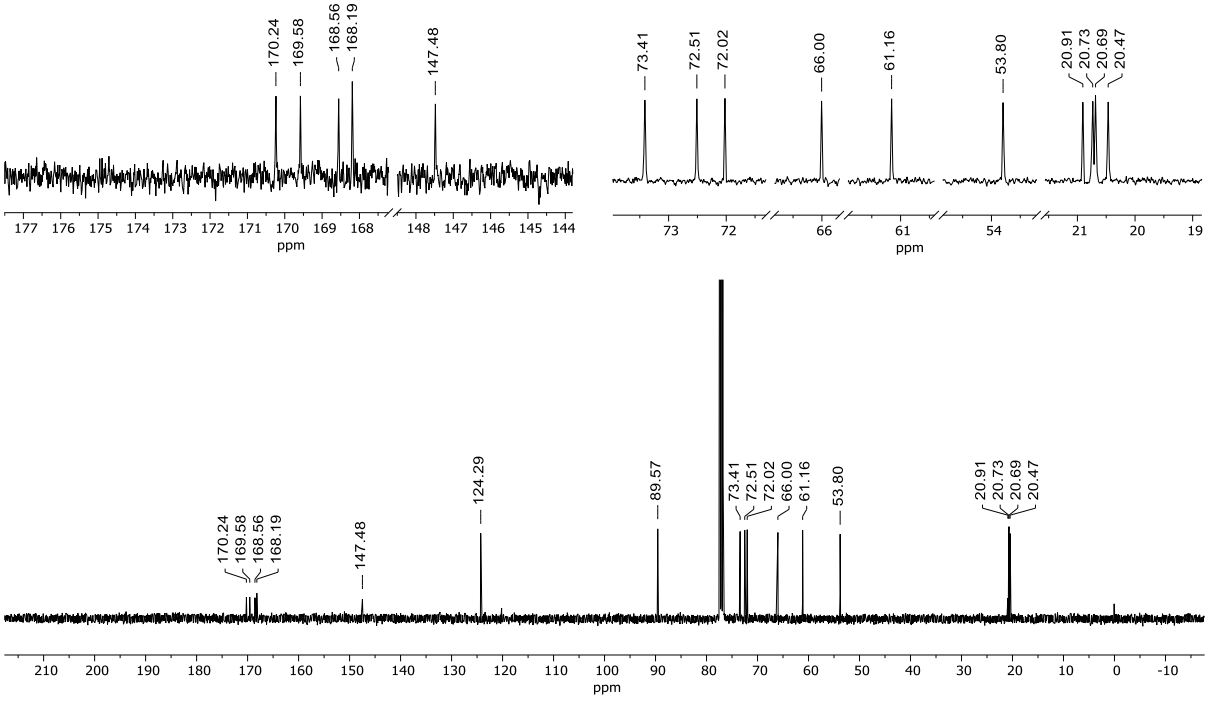


Figure S50. ^{13}C NMR of (2*R*,3*S*,4*S*,5*R*)-2-(acetoxymethyl)-6-(4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)tetrahydro-2*H*-pyran-3,4,5-triyl triacetate (**4a**) in $CDCl_3$ at 100MHz

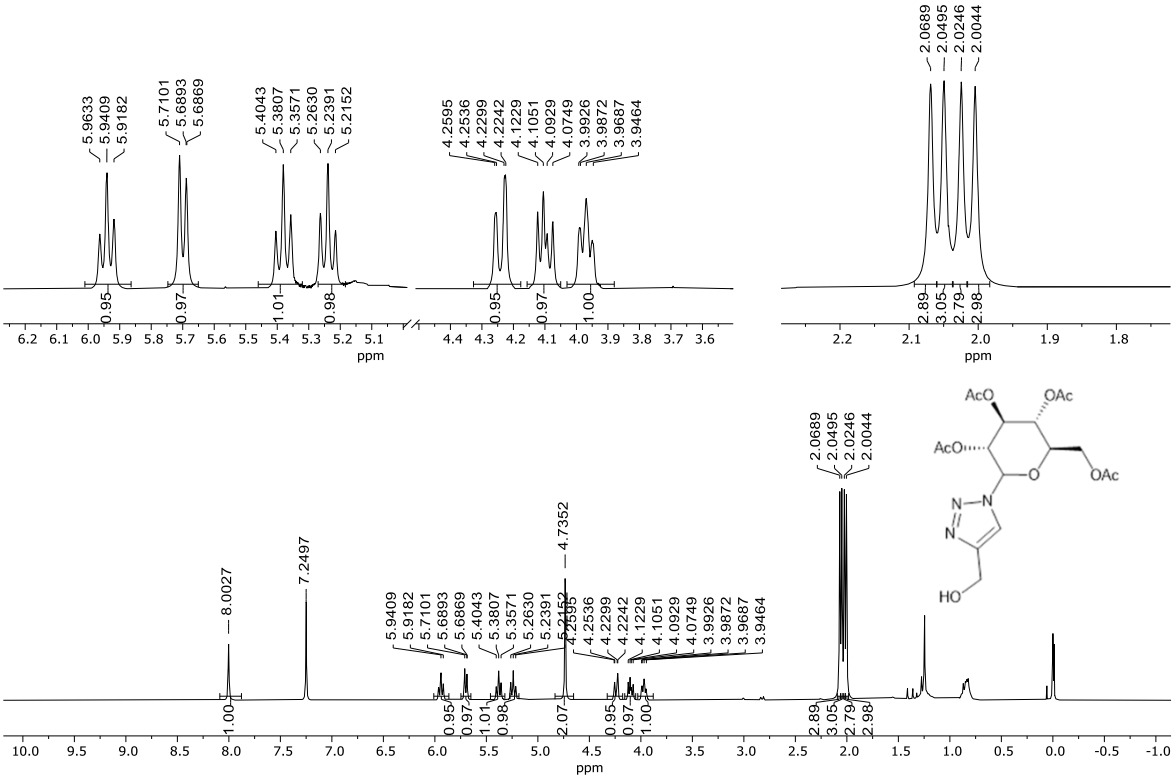


Figure S51. ^{1}H NMR of (2*R*,3*R*,4*S*,5*R*)-2-(acetoxymethyl)-6-(4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)tetrahydro-2*H*-pyran-3,4,5-triyl triacetate (**4b**) in $CDCl_3$ at 400MHz

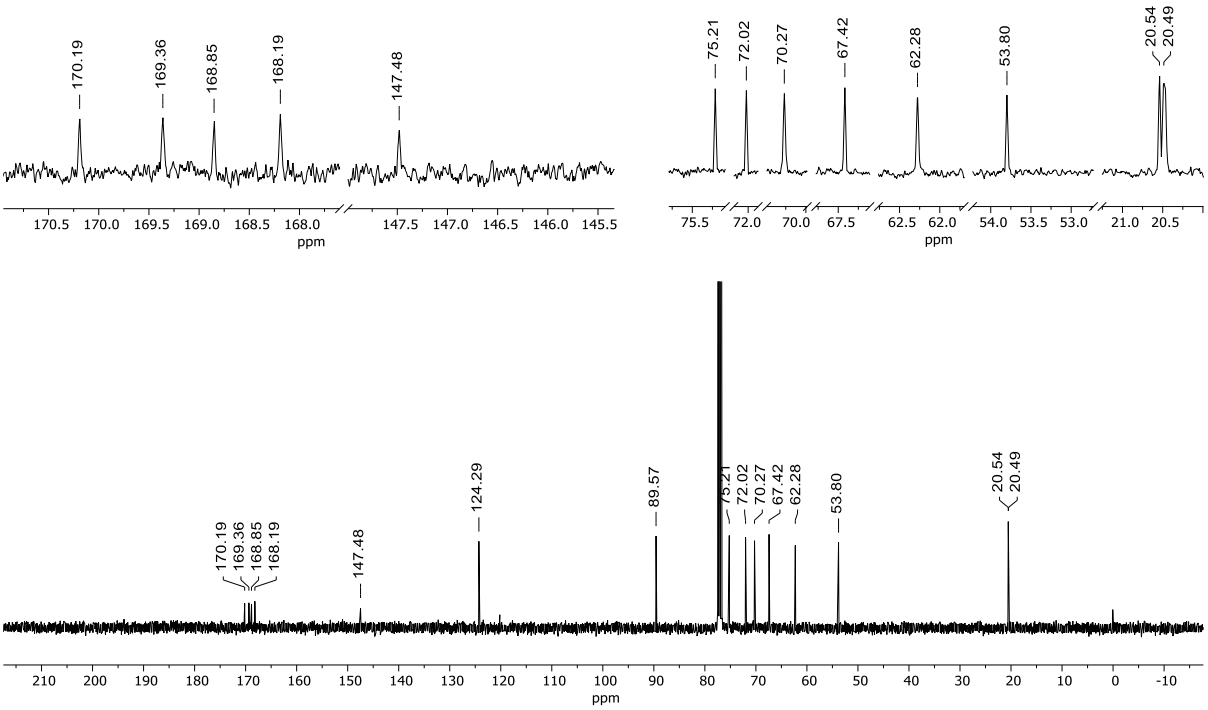


Figure S52. ^{13}C NMR of (2*R*,3*R*,4*S*,5*R*)-2-(acetoxymethyl)-6-(4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)tetrahydro-2*H*-pyran-3,4,5-triyl triacetate (**4b**) in $CDCl_3$ at 100 MHz

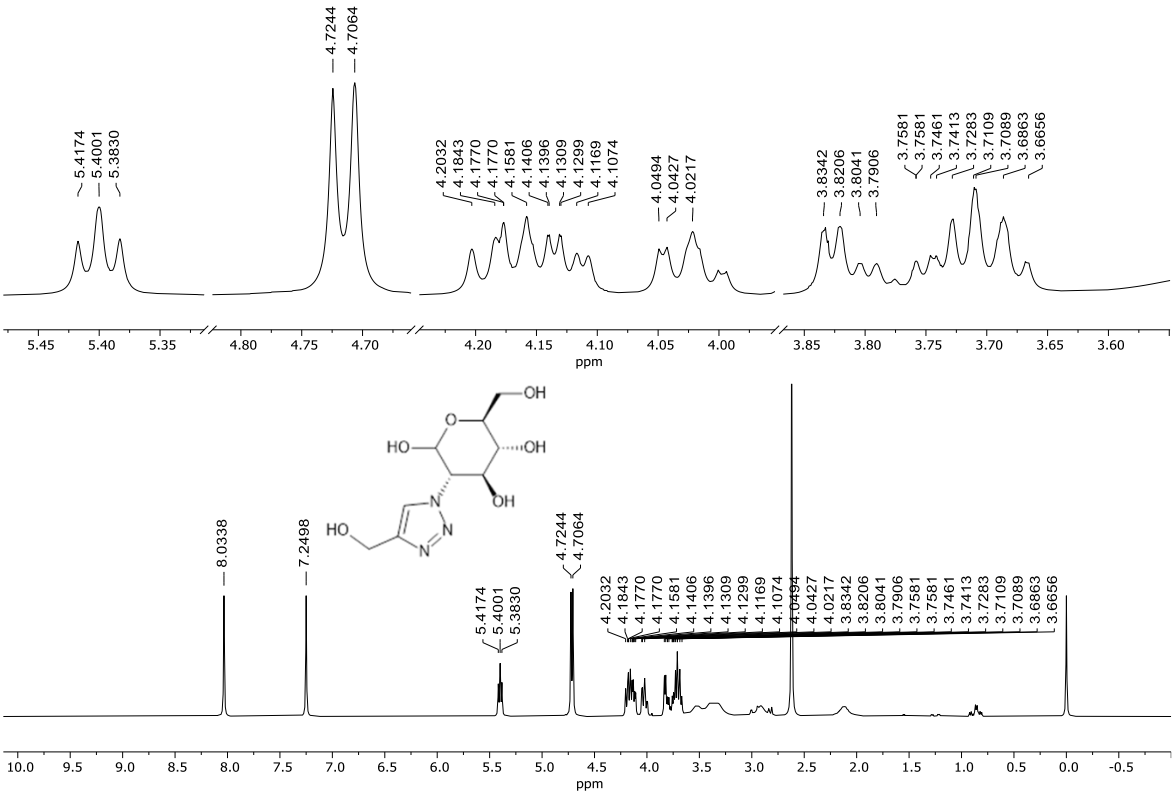


Figure S53. ^{1}H NMR of (3*R*,4*R*,5*S*)-6-(hydroxymethyl)-3-(4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)tetrahydro-2*H*-pyran-2,4,5-triol (**4c**) in $CDCl_3$ +DMSO-d_6 at 400MHz

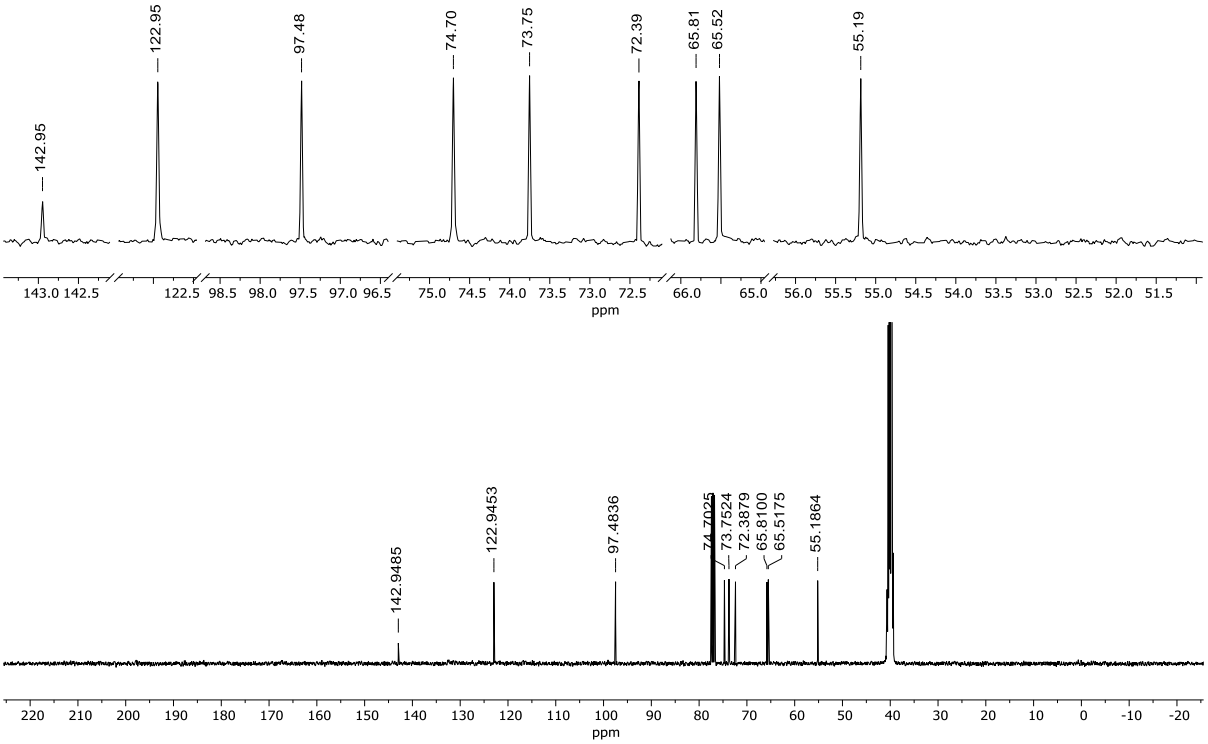


Figure S54. ^{13}C NMR of (3*R*,4*R*,5*S*)-6-(hydroxymethyl)-3-(4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)tetrahydro-2*H*-pyran-2,4,5-triol (**4c**) in $CDCl_3$ + DMSO-d_6 at 100 MHz

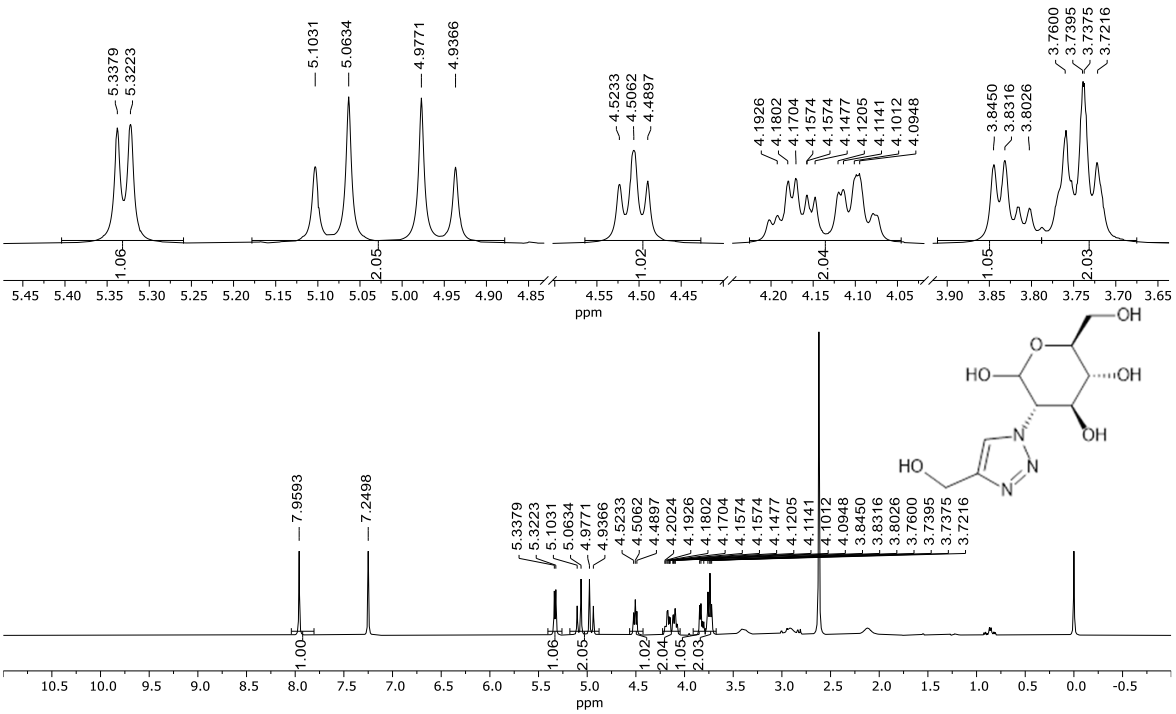


Figure S55. ^{1}H NMR of (8*S*,9*R*,9aR)-7-(hydroxymethyl)-5a,8,9,9a-tetrahydro-4*H*,7*H*-pyrano[2,3-b][1,2,3]triazolo[1,5-d][1,4]oxazine-8,9-diol (**4d**) in $CDCl_3$ +DMSO-d_6 at 400 MHz

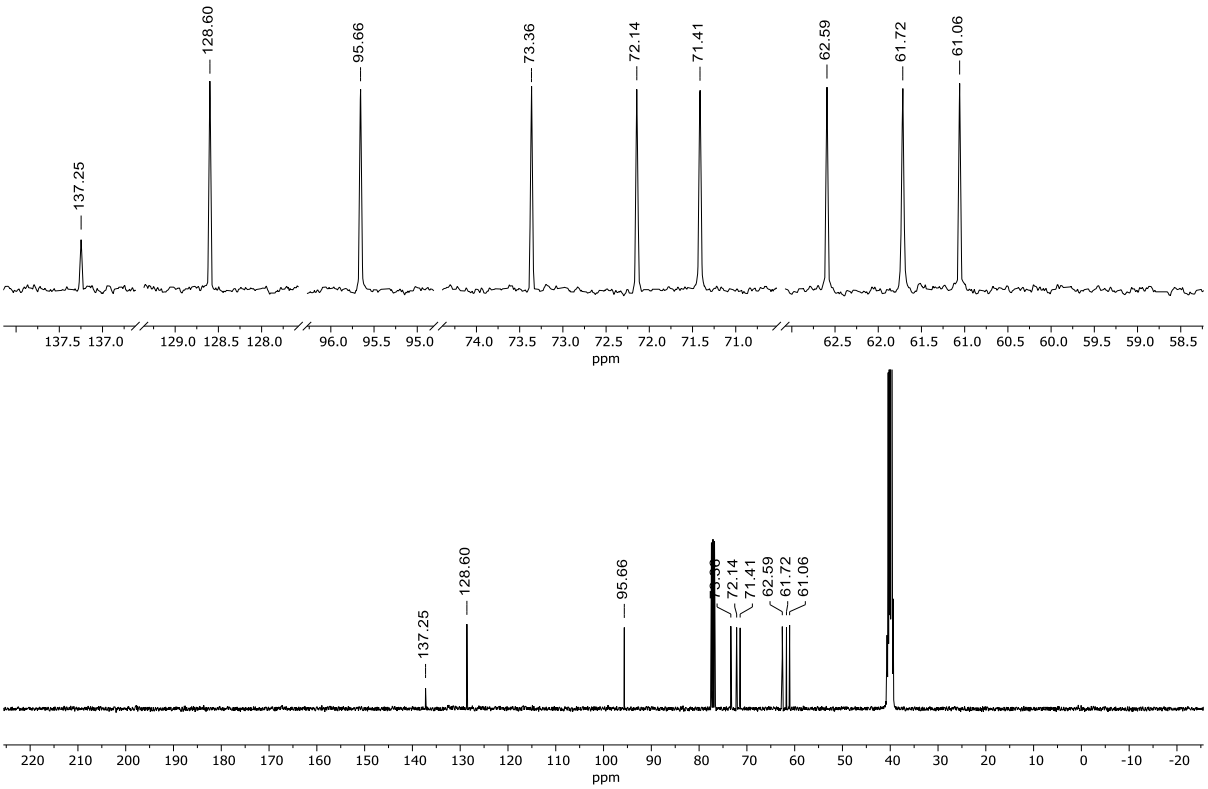


Figure S56. ^{13}C NMR of (8*S*,9*R*,9aR)-7-(hydroxymethyl)-5a,8,9,9a-tetrahydro-4*H*,7*H*-pyrano[2,3-b][1,2,3]triazolo[1,5-d][1,4]oxazine-8,9-diol (**4d**) in $CDCl_3$ +DMSO-d_6 at 100 MHz

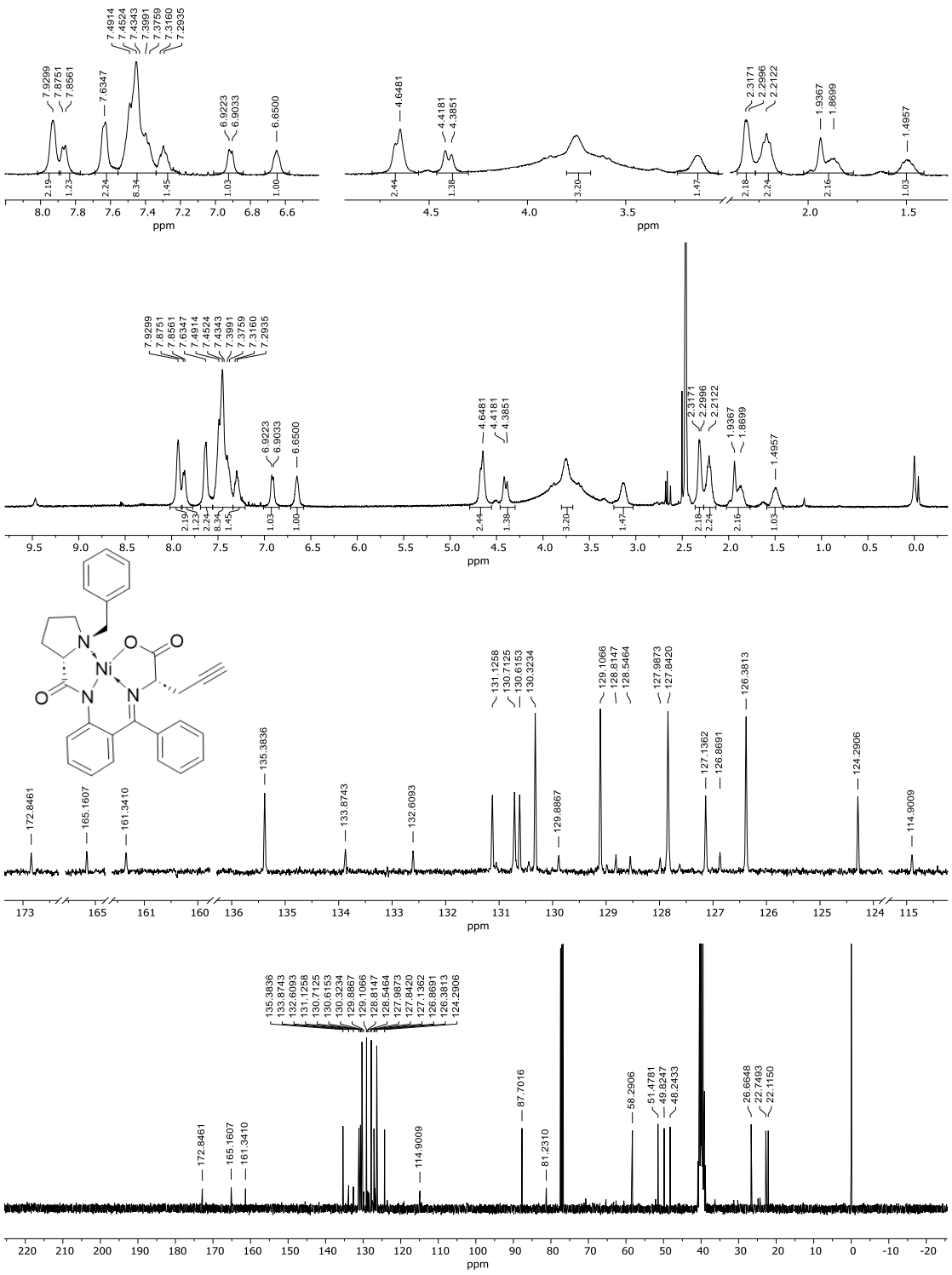


Figure S57: ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) of compound **P1** in DMSO-d_6

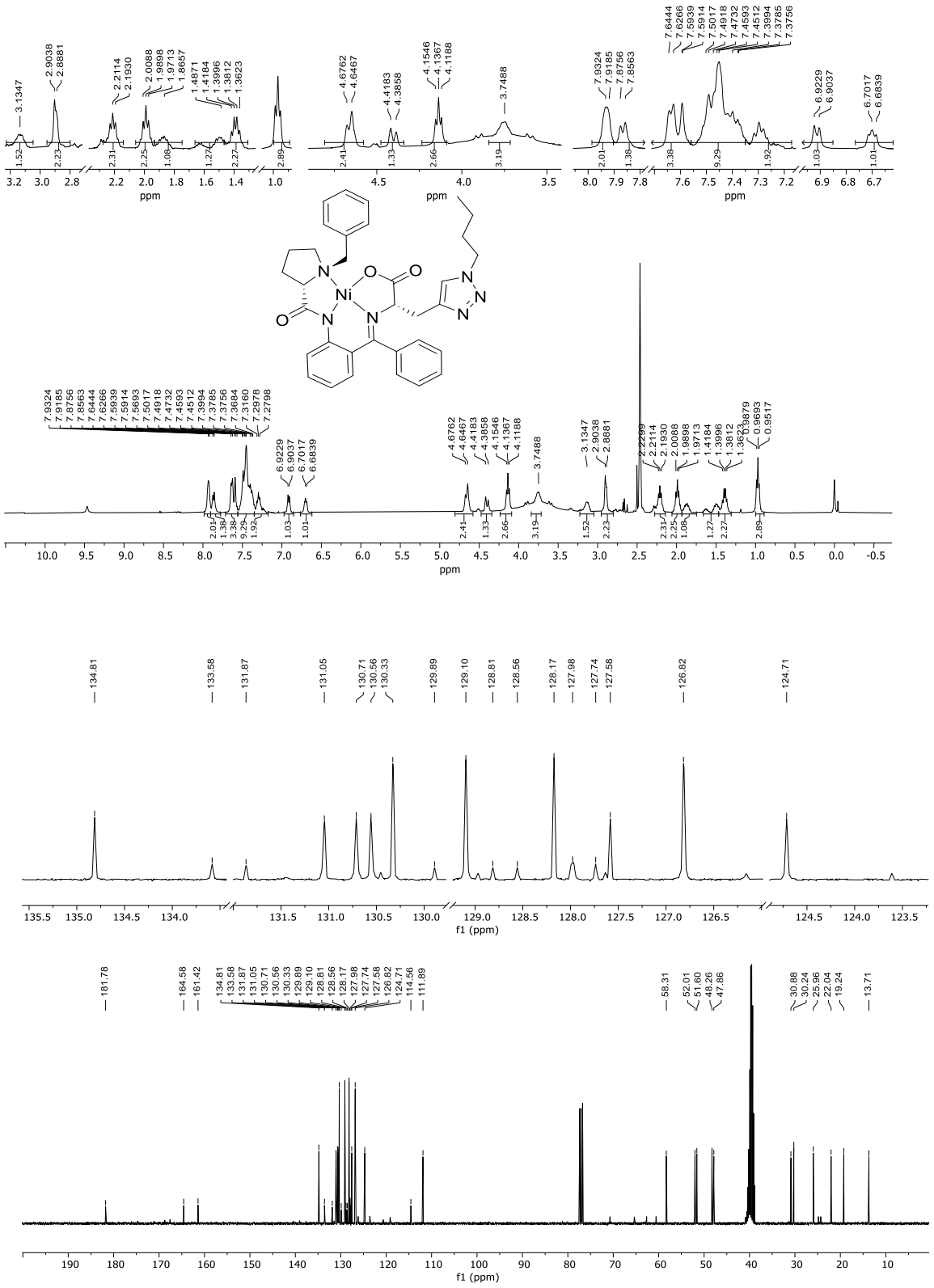


Figure S58: ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) of compound **5a** in DMSO-d_6

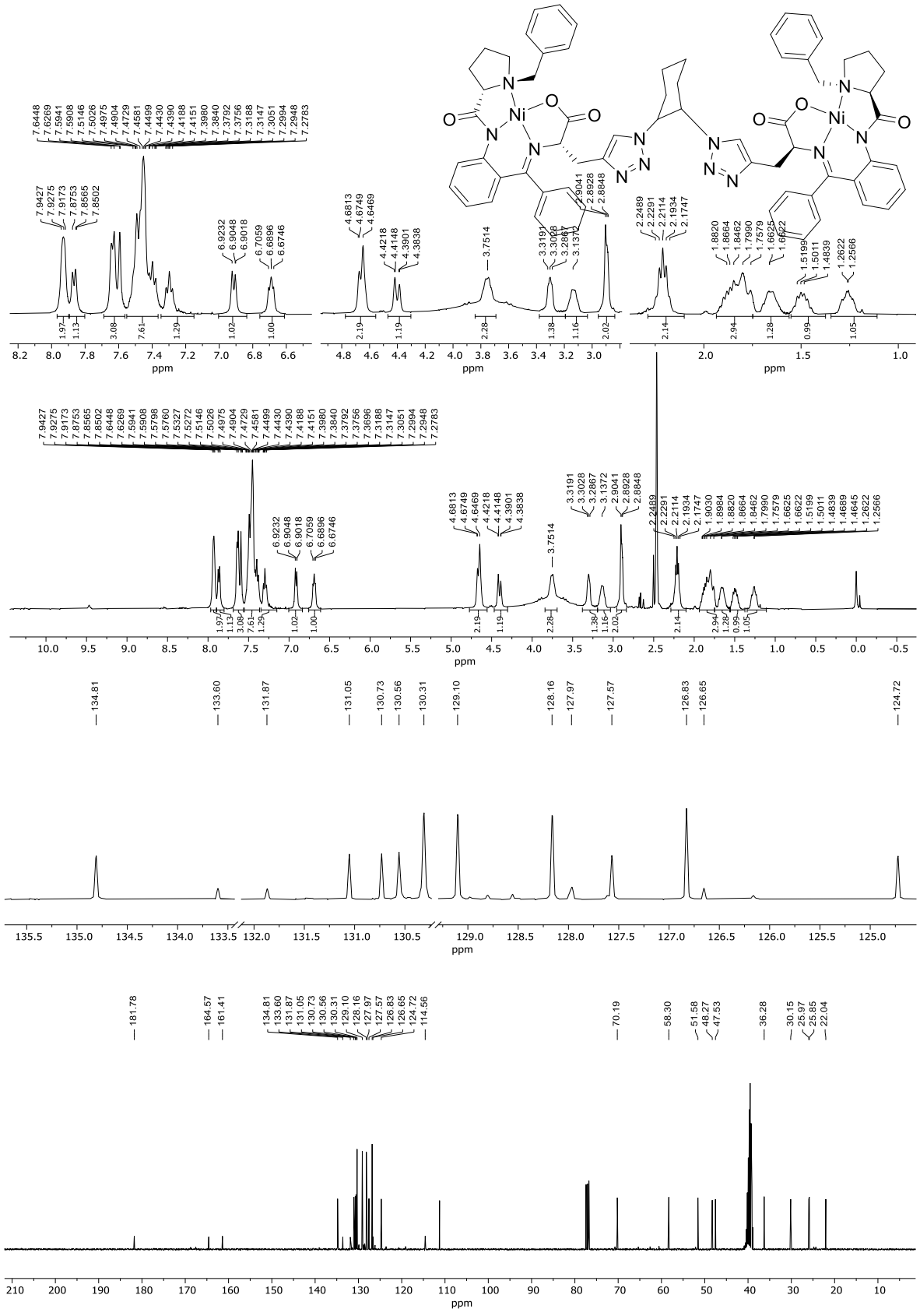


Figure S59: ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) of compound **5b** in DMSO-d_6

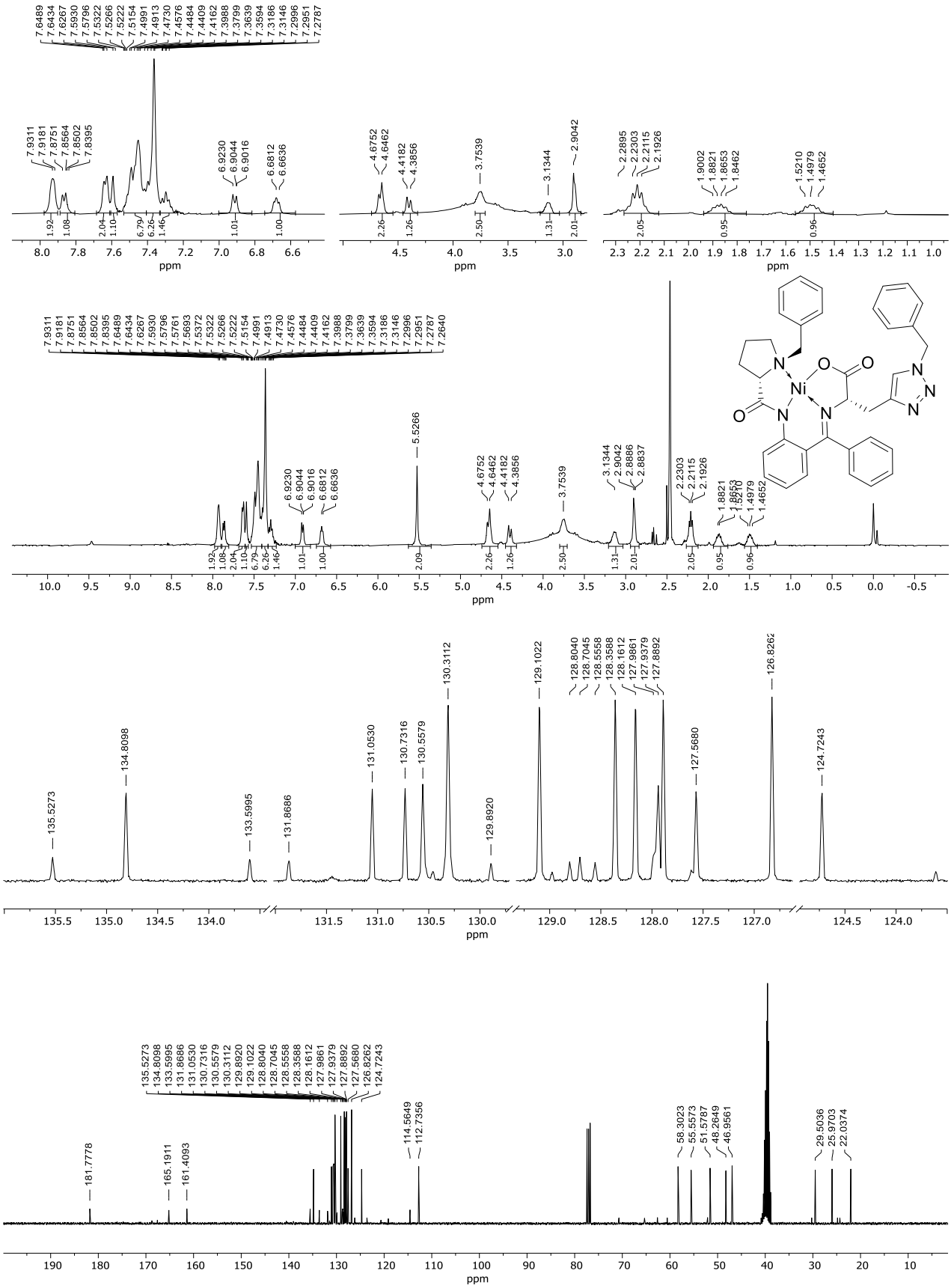


Figure S60: ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) of compound **5c** in DMSO-d_6

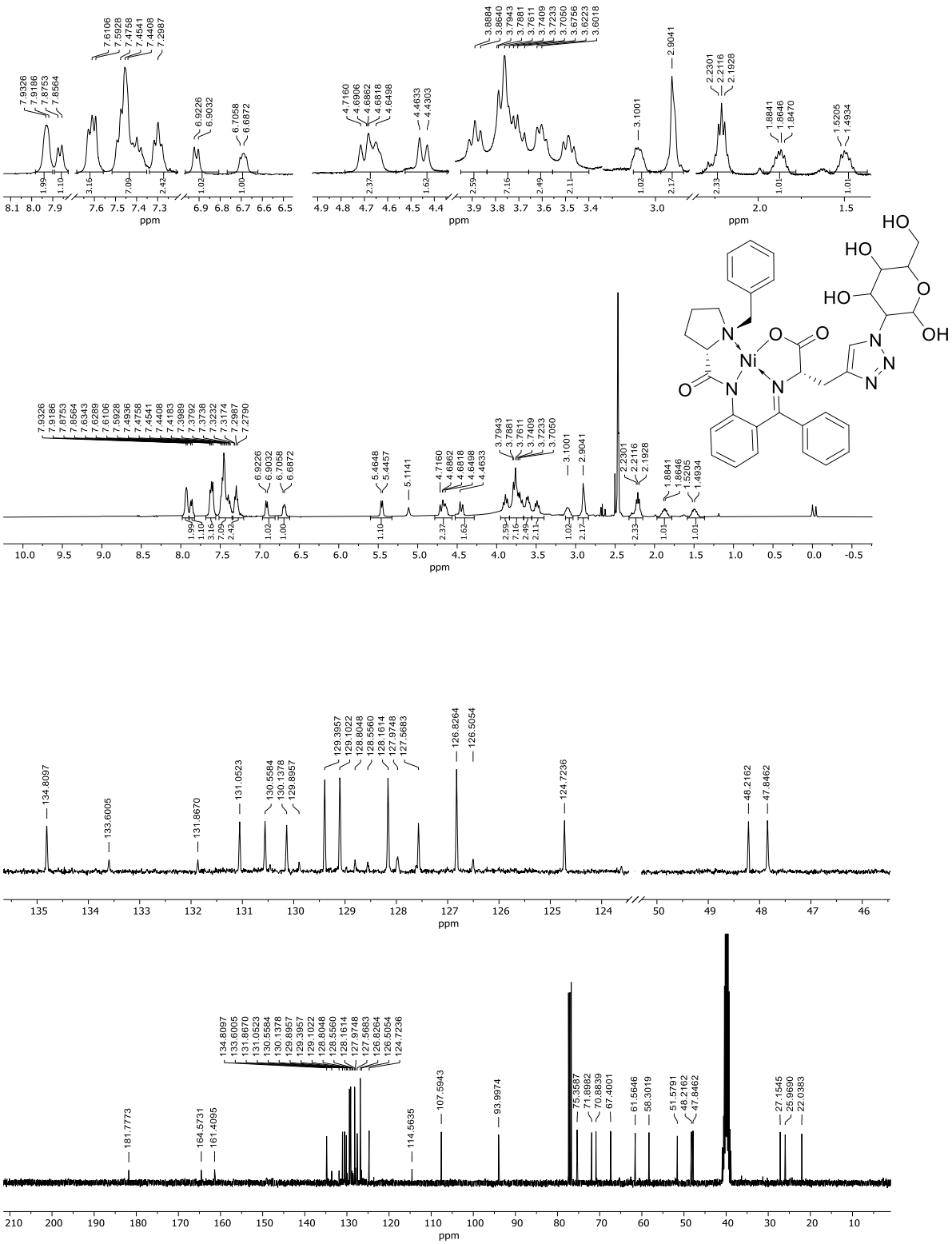


Figure S61: ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) of compound **5d** in DMSO-d_6

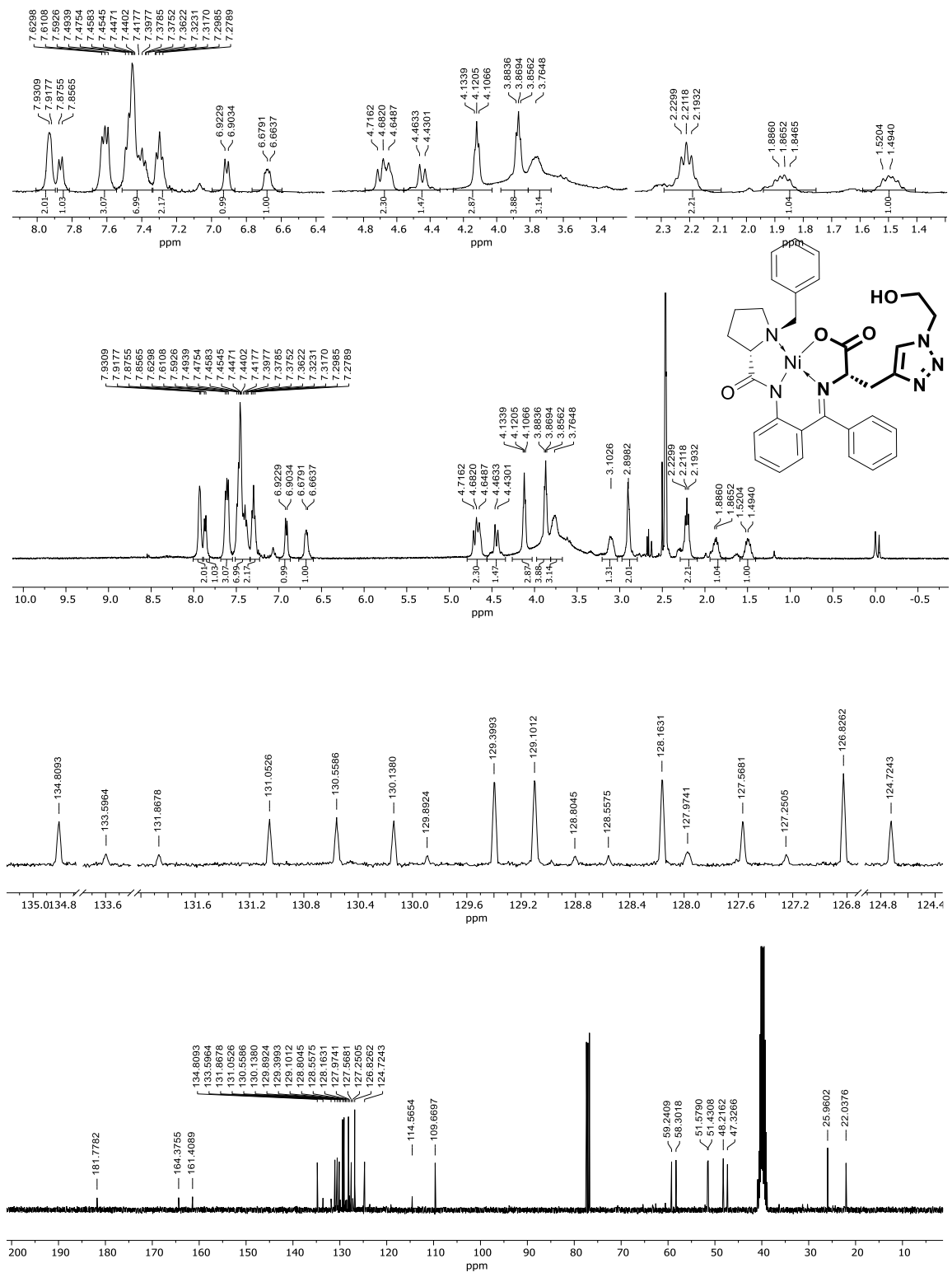


Figure S62: ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) of compound **5e** in DMSO-d_6

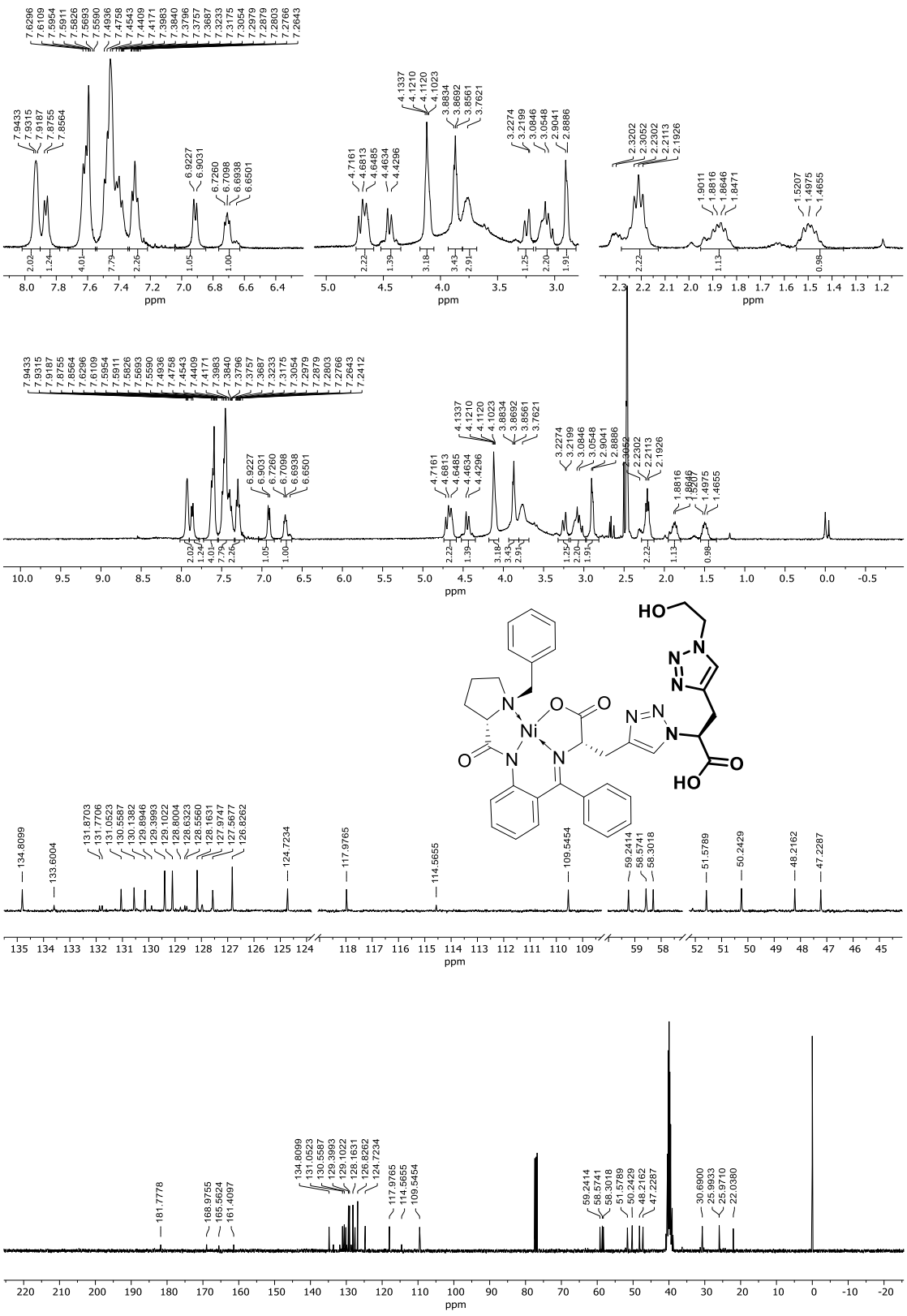


Figure S63: ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) of compound **5f** in DMSO-d_6

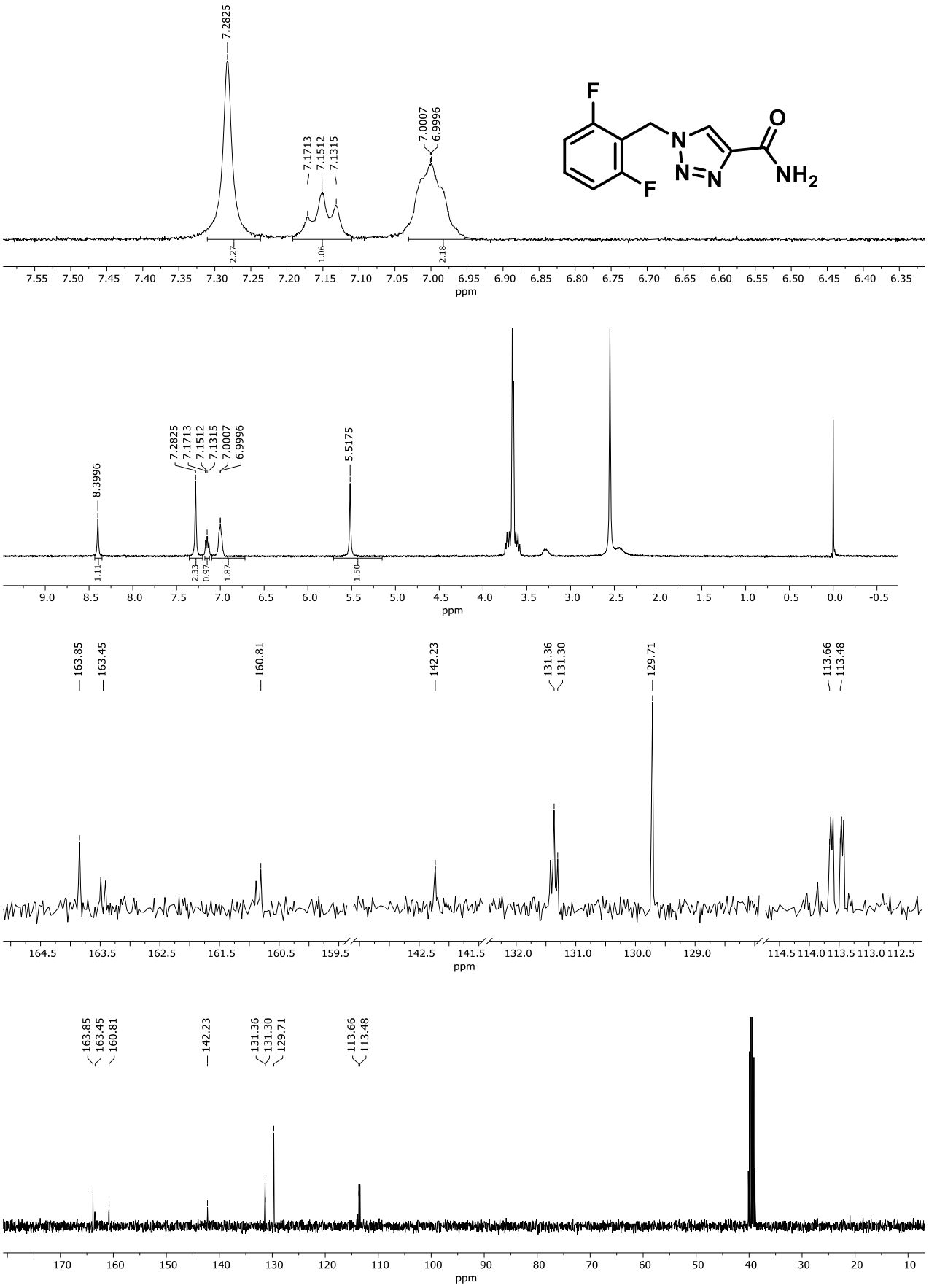


Figure S64: ^{1}H NMR (400MHz) and ^{13}CNMR (100 MHz) of *1-(2,6-difluorobenzyl)-1H-1,2,3-triazole-4-carboxamide* in DMSO-d_6

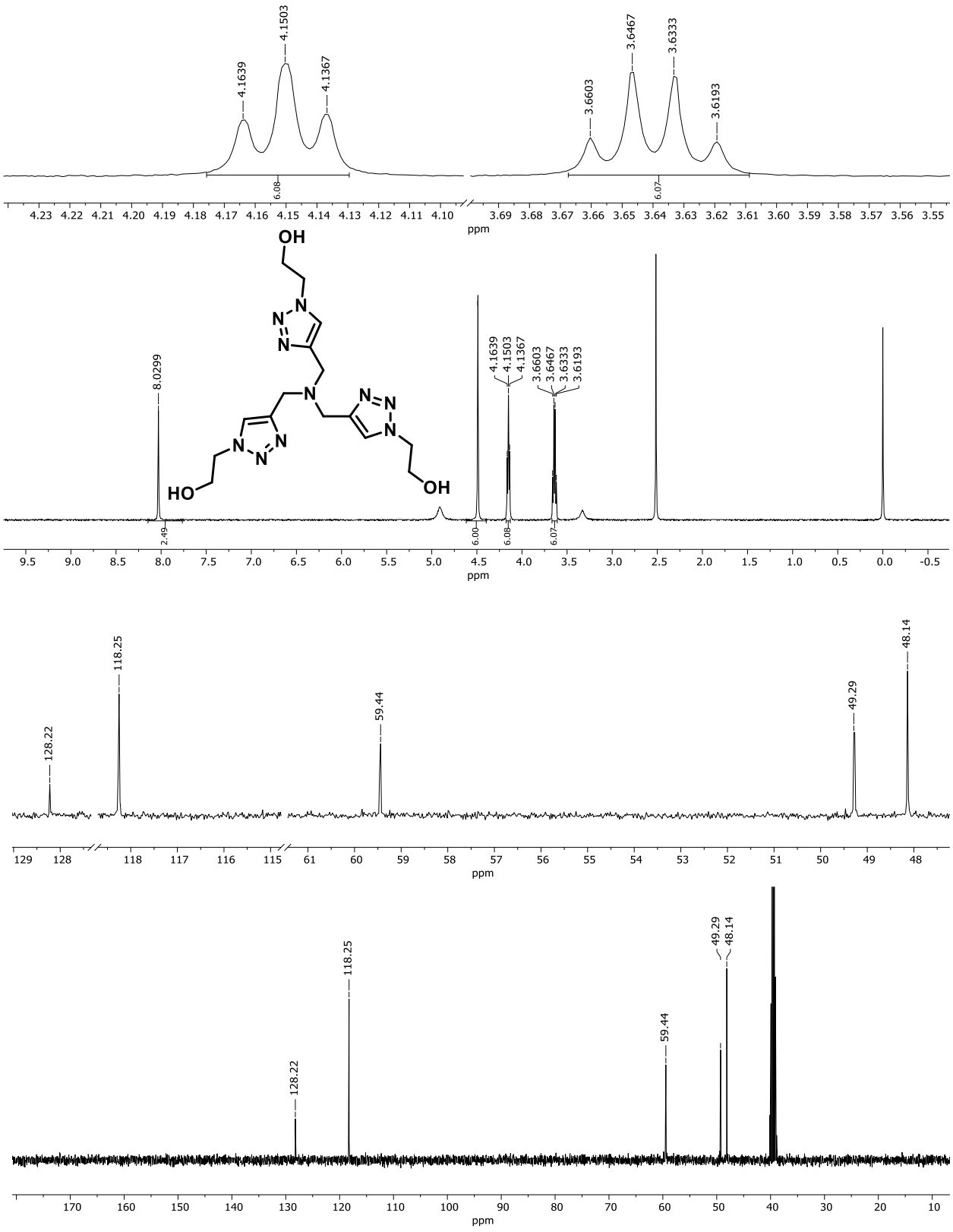


Figure S65:1H NMR and 13 CNMR of **2,2',2''-((nitrilotris(methylene))tris(1H-1,2,3-triazole-4,1-diyl))tris(ethan-1-ol) (THETA) in DMSO-d$_6$**

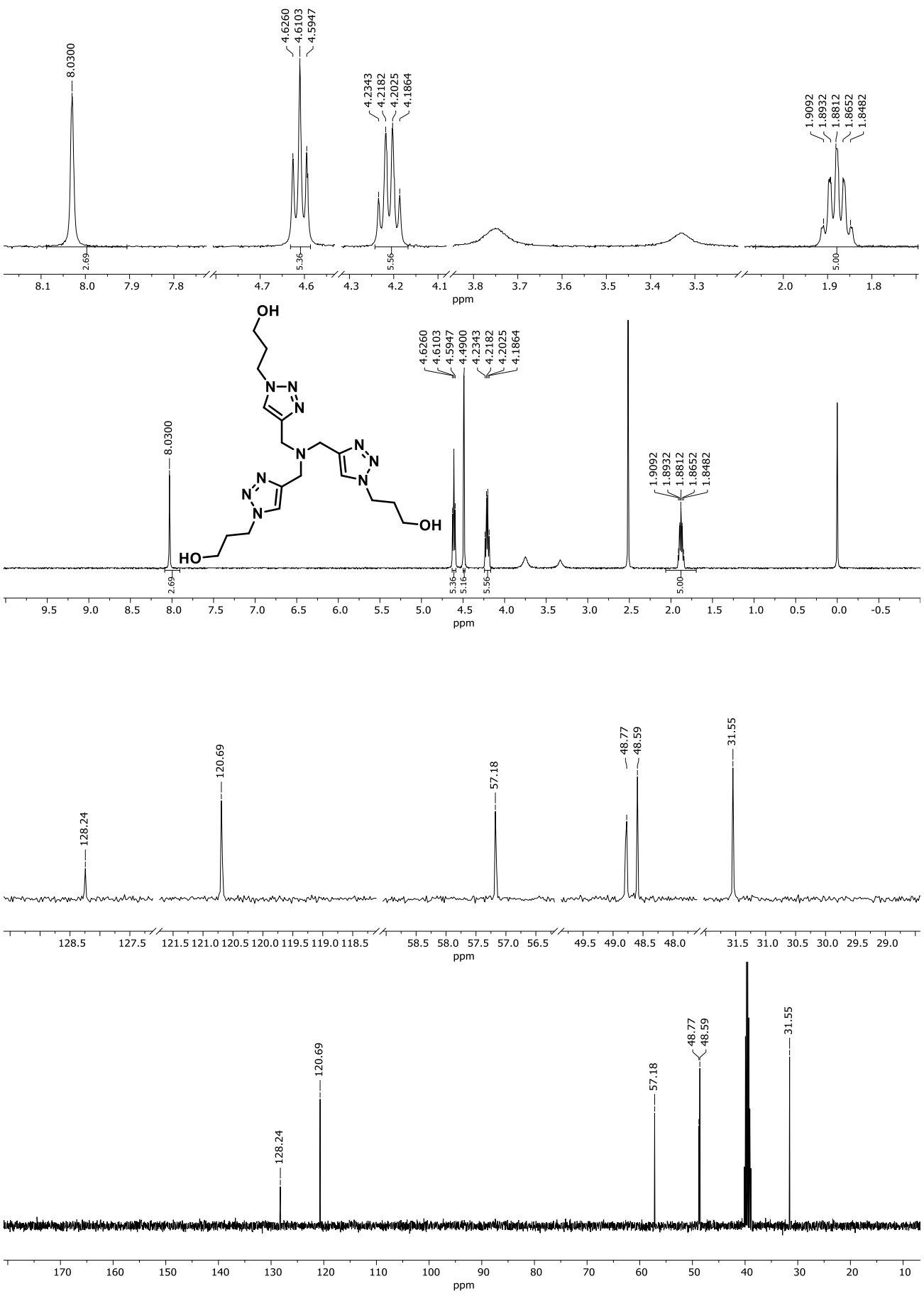


Figure S66:[1]H NMR and [13]C NMR of **3,3',3''-((nitrilotris(methylene))tris(1*H*-1,2,3-triazole-4,1-diyl))tris(propan-1-ol) THPTA**

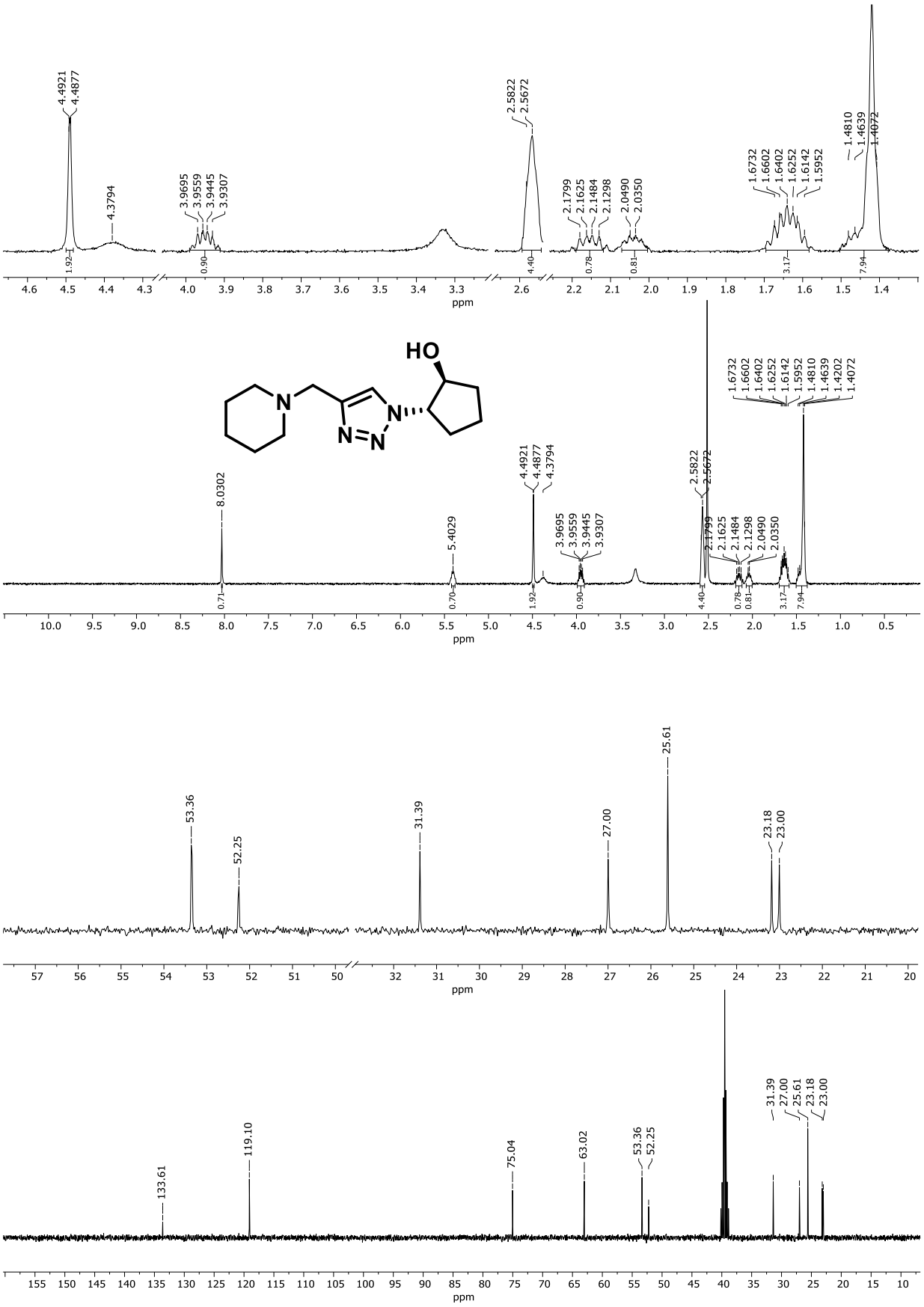


Figure S67:[1]H NMR and [13]CNMR of **(2-(4-(piperidin-1-ylmethyl)-1H-1,2,3-triazol-1-yl)cyclopentan-1-ol**

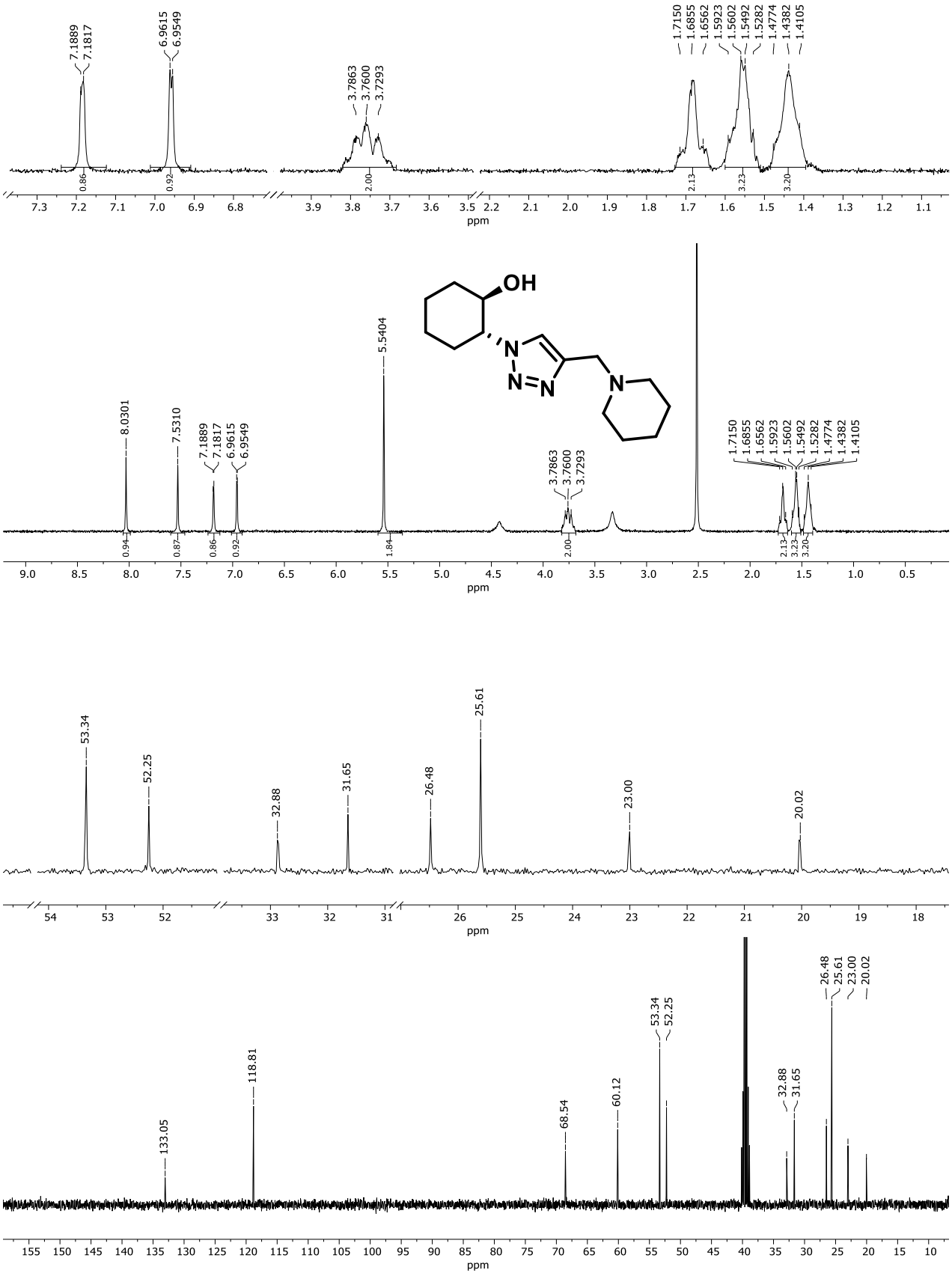


Figure S68:[1]H NMR and [13] CNMR of **2-(4-(piperidin-1-ylmethyl)-1H-1,2,3-triazol-1-yl)cyclohexan-1-ol**

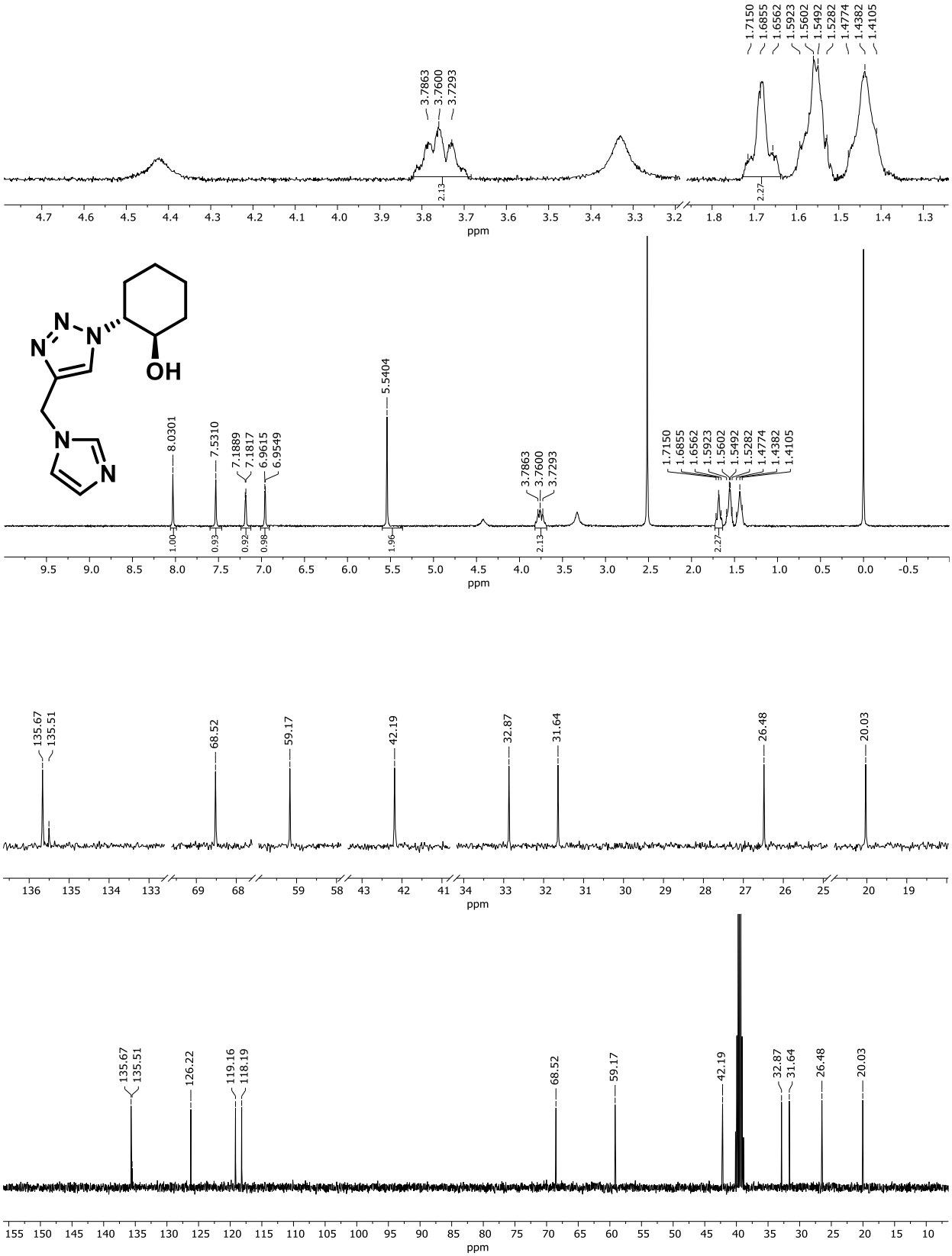
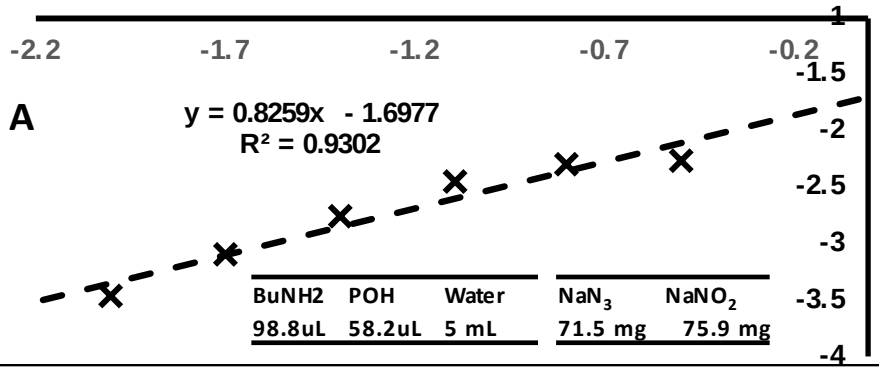


Figure S69:[1]H NMR and [13]CNMR of **2-(4-((1H-imidazol-1-yl)methyl)-1H-1,2,3-triazol-1-yl)cyclohexan-1-ol**



Conc of catalyst (in w/w in g)	0.005	0.01	0.02	0.04	0.08	0.16
Rate (in mmol/min)	0.00012	0.00033	0.000798	0.001757	0.003484	0.005056

B

Amount of Amine		0.38 mL	0.77 mL	0.97 mL	1.55mL	1.94 mL	3.1 mL
Amount of propargyl alcohol		0.2	0.4	0.5	0.8	1	1.6
0.39 mL	0.2	7.83E-05	0.000288	0.000333	0.000422	0.000481	0.000654
0.79 mL	0.4	3.73E-05	0.000271	0.000386	0.000533	0.000585	0.000729
0.98 mL	0.5	3.75E-05	0.000231	0.000371	0.000573	0.00063	0.000765
1.58 mL	0.8	1.47E-05	0.000135	0.000259	0.000634	0.000732	0.000867
1.97 mL	1	1.04E-05	9.78E-05	0.000195	0.000627	0.000772	0.000925
3.16 mL	1.6	6.7E-06	4.93E-05	9.56E-05	0.000455	0.000758	0.001071

C

Amount of Propargyl Alcohol		0.39 mL	0.79 mL	0.98 mL	1.58 mL	1.97 mL	3.16 mL
Amout of Amine		0.2	0.4	0.5	0.8	1	1.6
0.38 mL	0.2	7.83E-05	3.73E-05	3.75E-05	1.47E-05	1.04E-05	6.7E-06
0.77 mL	0.4	0.000288	0.000271	0.000231	0.000135	9.78E-05	4.93E-05
0.97 Ml	0.5	0.000333	0.000386	0.000371	0.000259	0.000195	9.56E-05
1.55mL	0.8	0.000422	0.000533	0.000573	0.000634	0.000627	0.000455
1.94 mL	1	0.000481	0.000585	0.00063	0.000732	0.000772	0.000758
3.1 mL	1.6	0.000654	0.000729	0.000765	0.000867	0.000925	0.001071

D

Conc of propargyl alcohol	Value	Standard	Error
	Vmax	0.00234	--
	Km	0	--
0.2	Ki	0.00649	--
	Vmax	81.9033	1.55E+07
	Km	28863.59511	5.45E+09
0.4	Ki	1.54E-06	0.28991
	Vmax	115.5511	1.49E+07
	Km	45988.70646	5.94E+09
0.5	Ki	2.03E-06	0.26166
	Vmax	0.00188	0.0013
	Km	0.6973	0.67063
0.8	Ki	0.6627	0.66988
	Vmax	9.32E-04	1.39E-04
	Km	0.20357	0.07503
1.0	Ki	20.27623	41.48472
	Vmax	0.00111	8.84E-05
	Km	0.1824	0.06113
1.6	Ki	1.98E+90	0

E

Conc of Amine	Value	Standard	Error
	Vmax	9.08E-04	3.30E-04
	k	0.83271	0.5119
0.2	n	1.31064	0.45386
	Vmax	7.64E-04	7.28E-05
	k	0.53175	0.06329
0.4	n	2.258	0.47377
	Vmax	8.03E-04	4.40E-05
	k	0.55819	0.03569
0.5	n	2.53836	0.32031
	Vmax	8.91E-04	1.65E-05
	k	0.63635	0.01174
0.8	n	3.66968	0.17036
	Vmax	9.51E-04	1.23E-05
	k	0.68813	0.00812
2.0	n	4.09921	0.13218
	Vmax	0.00115	2.35E-05
	k	0.86856	0.01223
1.6	n	4.44711	0.24431

Figure S70: A. Double log plot of catalyst loading vs initial rate; B & C datasheet of kinetic studies keeping amine and propargylalcohol constant respectively, D & E: fitting results of kinetic data

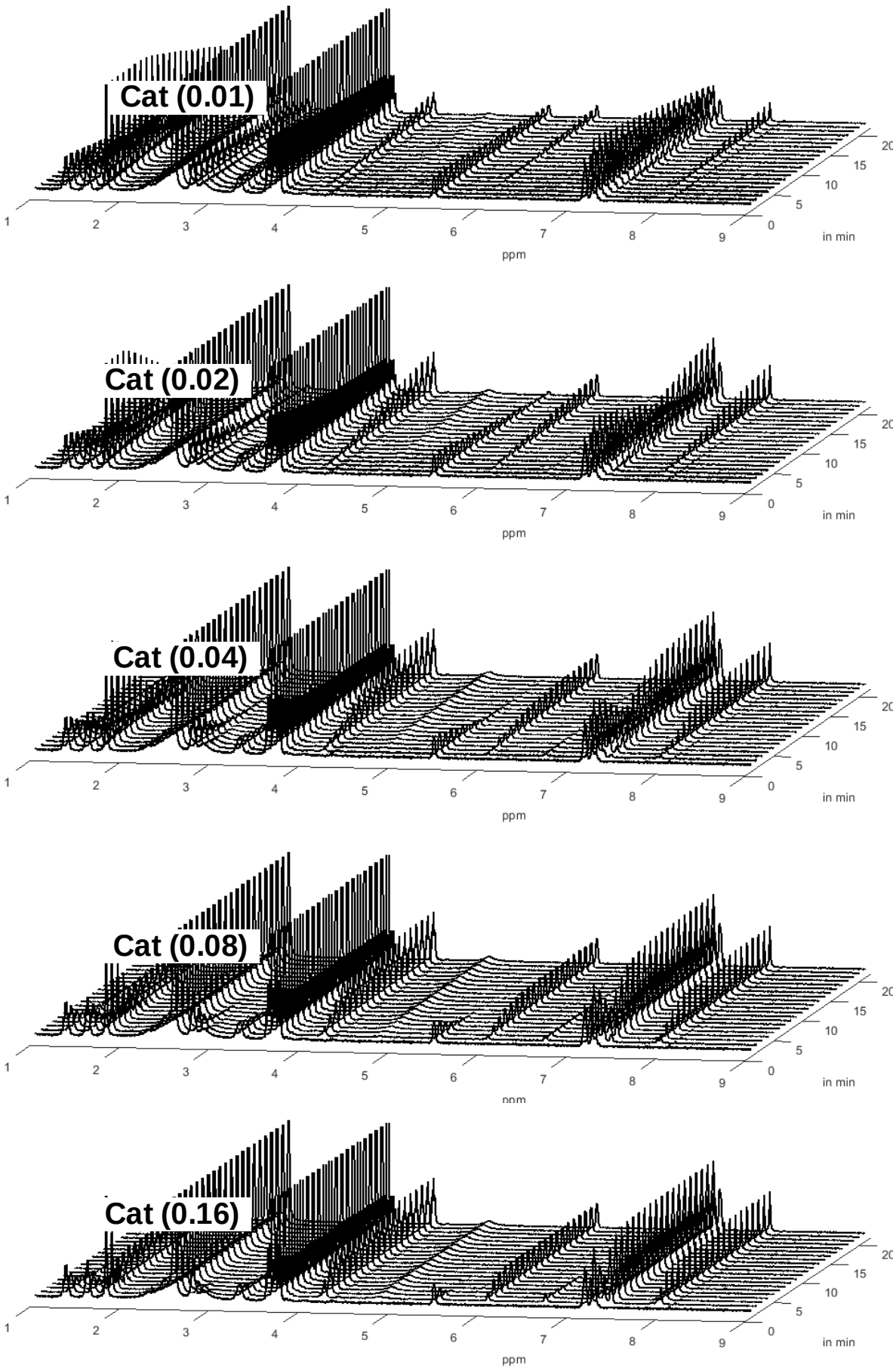


Figure S71: Stacked spectra obtained for the ex-situ NMR analysis with varying loading of Cu@Amberlyst

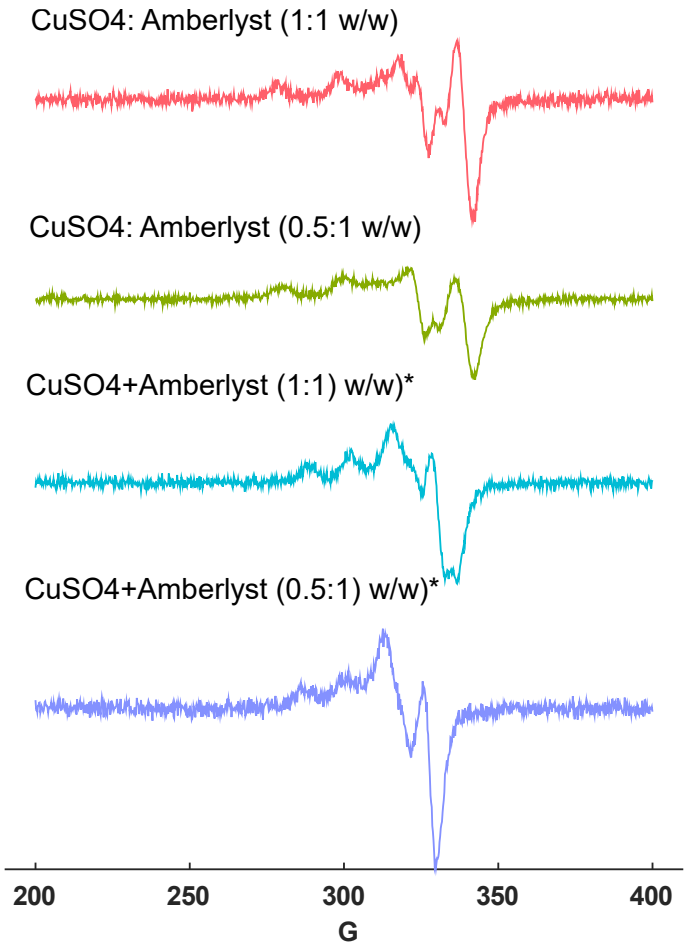
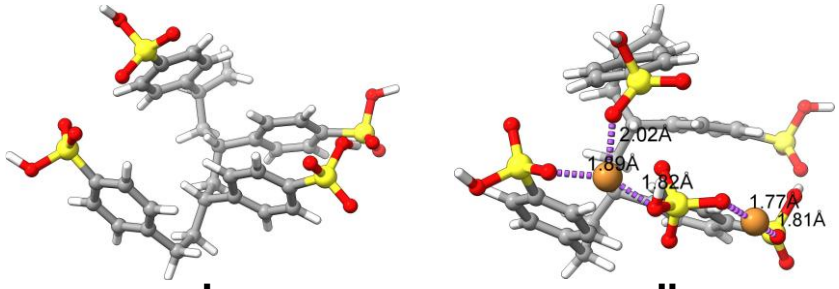


Figure S72: EPR of Cu@Amberlyst prepared using $CuSO_4$ and Amberlyst a) in 0.5:1 *w/w*; b) in 1:1 *w/w* ratio prepared using H_2O as solvent; c) 0.5:1.0 *w/w* and d) 1:1 *w/w* using mortar pestle. For sample preparation we used 0.08g of $CuSO_4$ and 0.08g of Amberlyst in 3 ml TDW (triple distilled water) was stirred for 30-40 min the solid was filtered and dried before EPR analysis



I

ΔG = 0.00 kJ/mol
ΔH = -50.21 kJ/mol
ΔS = -120.08 J/mol·K

II

ΔG = -9.37 kJ/mol
ΔH = -85.24 kJ/mol
ΔS = -140.16 J/mol·K

Figure S73. Structure of **I** and **II** in **Figure 8** of the manuscript

Table S9. XYZ coordinates of optmised structure shown in **Figure 8** of the manuscript

I			
symmetry c1			
C	0.748800000	-0.252900000	-4.565600000
C	-0.177200000	-1.457100000	-4.221500000
C	2.031500000	-0.291800000	-3.752400000
C	2.251800000	0.628600000	-2.742000000
C	3.334300000	0.493400000	-1.894200000
C	2.963000000	-1.313600000	-3.962900000
C	4.057600000	-1.446800000	-3.142200000
C	4.218500000	-0.545300000	-2.097600000
S	5.461100000	-0.719100000	-0.927100000
O	5.461800000	0.474500000	-0.114700000
O	5.435900000	-1.975100000	-0.238800000
O	6.739400000	-0.688100000	-1.833000000
C	-0.504400000	-1.547000000	-2.712800000
C	-1.172800000	-2.892200000	-2.331900000
C	-1.318700000	-0.357600000	-2.230900000
C	-2.595500000	-0.072700000	-2.725000000
C	-3.323300000	0.988400000	-2.229000000
C	-0.775200000	0.463700000	-1.263800000
C	-1.483700000	1.537900000	-0.781900000
C	-2.757300000	1.777400000	-1.235800000
S	-3.604600000	3.092000000	-0.496100000
O	-4.351900000	2.469600000	0.699900000
O	-2.593000000	3.930300000	0.127300000
O	-4.519800000	3.693400000	-1.403800000
C	-1.270200000	-3.066900000	-0.776000000
C	-0.909900000	-4.515900000	-0.357900000
C	-2.622400000	-2.581500000	-0.267100000
C	-2.675200000	-1.493900000	0.599700000
C	-3.876500000	-0.913600000	0.935800000
C	-3.816800000	-3.134200000	-0.717500000
C	-5.030100000	-2.567300000	-0.379600000
C	-5.051900000	-1.441900000	0.426900000
S	-6.537800000	-0.618700000	0.686200000
O	-7.586700000	-1.205200000	-0.079400000
O	-6.773700000	-0.896600000	2.212500000
O	-6.328100000	0.807200000	0.557800000
C	-0.575700000	-4.736000000	1.154600000
C	-1.846000000	-4.967700000	1.998800000
C	0.328100000	-3.620500000	1.687400000
C	-0.098200000	-2.718400000	2.651000000
C	0.728000000	-1.695800000	3.081000000
C	1.619600000	-3.480600000	1.175600000
C	2.452900000	-2.463800000	1.594800000
C	1.997600000	-1.574400000	2.556100000
S	2.999600000	-0.303900000	3.156600000
O	3.881500000	0.209800000	2.139900000
O	2.245500000	0.604100000	3.951000000
O	3.924900000	-1.163800000	4.106200000
H	0.979900000	-0.283000000	-5.625600000
H	0.225400000	0.672600000	-4.365900000
H	-1.090400000	-1.377000000	-4.801500000
H	0.317800000	-2.375300000	-4.522500000
H	1.580100000	1.436500000	-2.543100000
H	3.496800000	1.111400000	-1.042900000
H	2.816500000	-2.010000000	-4.765300000
H	4.767600000	-2.233900000	-3.300100000
H	7.590100000	-0.855900000	-1.390700000

II			
symmetry c1			
C	0.748800000	-0.252900000	-4.565600000
C	-0.177200000	-1.457100000	-4.221500000
C	2.031500000	-0.291800000	-3.752400000
C	2.251800000	0.628600000	-2.742000000
C	3.334300000	0.493400000	-1.894200000
C	2.963000000	-1.313600000	-3.962900000
C	4.057600000	-1.446800000	-3.142200000
C	4.218500000	-0.545300000	-2.097600000
S	5.461100000	-0.719100000	-0.927100000
O	5.461800000	0.474500000	-0.114700000
O	5.435900000	-1.975100000	-0.238800000
O	6.739400000	-0.688100000	-1.833000000
C	-0.504400000	-1.547000000	-2.712800000
C	-1.172800000	-2.892200000	-2.331900000
C	-1.318700000	-0.357600000	-2.230900000
C	-2.595500000	-0.072700000	-2.725000000
C	-3.323300000	0.988400000	-2.229000000
C	-0.775200000	0.463700000	-1.263800000
C	-1.483700000	1.537900000	-0.781900000
C	-2.757300000	1.777400000	-1.235800000
S	-3.604600000	3.092000000	-0.496100000
O	-4.351900000	2.469600000	0.699900000
O	-2.593000000	3.930300000	0.127300000
O	-4.519800000	3.693400000	-1.403800000
C	-1.270200000	-3.066900000	-0.776000000
C	-0.909900000	-4.515900000	-0.357900000
C	-2.622400000	-2.581500000	-0.267100000
C	-2.675200000	-1.493900000	0.599700000
C	-3.876500000	-0.913600000	0.935800000
C	-3.816800000	-3.134200000	-0.717500000
C	-5.030100000	-2.567300000	-0.379600000
C	-5.051900000	-1.441900000	0.426900000
S	-6.537800000	-0.618700000	0.686200000
O	-7.586700000	-1.205200000	-0.079400000
O	-6.773700000	-0.896600000	2.212500000
O	-6.328100000	0.807200000	0.557800000
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C	-1.846000000	-4.967700000	1.998800000
C	0.328100000	-3.620500000	1.687400000
C	-0.098200000	-2.718400000	2.651000000
C	0.728000000	-1.695800000	3.081000000
C	1.619600000	-3.480600000	1.175600000
C	2.452900000	-2.463800000	1.594800000
C	1.997600000	-1.574400000	2.556100000
S	2.999600000	-0.303900000	3.156600000
O	3.881500000	0.209800000	2.139900000
O	2.245500000	0.604100000	3.951000000
O	3.924900000	-1.163800000	4.106200000
Cu	4.165100000	1.591600000	0.689300000
O	3.011000000	2.999700000	0.629000000
O	1.190400000	2.862300000	-0.959100000
S	1.596400000	2.610700000	0.417900000
O	1.459300000	1.188000000	0.760700000
O	0.718900000	3.428100000	1.313500000
Cu	-0.916800000	3.873800000	0.810100000
H	0.979900000	-0.283000000	-5.625600000
H	0.225400000	0.672600000	-4.365900000

H	0.439900000	-1.515400000	-2.185500000
H	-2.149600000	-2.974000000	-2.791500000
H	-0.558600000	-3.690200000	-2.736400000
H	-3.024800000	-0.686600000	-3.491700000
H	-4.299600000	1.213400000	-2.610500000
H	0.200200000	0.304900000	-0.860300000
H	-1.077400000	2.233400000	-0.101500000
H	-5.182700000	1.920700000	0.577900000
H	-0.518400000	-2.425900000	-0.339800000
H	-1.699900000	-5.202400000	-0.645000000
H	-0.029800000	-4.794000000	-0.927500000
H	-1.766600000	-1.063100000	0.961100000
H	-3.891000000	-0.029700000	1.540800000
H	-3.802900000	-3.984800000	-1.369300000
H	-5.949000000	-2.961500000	-0.762100000
H	-7.551200000	-0.473300000	2.618300000
H	0.005000000	-5.653000000	1.202700000
H	-1.590100000	-5.167000000	3.033200000
H	-2.516400000	-4.121400000	1.959800000
H	-2.376900000	-5.831200000	1.613900000
H	-1.078600000	-2.796000000	3.069700000
H	0.390600000	-0.988300000	3.809600000
H	1.975700000	-4.171900000	0.437100000
H	3.433700000	-2.358900000	1.173800000
H	4.674700000	-0.685600000	4.500500000

H	-1.090400000	-1.377000000	-4.801500000
H	0.317800000	-2.375300000	-4.522500000
H	1.580100000	1.436500000	-2.543100000
H	3.496800000	1.111400000	-1.042900000
H	2.816500000	-2.010000000	-4.765300000
H	4.767600000	-2.233900000	-3.300100000
H	7.590100000	-0.855900000	-1.390700000
H	0.439900000	-1.515400000	-2.185500000
H	-2.149600000	-2.974000000	-2.791500000
H	-0.558600000	-3.690200000	-2.736400000
H	-3.024800000	-0.686600000	-3.491700000
H	-4.299600000	1.213400000	-2.610500000
H	0.200200000	0.304900000	-0.860300000
H	-1.077400000	2.233400000	-0.101500000
H	-5.182700000	1.920700000	0.577900000
H	-0.518400000	-2.425900000	-0.339800000
H	-1.699900000	-5.202400000	-0.645000000
H	-0.029800000	-4.794000000	-0.927500000
H	-1.766600000	-1.063100000	0.961100000
H	-3.891000000	-0.029700000	1.540800000
H	-3.802900000	-3.984800000	-1.369300000
H	-5.949000000	-2.961500000	-0.762100000
H	-7.551200000	-0.473300000	2.618300000
H	0.005000000	-5.653000000	1.202700000
H	-1.590100000	-5.167000000	3.033200000
H	-2.516400000	-4.121400000	1.959800000
H	-2.376900000	-5.831200000	1.613900000
H	-1.078600000	-2.796000000	3.069700000
H	0.390600000	-0.988300000	3.809600000
H	1.975700000	-4.171900000	0.437100000
H	3.433700000	-2.358900000	1.173800000
H	4.674700000	-0.685600000	4.500500000
H	6.148900000	0.407700000	0.552400000
H	-3.015900000	4.678900000	0.554400000
H	4.421500000	0.912400000	2.509200000
H	3.258400000	2.826500000	1.540200000

III

symmetry c1

C	0.748800000	-0.252900000	-4.565600000
C	-0.177200000	-1.457100000	-4.221500000
C	2.031500000	-0.291800000	-3.752400000
C	2.251800000	0.628600000	-2.742000000
C	3.334300000	0.493400000	-1.894200000
C	2.963000000	-1.313600000	-3.962900000
C	4.057600000	-1.446800000	-3.142200000
C	4.218500000	-0.545300000	-2.097600000
S	5.461100000	-0.719100000	-0.927100000
O	5.461800000	0.474500000	-0.114700000
O	5.435900000	-1.975100000	-0.238800000
O	6.739400000	-0.688100000	-1.833000000
C	-0.504400000	-1.547000000	-2.712800000
C	-1.172800000	-2.892200000	-2.331900000
C	-1.318700000	-0.357600000	-2.230900000
C	-2.595500000	-0.072700000	-2.725000000
C	-3.323300000	0.988400000	-2.229000000
C	-0.775200000	0.463700000	-1.263800000
C	-1.483700000	1.537900000	-0.781900000
C	-2.757300000	1.777400000	-1.235800000
S	-3.604600000	3.092000000	-0.496100000
O	-4.351900000	2.469600000	0.699900000
O	-2.593000000	3.930300000	0.127300000
O	-4.519800000	3.693400000	-1.403800000
C	-1.270200000	-3.066900000	-0.776000000
C	-0.909900000	-4.515900000	-0.357900000
C	-2.622400000	-2.581500000	-0.267100000
C	-2.675200000	-1.493900000	0.599700000
C	-3.876500000	-0.913600000	0.935800000
C	-3.816800000	-3.134200000	-0.717500000
C	-5.030100000	-2.567300000	-0.379600000
C	-5.051900000	-1.441900000	0.426900000
S	-6.537800000	-0.618700000	0.686200000
O	-7.586700000	-1.205200000	-0.079400000
O	-6.773700000	-0.896600000	2.212500000
O	-6.328100000	0.807200000	0.557800000
C	-0.575700000	-4.736000000	1.154600000
C	-1.846000000	-4.967700000	1.998800000
C	0.328100000	-3.620500000	1.687400000
C	-0.098200000	-2.718400000	2.651000000
C	0.728000000	-1.695800000	3.081000000
C	1.619600000	-3.480600000	1.175600000
C	2.452900000	-2.463800000	1.594800000
C	1.997600000	-1.574400000	2.556100000
S	2.999600000	-0.303900000	3.156600000

IV

symmetry c1

C	4.139000000	-0.676000000	-3.262000000
C	4.232000000	0.873000000	-3.390000000
C	2.767000000	-1.251000000	-2.953000000
C	1.716000000	-1.281000000	-3.897000000
C	0.463000000	-1.832000000	-3.567000000
C	2.533000000	-1.782000000	-1.671000000
C	1.287000000	-2.294000000	-1.290000000
C	0.288000000	-2.314000000	-2.261000000
S	-1.334000000	-3.174000000	-1.871000000
O	-2.535000000	-2.191000000	-1.321000000
O	-1.760000000	-4.070000000	-3.138000000
O	-0.997000000	-4.248000000	-0.546000000
C	3.664000000	1.756000000	-2.221000000
C	4.131000000	1.276000000	-0.819000000
C	2.163000000	1.979000000	-2.417000000
C	1.768000000	2.925000000	-3.393000000
C	0.417000000	3.183000000	-3.662000000
C	1.165000000	1.273000000	-1.719000000
C	-0.194000000	1.510000000	-1.964000000
C	-0.532000000	2.468000000	-2.922000000
S	-2.321000000	2.839000000	-3.230000000
O	-2.592000000	4.346000000	-2.365000000
O	-2.583000000	3.137000000	-4.789000000
O	-3.183000000	1.672000000	-2.443000000
C	4.113000000	2.384000000	0.284000000
C	4.955000000	2.083000000	1.594000000
C	2.679000000	2.805000000	0.622000000
C	1.856000000	1.979000000	1.415000000
C	0.524000000	2.314000000	1.692000000
C	2.139000000	4.010000000	0.119000000
C	0.798000000	4.362000000	0.351000000
C	0.023000000	3.488000000	1.125000000
S	-1.777000000	3.911000000	1.370000000
O	-2.599000000	3.356000000	0.014000000
O	-2.290000000	2.875000000	2.652000000
O	-1.992000000	5.461000000	1.731000000
C	5.528000000	0.670000000	1.998000000
C	6.720000000	0.203000000	1.130000000
C	4.467000000	-0.408000000	2.237000000
C	4.358000000	-1.570000000	1.442000000
C	3.337000000	-2.512000000	1.660000000
C	3.564000000	-0.256000000	3.316000000
C	2.531000000	-1.179000000	3.550000000
C	2.424000000	-2.278000000	2.691000000
S	0.954000000	-3.428000000	2.865000000

O	3.881500000	0.209800000	2.139900000
O	2.245500000	0.604100000	3.951000000
O	3.924900000	-1.163800000	4.106200000
Cu	4.165100000	1.591600000	0.689300000
O	3.011000000	2.999700000	0.629000000
O	1.190400000	2.862300000	-0.959100000
S	1.596400000	2.610700000	0.417900000
O	1.459300000	1.188000000	0.760700000
O	0.718900000	3.428100000	1.313500000
Cu	-0.916800000	3.873800000	0.810100000
H	0.979900000	-0.283000000	-5.625600000
H	0.225400000	0.672600000	-4.365900000
H	-1.090400000	-1.377000000	-4.801500000
H	0.317800000	-2.375300000	-4.522500000
H	1.580100000	1.436500000	-2.543100000
H	3.496800000	1.111400000	-1.042900000
H	2.816500000	-2.010000000	-4.765300000
H	4.767600000	-2.233900000	-3.300100000
H	7.590100000	-0.855900000	-1.390700000
H	0.439900000	-1.515400000	-2.185500000
H	-2.149600000	-2.974000000	-2.791500000
H	-0.558600000	-3.690200000	-2.736400000
H	-3.024800000	-0.686600000	-3.491700000
H	-4.299600000	1.213400000	-2.610500000
H	0.200200000	0.304900000	-0.860300000
H	-1.077400000	2.233400000	-0.101500000
H	-5.182700000	1.920700000	0.577900000
H	-0.518400000	-2.425900000	-0.339800000
H	-1.699900000	-5.202400000	-0.645000000
H	-0.029800000	-4.794000000	-0.927500000
H	-1.766600000	-1.063100000	0.961100000
H	-3.891000000	-0.029700000	1.540800000
H	-3.802900000	-3.984800000	-1.369300000
H	-5.949000000	-2.961500000	-0.762100000
H	-7.551200000	-0.473300000	2.618300000
H	0.005000000	-5.653000000	1.202700000
H	-1.590100000	-5.167000000	3.033200000
H	-2.516400000	-4.121400000	1.959800000
H	-2.376900000	-5.831200000	1.613900000
H	-1.078600000	-2.796000000	3.069700000
H	0.390600000	-0.988300000	3.809600000
H	1.975700000	-4.171900000	0.437100000
H	3.433700000	-2.358900000	1.173800000
H	4.674700000	-0.685600000	4.500500000
H	6.148900000	0.407700000	0.552400000
H	-3.015900000	4.678900000	0.554400000
H	4.421500000	0.912400000	2.509200000
H	3.258400000	2.826500000	1.540200000

O	0.365000000	-3.390000000	1.316000000
O	1.356000000	-4.895000000	3.402000000
O	-0.076000000	-2.595000000	3.886000000
Cu	-3.871000000	-2.862000000	0.451000000
O	-2.502000000	-1.955000000	1.687000000
O	-2.553000000	0.744000000	1.389000000
S	-1.576000000	-0.623000000	1.495000000
O	-0.720000000	-0.403000000	2.963000000
O	-0.538000000	-0.624000000	0.252000000
Cu	-3.376000000	1.454000000	-0.395000000
N	-4.939000000	-1.292000000	-0.034000000
N	-3.487000000	-4.785000000	0.855000000
C	-3.062000000	-4.926000000	2.297000000
O	-5.791000000	-0.709000000	0.634000000
O	-4.274000000	-0.383000000	-0.988000000
H	4.511000000	-1.095000000	-4.208000000
H	4.838000000	-1.004000000	-2.482000000
H	5.300000000	1.111000000	-3.507000000
H	3.740000000	1.186000000	-4.320000000
H	1.870000000	-0.884000000	-4.897000000
H	-0.331000000	-1.898000000	-4.304000000
H	3.332000000	-1.779000000	-0.941000000
H	1.123000000	-2.638000000	-0.275000000
H	-0.463000000	-3.885000000	0.312000000
H	4.136000000	2.741000000	-2.377000000
H	3.555000000	0.411000000	-0.478000000
H	5.166000000	0.939000000	-0.935000000
H	2.529000000	3.476000000	-3.943000000
H	0.113000000	3.908000000	-4.411000000
H	1.409000000	0.539000000	-0.966000000
H	-0.931000000	0.939000000	-1.415000000
H	-2.674000000	4.123000000	-1.363000000
H	4.597000000	3.261000000	-0.173000000
H	5.837000000	2.738000000	1.562000000
H	4.360000000	2.438000000	2.446000000
H	2.236000000	1.048000000	1.812000000
H	-0.065000000	1.674000000	2.338000000
H	2.757000000	4.670000000	-0.484000000
H	0.383000000	5.280000000	-0.053000000
H	-2.452000000	1.898000000	2.260000000
H	5.962000000	0.874000000	2.991000000
H	7.222000000	-0.654000000	1.596000000
H	6.433000000	-0.094000000	0.117000000
H	7.454000000	1.013000000	1.039000000
H	5.071000000	-1.750000000	0.644000000
H	3.248000000	-3.391000000	1.028000000
H	3.653000000	0.606000000	3.973000000
H	1.822000000	-1.034000000	4.358000000
H	-0.452000000	-1.397000000	3.405000000
H	-2.697000000	-5.937000000	2.515000000
H	-2.275000000	-4.198000000	2.501000000
H	-3.912000000	-4.694000000	2.945000000
H	-4.252000000	-5.428000000	0.637000000
H	-2.687000000	-4.992000000	0.240000000
H	-3.597000000	-0.964000000	-1.476000000

V			
symmetry c1			
C	3.992000000	-0.165000000	-3.011000000
C	3.687000000	1.360000000	-3.009000000
C	2.800000000	-1.076000000	-2.788000000
C	1.837000000	-1.340000000	-3.789000000
C	0.723000000	-2.154000000	-3.517000000
C	2.642000000	-1.667000000	-1.522000000
C	1.538000000	-2.470000000	-1.219000000
C	0.599000000	-2.686000000	-2.226000000
S	-0.898000000	-3.712000000	-1.808000000
O	-2.034000000	-2.563000000	-1.258000000
O	-1.448000000	-4.440000000	-3.139000000
O	-0.512000000	-4.654000000	-0.515000000
C	2.813000000	1.972000000	-1.853000000
C	3.187000000	1.494000000	-0.411000000
C	1.320000000	1.898000000	-2.203000000
C	0.807000000	2.843000000	-3.124000000
C	-0.553000000	2.886000000	-3.460000000
C	0.434000000	0.952000000	-1.649000000
C	-0.932000000	0.958000000	-1.961000000
C	-1.384000000	1.941000000	-2.847000000
S	-3.220000000	2.062000000	-3.123000000
O	-3.519000000	3.651000000	-3.712000000
O	-3.868000000	1.010000000	-4.156000000
O	-3.876000000	1.998000000	-1.572000000
C	3.205000000	2.668000000	0.631000000
C	3.499000000	2.267000000	2.114000000

VIA			
symmetry c1			
C	0.378300000	0.473300000	-4.842300000
C	1.860000000	0.606600000	-4.394700000
C	-0.535100000	-0.477900000	-4.082100000
C	-1.885400000	-0.148300000	-3.967900000
C	-2.730700000	-0.879300000	-3.165100000
C	-0.083600000	-1.633100000	-3.463300000
C	-0.919900000	-2.361700000	-2.635000000
C	-2.224500000	-1.952100000	-2.445600000
S	-3.218300000	-2.756200000	-1.271500000
O	-4.539600000	-2.923500000	-1.770900000
O	-2.489200000	-3.858000000	-0.723200000
O	-3.268600000	-1.675200000	-0.119300000
C	2.239100000	1.152300000	-2.961700000
C	2.582300000	-0.008300000	-1.972500000
C	1.232700000	2.149900000	-2.400100000
C	-0.010900000	1.724300000	-1.968600000
C	-0.908600000	2.592100000	-1.391800000
C	1.547700000	3.497600000	-2.256400000
C	0.662300000	4.377200000	-1.657800000
C	-0.566500000	3.916700000	-1.214400000
S	-1.690100000	4.960200000	-0.392500000
O	-2.595800000	4.060000000	0.323400000
O	-0.829400000	5.678500000	0.636400000
O	-2.286000000	5.907000000	-1.269400000
C	3.502700000	0.400800000	-0.794600000
C	4.307200000	-0.782000000	-0.143600000

C	1.861000000	3.403000000	0.564000000
C	0.708000000	2.789000000	1.096000000
C	-0.578000000	3.295000000	0.863000000
C	1.711000000	4.619000000	-0.138000000
C	0.439000000	5.166000000	-0.380000000
C	-0.673000000	4.461000000	0.099000000
S	-2.359000000	5.099000000	-0.371000000
O	-2.380000000	5.055000000	-2.017000000
O	-3.429000000	3.840000000	0.214000000
O	-2.755000000	6.492000000	0.314000000
C	4.630000000	1.238000000	2.461000000
C	5.950000000	1.500000000	1.707000000
C	4.120000000	-0.210000000	2.421000000
C	4.603000000	-1.185000000	1.525000000
C	4.060000000	-2.484000000	1.497000000
C	3.116000000	-0.589000000	3.347000000
C	2.568000000	-1.877000000	3.354000000
C	3.040000000	-2.785000000	2.401000000
S	2.246000000	-4.464000000	2.290000000
O	2.990000000	-5.322000000	1.141000000
O	1.944000000	-5.061000000	3.753000000
O	0.649000000	-3.945000000	1.622000000
Cu	-2.422000000	-2.132000000	0.602000000
O	-0.991000000	-2.137000000	2.123000000
O	-1.604000000	0.097000000	1.006000000
S	-0.322000000	-0.455000000	1.884000000
O	-0.107000000	0.233000000	3.330000000
O	1.021000000	-0.650000000	0.994000000
Cu	-4.318000000	0.247000000	-0.662000000
N	-4.638000000	-0.533000000	1.040000000
N	-4.012000000	-1.440000000	1.588000000
C	-4.184000000	-1.824000000	3.029000000
O	-3.784000000	-0.980000000	-2.189000000
H	4.469000000	-0.395000000	-3.974000000
H	4.741000000	-0.375000000	-2.237000000
H	4.661000000	1.872000000	-2.996000000
H	3.209000000	1.629000000	-3.961000000
H	1.953000000	-0.907000000	-4.780000000
H	-0.015000000	-2.380000000	-4.281000000
H	3.367000000	-1.472000000	-0.744000000
H	1.422000000	-2.869000000	-0.224000000
H	-0.265000000	-2.886000000	2.075000000
H	3.060000000	3.043000000	-1.899000000
H	2.515000000	0.713000000	-0.048000000
H	4.186000000	1.050000000	-0.435000000
H	1.471000000	3.587000000	-3.557000000
H	-0.943000000	3.645000000	-4.129000000
H	0.773000000	0.221000000	-0.928000000
H	-1.588000000	0.240000000	-1.483000000
H	-3.148000000	4.352000000	-3.002000000
H	3.996000000	3.363000000	0.308000000
H	3.736000000	3.205000000	2.638000000
H	2.580000000	1.894000000	2.574000000
H	0.804000000	1.888000000	1.683000000
H	-1.451000000	2.762000000	1.225000000
H	2.588000000	5.133000000	-0.524000000
H	0.326000000	6.082000000	-0.952000000
H	-3.632000000	3.140000000	-0.516000000
H	4.844000000	1.433000000	3.524000000
H	6.749000000	0.841000000	2.070000000
H	5.859000000	1.351000000	0.625000000
H	6.269000000	2.537000000	1.869000000
H	5.402000000	-0.941000000	0.830000000
H	4.408000000	-3.234000000	0.792000000
H	2.729000000	0.137000000	4.056000000
H	1.788000000	-2.144000000	4.060000000
H	0.277000000	-4.393000000	0.762000000
H	-3.183000000	-1.801000000	3.471000000
H	-4.869000000	-1.134000000	3.530000000
H	-4.562000000	-2.851000000	3.052000000
H	-3.136000000	-1.743000000	-2.032000000
H	-3.958000000	-0.761000000	-3.126000000
H	-1.454000000	1.013000000	0.761000000

C	2.847900000	1.267200000	0.277900000
C	3.592500000	2.290100000	0.851300000
C	3.049000000	3.128200000	1.811200000
C	1.537700000	1.085300000	0.698800000
C	0.985100000	1.932700000	1.621300000
C	1.738800000	2.943800000	2.182400000
S	0.939600000	3.953000000	3.353400000
O	1.717900000	5.134800000	3.549700000
O	-0.365300000	4.249700000	2.608300000
O	0.589700000	3.134500000	4.481300000
C	3.691300000	-2.186100000	0.175100000
C	3.616600000	-3.096800000	-1.069900000
C	2.402000000	-2.173300000	0.996400000
C	1.223000000	-2.744100000	0.529900000
C	0.084600000	-2.785700000	1.311000000
C	2.415400000	-1.651700000	2.286100000
C	1.284200000	-1.672400000	3.073900000
C	0.117300000	-2.232900000	2.579000000
S	-1.296500000	-2.267600000	3.570700000
O	-1.988900000	-3.504600000	3.408800000
O	-0.992900000	-1.750900000	4.861800000
O	-2.249400000	-1.226000000	2.836100000
Cu	-3.831500000	-1.853500000	1.780900000
O	-3.036700000	0.796800000	0.033600000
O	-2.427100000	1.361300000	2.304700000
S	-3.558300000	1.152000000	1.352900000
O	-4.431000000	0.128900000	1.864700000
O	-4.303000000	2.471300000	1.245500000
Cu	-1.539600000	2.867500000	2.712000000
N	-4.820100000	-3.175400000	2.468600000
N	-4.961500000	-4.161800000	2.970100000
N	-5.191300000	-5.269200000	3.453900000
C	-4.363300000	-5.569600000	4.681900000
H	-0.075200000	1.455400000	-4.820900000
H	0.399800000	0.160500000	-5.883700000
H	2.367600000	-0.340400000	-4.538700000
H	2.301300000	1.291300000	-5.111500000
H	-2.261200000	0.716800000	-4.476700000
H	-3.763900000	-0.607500000	-3.072700000
H	0.931200000	-1.948900000	-3.588400000
H	-0.567400000	-3.232300000	-2.123700000
H	-3.147800000	-0.674800000	-0.297200000
H	3.169200000	1.690500000	-3.111400000
H	1.684200000	-0.489500000	-1.616500000
H	3.130600000	-0.742800000	-2.549400000
H	-0.278300000	0.697600000	-2.045500000
H	-1.840800000	2.218100000	-1.036900000
H	2.504400000	3.859400000	-2.576400000
H	0.939200000	5.401700000	-1.509500000
H	-3.803400000	3.253000000	0.825200000
H	4.279400000	1.022800000	-1.230300000
H	5.153300000	-0.986000000	-0.793400000
H	4.726000000	-0.388200000	0.775100000
H	4.604100000	2.450600000	0.531000000
H	3.617000000	3.928300000	2.239400000
H	0.937500000	0.306900000	0.284800000
H	-0.035800000	1.914000000	1.902500000
H	-0.578800000	5.196600000	1.528700000
H	4.431200000	-2.649200000	0.823200000
H	3.372200000	-4.112200000	-0.780800000
H	2.884100000	-2.760100000	-1.788600000
H	4.583100000	-3.115000000	-1.559400000
H	1.188600000	-3.188600000	-0.439900000
H	-0.803400000	-3.254000000	0.933400000
H	3.313900000	-1.219700000	2.678000000
H	1.299400000	-1.267100000	4.064300000
H	-2.119800000	-0.248200000	2.948200000
H	-4.470100000	-6.626600000	4.853500000
H	-3.329700000	-5.309300000	4.513400000
H	-4.747800000	-5.019700000	5.531500000

VIB

symmetry c1

C	4.981400000	2.051100000	-2.632300000
C	3.784900000	3.001200000	-2.898200000
C	4.608200000	0.592600000	-2.476800000
C	3.924700000	-0.085600000	-3.474300000
C	3.450500000	-1.365900000	-3.255600000
C	4.917300000	-0.079100000	-1.299000000
C	4.473000000	-1.365700000	-1.084000000
C	3.692300000	-1.985400000	-2.045500000

VII

symmetry c1

C	-4.119800000	-3.351200000	-5.424300000
C	-3.038100000	-2.307100000	-5.805900000
C	-5.476900000	-2.850800000	-4.949500000
C	-6.087000000	-1.721100000	-5.473900000
C	-7.292500000	-1.270900000	-4.967900000
C	-6.155800000	-3.584500000	-3.978400000
C	-7.370800000	-3.160000000	-3.485600000
C	-7.910100000	-1.970800000	-3.949000000

S	2.916600000	-3.498500000	-1.673300000
O	1.969600000	-3.767800000	-2.716600000
O	3.879500000	-4.483100000	-1.302300000
O	2.125800000	-3.083300000	-0.412700000
C	2.602600000	3.086000000	-1.869000000
C	3.023000000	3.073500000	-0.372800000
C	1.456400000	2.125600000	-2.196400000
C	0.429000000	2.611000000	-2.991400000
C	-0.694700000	1.858300000	-3.235900000
C	1.348100000	0.827000000	-1.712300000
C	0.229400000	0.049000000	-1.950600000
C	-0.807700000	0.585800000	-2.698600000
S	-2.321500000	-0.211300000	-3.023700000
O	-2.667500000	-0.942500000	-1.714400000
O	-3.304600000	0.864300000	-3.082400000
O	-2.249100000	-1.112000000	-4.119400000
C	2.179400000	4.066200000	0.486700000
C	2.804900000	4.321700000	1.907700000
C	0.686100000	3.740000000	0.491800000
C	0.211600000	2.492300000	0.887700000
C	-1.129200000	2.184700000	0.836200000
C	-0.234700000	4.681000000	0.049300000
C	-1.583900000	4.377200000	-0.034800000
C	-2.025700000	3.125100000	0.348700000
S	-3.716300000	2.750400000	0.262800000
O	-4.408700000	3.841900000	-0.333900000
O	-3.770800000	1.496400000	-0.699600000
O	-4.156600000	2.162900000	1.491600000
C	2.300000000	3.570200000	3.166500000
C	3.032500000	4.148800000	4.405800000
C	2.462800000	2.056300000	3.177000000
C	3.569000000	1.402000000	2.651400000
C	3.623700000	0.019200000	2.620200000
C	1.455100000	1.290700000	3.754300000
C	1.502400000	-0.085200000	3.731700000
C	2.575600000	-0.725100000	3.131900000
S	2.557400000	-2.463200000	3.018200000
O	3.308300000	-2.721700000	1.720200000
O	3.204200000	-3.088300000	4.116500000
O	1.155500000	-2.822000000	2.797800000
Cu	0.383100000	-2.718300000	-0.393500000
O	-2.632500000	-3.146000000	1.743100000
O	-2.799500000	-0.799400000	1.088300000
S	-1.970700000	-1.986300000	1.260500000
O	-0.847300000	-1.533000000	2.176300000
O	-1.300300000	-2.233000000	-0.076100000
Cu	-4.381000000	-0.129800000	0.255500000
O	-7.190000000	-3.124300000	1.069800000
C	-6.001700000	-2.454000000	1.538000000
C	-5.778200000	-1.283700000	0.679100000
C	-6.172100000	-0.461100000	-0.167700000
H	5.667100000	2.161100000	-3.467600000
H	5.514100000	2.378300000	-1.748100000
H	4.204400000	4.000400000	-2.974900000
H	3.358800000	2.773500000	-3.868300000
H	3.709100000	0.401700000	-4.404100000
H	2.858900000	-1.869900000	-3.991400000
H	5.491600000	0.417100000	-0.541400000
H	4.693800000	-1.869300000	-0.164800000
H	2.802900000	-2.972200000	0.823600000
H	2.185500000	4.070900000	-2.049600000
H	2.986200000	2.077400000	0.039600000
H	4.051900000	3.409900000	-0.303000000
H	0.483000000	3.606600000	-3.384800000
H	-1.502700000	2.267100000	-3.804900000
H	2.134400000	0.410700000	-1.120400000
H	0.194200000	-0.921800000	-1.501100000
H	-2.075300000	-1.585400000	-1.198200000
H	2.275300000	5.020700000	-0.021200000
H	3.880000000	4.198200000	1.825300000
H	2.641900000	5.371900000	2.127000000
H	0.893200000	1.749300000	1.231800000
H	-1.472800000	1.220400000	1.152900000
H	0.098900000	5.654400000	-0.251900000
H	-2.287900000	5.098500000	-0.395600000
H	-3.663900000	1.466700000	-1.721400000
H	1.242700000	3.779500000	3.271700000
H	2.667700000	3.684700000	5.313800000
H	4.097900000	3.961800000	4.333300000
H	2.872200000	5.218800000	4.478900000
H	4.381100000	1.963600000	2.236800000
H	4.461500000	-0.478200000	2.177600000
H	0.601000000	1.777000000	4.181900000
S	-9.342800000	-1.344000000	-3.206700000
O	-9.865900000	-0.282300000	-4.000200000
O	-10.157600000	-2.417300000	-2.746400000
O	-8.742000000	-0.627100000	-1.919700000
C	-2.499400000	-1.314800000	-4.715000000
C	-2.223300000	-2.023400000	-3.360700000
C	-3.361800000	-0.049700000	-4.666600000
C	-3.166500000	0.897300000	-5.666300000
C	-3.905500000	2.062800000	-5.705800000
C	-4.339200000	0.194800000	-3.711600000
C	-5.076000000	1.362100000	-3.735400000
C	-4.852100000	2.299900000	-4.727900000
S	-5.717700000	3.808500000	-4.722000000
O	-5.165100000	4.513900000	-3.493000000
O	-5.400000000	4.504800000	-5.931600000
O	-7.110800000	3.547200000	-4.420800000
C	-1.094600000	-1.367400000	-2.509300000
C	-0.563900000	-2.193800000	-1.261900000
C	-1.460500000	0.058700000	-2.101400000
C	-2.393600000	0.302200000	-1.104400000
C	-2.794200000	1.585900000	-0.802100000
C	-0.892300000	1.143900000	-2.754300000
C	-1.286600000	2.434800000	-2.459800000
C	-2.251300000	2.655100000	-1.492300000
S	-2.771000000	4.280300000	-1.152200000
O	-2.915700000	4.887100000	-2.541600000
O	-4.108400000	4.175100000	-0.570700000
O	-1.797700000	4.997300000	-0.405700000
C	-1.310600000	-3.410300000	-0.603100000
C	-1.208800000	-4.711100000	-1.429900000
C	-2.725600000	-3.090000000	-0.129600000
C	-3.853700000	-3.516700000	-0.811700000
C	-5.116300000	-3.120100000	-0.414700000
C	-2.904300000	-2.325300000	1.023600000
C	-4.161500000	-1.933600000	1.435500000
C	-5.269700000	-2.312400000	0.693200000
S	-6.869500000	-1.801500000	1.137000000
O	-7.670900000	-1.919500000	-0.076200000
O	-7.345700000	-2.480300000	2.289400000
O	-6.667000000	-0.317600000	1.438800000
H	-4.284500000	-3.965000000	-6.307200000
H	-3.719100000	-4.013700000	-4.666500000
H	-2.187000000	-2.885900000	-6.154300000
H	-3.376800000	-1.725800000	-6.654900000
H	-5.607200000	-1.156600000	-6.245100000
H	-7.743400000	-0.375400000	-5.343600000
H	-5.728400000	-4.496800000	-3.610200000
H	-7.897300000	-3.731600000	-2.747200000
H	-8.346100000	-1.209200000	-1.173700000
H	-1.535700000	-0.991700000	-5.098400000
H	-3.126900000	-2.108300000	-2.781400000
H	-1.896500000	-3.027000000	-3.598200000
H	-2.417400000	0.729200000	-6.416100000
H	-3.750700000	2.792600000	-6.473000000
H	-4.531200000	-0.519500000	-2.941000000
H	-5.815700000	1.557800000	-2.984700000
H	-3.817900000	4.776800000	-3.053400000
H	-0.240400000	-1.281400000	-3.172600000
H	0.411000000	-2.583300000	-1.537100000
H	-0.380700000	-1.474600000	-0.473600000
H	-2.826700000	-0.514800000	-0.574400000
H	-3.551000000	1.742600000	-0.063000000
H	-0.156700000	0.984500000	-3.517600000
H	-0.871000000	3.263100000	-2.997000000
H	-5.022800000	3.364900000	0.272100000
H	-0.734300000	-3.595800000	0.299100000
H	-1.630900000	-5.541300000	-0.875300000
H	-1.713100000	-4.646300000	-2.382100000
H	-0.164900000	-4.932000000	-1.621700000
H	-3.759200000	-4.142300000	-1.673200000
H	-5.976100000	-3.413800000	-0.974700000
H	-2.048200000	-2.011500000	1.588500000
H	-4.280700000	-1.316600000	2.303400000
H	-7.069500000	0.425800000	0.861900000
Cu	-8.895800000	1.229500000	-1.516900000
O	-7.637800000	1.477400000	-0.073000000
O	-6.935000000	3.368600000	-1.352400000
S	-7.144900000	2.884700000	0.015600000
O	-7.996900000	3.711300000	0.804700000
O	-5.754200000	2.747400000	0.638600000
Cu	-6.576800000	5.015000000	-2.268000000
O	-8.567300000	6.500300000	0.598500000
C	-8.853500000	6.687500000	-0.791200000

H	0.690000000	-0.651500000	4.136500000
H	-0.057700000	-2.139300000	2.470300000
H	-7.289700000	-3.972800000	1.522100000
H	-6.123000000	-2.116900000	2.563000000
H	-5.135300000	-3.101400000	1.509100000
H	-6.942800000	-0.071200000	-0.774900000

C	-7.701200000	6.412900000	-1.690100000
C	-6.876500000	6.819300000	-2.533900000
H	-8.415200000	5.563700000	0.795300000
H	-9.695000000	6.088800000	-1.119700000
H	-9.122900000	7.727700000	-0.898200000
H	-6.475400000	7.594000000	-3.129700000
N	-9.870000000	2.508800000	-2.290200000
N	-10.021900000	3.429500000	-2.906800000
N	-10.212800000	4.503400000	-3.455500000
C	-10.189400000	4.465200000	-4.967000000
H	-10.460800000	5.456800000	-5.284200000
H	-9.187000000	4.222700000	-5.282400000
H	-10.901800000	3.744100000	-5.345100000

VIII

symmetry c1

C	-4.289900000	-0.735200000	-0.030000000
C	-3.834300000	-0.755100000	1.452000000
C	-3.287800000	-1.344000000	-0.994100000
C	-2.749500000	-0.565200000	-2.009800000
C	-1.823000000	-1.082600000	-2.890900000
C	-2.890200000	-2.672100000	-0.882000000
C	-1.968200000	-3.208300000	-1.757700000
C	-1.436000000	-2.406200000	-2.756900000
S	-0.291900000	-3.076200000	-3.861000000
O	-0.426700000	-4.490400000	-3.919700000
O	-0.254800000	-2.281800000	-5.048100000
O	1.099100000	-2.753100000	-3.148400000
C	-2.385500000	-0.261500000	1.702000000
C	-2.113200000	-0.188900000	3.234700000
C	-2.097000000	1.048200000	0.990000000
C	-2.911200000	2.159800000	1.155900000
C	-2.658300000	3.333300000	0.467600000
C	-1.002400000	1.139700000	0.138200000
C	-0.742200000	2.303700000	-0.539700000
C	-1.577300000	3.392400000	-0.385700000
S	-1.274000000	4.802700000	-1.349200000
O	0.241800000	4.981800000	-1.175100000
O	-1.468300000	4.447900000	-2.729500000
O	-2.014700000	5.894800000	-0.805200000
C	-0.630500000	-0.474500000	3.598700000
C	-0.490900000	-0.948000000	5.074300000
C	0.314700000	0.653000000	3.197500000
C	1.467200000	0.313900000	2.503100000
C	2.266200000	1.275000000	1.932200000
C	0.034100000	2.001200000	3.379900000
C	0.803200000	2.971800000	2.760500000
C	1.899300000	2.603700000	2.000300000
S	2.735300000	3.769000000	1.006200000
O	3.995000000	4.149400000	1.555000000
O	2.920500000	3.002400000	-0.291000000
O	1.768600000	4.842200000	0.792700000
C	0.722800000	-1.909000000	5.392400000
C	1.932200000	-1.113100000	5.921600000
C	1.049600000	-2.799000000	4.190300000
C	0.036900000	-3.565800000	3.612200000
C	0.212200000	-4.168900000	2.386100000
C	2.296600000	-2.800400000	3.581000000
C	2.494600000	-3.432600000	2.366200000
C	1.432500000	-4.053400000	1.739200000
S	1.615500000	-4.657700000	0.124400000
O	2.920600000	-5.202300000	-0.041500000
O	0.448500000	-5.396100000	-0.237700000
O	1.543200000	-3.322800000	-0.726700000
Cu	2.364100000	-1.551600000	-3.962800000
O	3.343200000	-0.861600000	-2.489200000
O	1.797800000	0.811300000	-1.708500000
S	2.858700000	-0.129200000	-1.337400000
O	2.441100000	-1.026400000	-0.267600000
O	4.020300000	0.733500000	-0.820200000
Cu	1.959200000	2.763200000	-1.951300000
O	-0.538400000	2.227100000	-4.270300000
C	0.609700000	2.948900000	-4.767500000
C	1.543900000	3.353300000	-3.700900000
C	2.370900000	4.118700000	-3.194800000
N	2.162200000	-0.903500000	-5.602000000
N	1.583100000	-0.280000000	-6.327500000
N	1.016400000	0.443700000	-7.137700000
C	-0.494900000	0.274400000	-7.147100000
H	2.977100000	4.981400000	-3.164000000
H	-5.229500000	-1.273800000	-0.105300000
H	-4.479500000	0.286500000	-0.328200000
H	-4.531700000	-0.153600000	2.026500000
H	-3.905200000	-1.767600000	1.835800000

IX

symmetry c1

C	-4.881400000	-1.515100000	0.393000000
C	-4.312000000	-1.329000000	1.828600000
C	-3.891200000	-1.937700000	-0.692000000
C	-4.108400000	-1.505600000	-1.997300000
C	-3.180000000	-1.734300000	-2.990900000
C	-2.747700000	-2.681100000	-0.430300000
C	-1.794400000	-2.884500000	-1.410600000
C	-1.999100000	-2.387400000	-2.685000000
S	-0.774800000	-2.528600000	-3.910200000
O	-0.018300000	-3.788800000	-3.523100000
O	-1.390600000	-2.625900000	-5.188200000
O	0.187700000	-1.424000000	-3.758100000
C	-2.994400000	-0.512900000	1.952300000
C	-2.361300000	-0.669400000	3.369200000
C	-3.099100000	0.926200000	1.443100000
C	-3.029100000	1.104700000	0.070500000
C	-2.877700000	2.350800000	-0.487500000
C	-3.108500000	2.062400000	2.248400000
C	-2.888100000	3.313600000	1.703900000
C	-2.731700000	3.448800000	0.333200000
S	-2.161400000	4.931400000	-0.353800000
O	-1.461400000	4.450100000	-1.649000000
O	-3.170900000	5.859000000	-0.713300000
O	-1.119200000	5.412500000	0.553000000
C	-0.826200000	-0.866100000	3.269500000
C	-0.181900000	-1.439500000	4.569000000
C	-0.095600000	0.374800000	2.783200000
C	0.046500000	1.520300000	3.563200000
C	0.736900000	2.619100000	3.088000000
C	0.494000000	0.344300000	1.528400000
C	1.203800000	1.423000000	1.056800000
C	1.302900000	2.566700000	1.824000000
S	2.165900000	3.898300000	1.151100000
O	3.145300000	3.383800000	0.232000000
O	1.141200000	4.533200000	0.124300000
O	2.489600000	4.851900000	2.154200000
C	0.105300000	-2.964600000	4.461900000
C	0.907200000	-3.447900000	5.688600000
C	0.833100000	-3.288600000	3.160900000
C	1.979200000	-2.600000000	2.787600000
C	2.539200000	-2.782600000	1.537000000
C	0.316700000	-4.237400000	2.284500000
C	0.887600000	-4.442500000	1.042900000
C	1.969200000	-3.674600000	0.649200000
S	2.601700000	-3.815600000	-0.971200000
O	3.840300000	-3.088900000	-1.006200000
O	2.576600000	-5.197500000	-1.350400000
O	1.565800000	-3.065500000	-1.802500000
Cu	1.911400000	-1.314800000	-2.527800000
O	-1.225600000	0.940000000	-2.384900000
O	1.010300000	0.234500000	-1.707400000
S	0.176600000	1.200000000	-2.406500000
O	0.659900000	1.189800000	-3.888700000
O	0.492600000	2.584100000	-1.955500000
Cu	1.807700000	3.972500000	-1.684000000
O	3.389200000	4.642600000	-5.503900000
C	3.030000000	3.638600000	-4.530300000
C	2.726600000	4.334400000	-3.273600000
C	2.733200000	5.346500000	-2.554800000
N	3.399400000	-0.765500000	-3.396400000
N	4.248600000	-0.187100000	-3.833200000
N	5.098500000	0.585900000	-4.305500000
C	6.419800000	-0.066100000	-4.613700000
H	-5.674300000	-2.256100000	0.451600000
H	-5.341700000	-0.588800000	0.073500000
H	-5.085100000	-0.869800000	2.435800000
H	-4.121200000	-2.310700000	2.249800000
H	-4.998600000	-0.954400000	-2.230300000

H	-3.043300000	0.459400000	-2.105000000
H	-1.404500000	-0.453400000	-3.651500000
H	-3.306600000	-3.292900000	-0.113600000
H	-1.651200000	-4.228000000	-1.663200000
H	1.249400000	-3.138500000	-2.216100000
H	-1.720900000	-1.008200000	1.285800000
H	-2.452600000	0.759100000	3.633000000
H	-2.711700000	-0.961500000	3.707500000
H	-3.752300000	2.114700000	1.819400000
H	-3.282800000	4.194900000	0.586500000
H	-0.343600000	0.308700000	0.006000000
H	0.113600000	2.389500000	-1.157800000
H	0.763700000	5.074900000	-0.299900000
H	-0.356700000	-1.314700000	2.985400000
H	-0.433200000	-0.093400000	5.737900000
H	-1.399400000	-1.482000000	5.329700000
H	1.713200000	-0.711000000	2.345400000
H	3.127500000	0.967700000	1.384000000
H	-0.832200000	2.305100000	3.931100000
H	0.521700000	4.002700000	2.815600000
H	3.802200000	1.680500000	-0.536700000
H	0.390700000	-2.561300000	6.194500000
H	2.743800000	-1.771800000	6.208100000
H	2.291600000	-0.404600000	5.187200000
H	1.633400000	-0.558500000	6.803200000
H	-0.916100000	-3.636700000	4.099000000
H	-0.582200000	-4.709900000	1.915100000
H	3.114200000	-2.272100000	4.021900000
H	3.458100000	-3.412000000	1.896900000
H	1.951300000	-2.431700000	-0.415200000
H	-1.087200000	2.858200000	-3.770700000
H	1.095500000	2.303900000	-5.478900000
H	0.296600000	3.848200000	-5.283700000
H	-0.825000000	0.600700000	-8.118400000
H	-0.768500000	-0.753400000	-6.965000000
H	-0.897400000	0.911100000	-6.371600000
H	-3.356400000	-1.392500000	-3.990300000
H	-2.569000000	-3.077100000	0.548500000
H	-0.887400000	-3.397400000	-1.173100000
H	0.470000000	0.327000000	-4.327600000
H	-2.297500000	-0.976000000	1.271800000
H	-2.602300000	0.155300000	4.025400000
H	-2.770000000	-1.562500000	3.830900000
H	-2.990600000	0.265600000	-0.581300000
H	-2.765900000	2.429600000	-1.543900000
H	-3.195400000	1.979500000	3.310100000
H	-2.777000000	4.165000000	2.344800000
H	-0.797000000	3.709700000	-1.692400000
H	-0.676200000	-1.610600000	2.503800000
H	0.752400000	-0.930300000	4.766800000
H	-0.826300000	-1.265200000	5.425100000
H	-0.380700000	1.555300000	4.545800000
H	0.850400000	3.499600000	3.687600000
H	0.417900000	-0.525700000	0.911300000
H	1.672500000	1.360500000	0.103700000
H	0.259700000	5.013900000	0.409400000
H	-0.844500000	-3.489300000	4.445800000
H	1.075700000	-4.516700000	5.637700000
H	1.870700000	-2.953300000	5.728900000
H	0.370500000	-3.227500000	6.605700000
H	2.419700000	-1.886300000	3.454300000
H	3.405900000	-2.232000000	1.235200000
H	-0.541800000	-4.813700000	2.571900000
H	0.498700000	-5.190200000	0.380100000
H	0.750400000	-3.673500000	-2.811700000
H	3.714100000	4.217000000	-6.309000000
H	2.165300000	3.069400000	-4.847700000
H	3.843600000	2.940600000	-4.368600000
H	3.032800000	6.340100000	-2.364000000
H	7.135600000	0.737000000	-4.676200000
H	6.714900000	-0.761900000	-3.839000000
H	6.368900000	-0.578400000	-5.566000000

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symmetry c1

C	2.290900000	-0.021600000	3.833300000
C	2.922600000	-0.829900000	2.645400000
C	1.481600000	1.180900000	3.366400000
C	0.119900000	1.274300000	3.613400000
C	-0.631300000	2.302400000	3.073100000
C	2.097400000	2.189300000	2.630100000
C	1.361200000	3.226100000	2.096700000
C	-0.010200000	3.259700000	2.292900000
S	-0.953600000	4.486200000	1.510400000
O	-2.248300000	4.537600000	2.108300000
O	-0.162700000	5.657400000	1.335100000
O	-1.190900000	3.846100000	0.088800000
C	2.283900000	-2.222300000	2.411300000
C	3.094400000	-3.151500000	1.433200000
C	0.791900000	-2.172700000	2.093100000
C	-0.014300000	-3.264000000	2.403100000
C	-1.365700000	-3.264700000	2.109000000
C	0.203600000	-1.070500000	1.495600000
C	-1.130500000	-1.064400000	1.193300000
C	-1.913500000	-2.152400000	1.505100000
S	-3.601900000	-2.043900000	1.120500000
O	-3.506700000	-1.279700000	-0.248400000
O	-4.139000000	-3.349400000	0.938300000
O	-4.247500000	-1.129900000	2.013000000
C	3.345600000	-2.842600000	-0.085500000
C	4.254000000	-1.605000000	-0.305400000
C	2.060900000	-2.833400000	-0.906600000
C	1.386300000	-1.659600000	-1.181400000
C	0.209700000	-1.660200000	-1.896900000
C	1.538900000	-4.023800000	-1.406600000
C	0.362300000	-4.038000000	-2.132800000
C	-0.310700000	-2.849600000	-2.361900000
S	-1.847700000	-2.856200000	-3.173200000
O	-2.885900000	-2.663600000	-2.160800000
O	-1.818800000	-1.603700000	-4.022400000
O	-1.957800000	-4.043600000	-3.949000000
C	4.615300000	-1.295000000	-1.802500000
C	6.141900000	-1.331000000	-2.029000000
C	4.022100000	0.055200000	-2.196600000
C	3.016200000	0.134600000	-3.144500000
C	2.298800000	1.304200000	-3.328500000
C	4.392700000	1.219700000	-1.525900000
C	3.705400000	2.396700000	-1.724000000
C	2.619300000	2.423000000	-2.587300000
S	1.616800000	3.841700000	-2.604000000

O	0.744300000	3.731300000	-1.442300000
O	2.427100000	5.008100000	-2.668600000
O	0.760500000	3.685200000	-3.849500000
Cu	-2.815800000	2.897400000	-0.310100000
O	-2.865200000	2.690700000	-2.266600000
O	-1.332200000	1.088800000	-1.417700000
S	-1.995900000	1.576000000	-2.661700000
O	-0.995700000	1.973200000	-3.649700000
O	-2.824400000	0.457200000	-3.163400000
Cu	-2.771700000	0.634900000	-0.224900000
O	-7.013700000	1.164100000	-1.329700000
C	-5.621600000	1.523200000	-1.309000000
C	-5.283900000	1.579500000	0.144700000
C	-6.108900000	1.378500000	1.194900000
N	-4.033900000	1.834300000	0.641300000
N	-4.080600000	1.798500000	1.971900000
N	-5.333800000	1.525200000	2.296700000
C	-5.661300000	1.227900000	3.696500000
H	1.661300000	-0.671500000	4.427900000
H	3.088600000	0.330500000	4.478300000
H	2.872700000	-0.230300000	1.752500000
H	3.974200000	-0.992400000	2.853700000
H	-0.367800000	0.516100000	4.191700000
H	-1.690500000	2.348300000	3.223900000
H	3.155900000	2.155200000	2.461200000
H	1.833100000	3.996600000	1.521900000
H	-0.413900000	3.864600000	-0.589300000
H	2.363600000	-2.742000000	3.363500000
H	4.075700000	-3.278700000	1.884400000
H	2.613900000	-4.123400000	1.472500000
H	0.418800000	-4.127000000	2.870200000
H	-1.979400000	-4.115300000	2.325100000
H	0.780900000	-0.214200000	1.238000000
H	-1.592300000	-0.280600000	0.665100000
H	-3.306000000	-1.856000000	-1.111700000
H	3.917300000	-3.701100000	-0.430000000
H	3.795200000	-0.732100000	0.121900000
H	5.169900000	-1.779500000	0.250500000
H	1.770400000	-0.724600000	-0.843000000
H	-0.294100000	-0.732300000	-2.050600000
H	2.057500000	-4.946900000	-1.233600000
H	-0.031600000	-4.952200000	-2.527000000
H	-2.315700000	-0.699700000	-3.730000000
H	4.163200000	-2.050000000	-2.433000000
H	6.378400000	-1.121500000	-3.065100000
H	6.643800000	-0.596900000	-1.409500000
H	6.535200000	-2.310700000	-1.778800000
H	2.733800000	-0.739200000	-3.694800000
H	1.469800000	1.320800000	-4.003200000
H	5.201700000	1.199300000	-0.822900000
H	3.990400000	3.288300000	-1.201800000
H	-0.067200000	3.049400000	-3.821200000
H	-7.311600000	0.967700000	-2.226200000
H	-5.000200000	0.792300000	-1.808500000
H	-5.443400000	2.481100000	-1.776900000
H	-5.422800000	0.190600000	3.870000000
H	-5.066900000	1.871700000	4.323600000
H	-6.710700000	1.417300000	3.855100000
H	-7.141100000	1.141300000	1.217200000