Electronic supplementary materials *Mendeleev Commun.*, 2026, **36**, 107–109

Instability of thermoplastics as a key feature in catalyst preparation

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Experimental details

General information. All reagents except azides were purchased from commercial sources and were checked by NMR before use. Initial azides were synthesized according to published procedure.[S1] Briefly, NaN_3 (2.2 mmol) was dissolved in DMSO (4.4 ml). Then corresponding alkyl or benzyl bromide (2 mmol) was added. Completion of the reaction was monitored by TLC. After the reaction completed (~1-3 h), water (10 ml) was added to the reaction solution. Target azide was extracted with diethyl ether (3 × 10 ml). The organic layer was dried over Na_2SO_4. The solvent was evaporated *in vacuo*.

3D printing of catalytic sleeve. Materials for 3D printing were purchased from commercial sources. Sleeves were manufactured using the FFF method with a Picaso Designer X-Pro desktop 3D printer. Printing was performed with PLA, PETG and ABS with a primary filament diameter of 1.75 mm. Printing was carried out at a layer height of 0.25 mm using a 0.5 mm nozzle. Extrusion multiplier 0.95 was used. Printing with raft was performed for better adhesion to the printing bed. Printing temperatures are indicated in Table S1.

Table S1. 3D printing parameters

Material	Nozzle temperature, °C	Bed temperature, °C	Cooling intensity, %
PLA	220	60	40
PETG	240	80	30
ABS	230	100	0

Preparation of catalytic stir bar. Two sleeves were fixed on magnetic stir bar (3 × 6 mm). Obtained stir bar was immersed in suspension of CuI (50 mg) in DMF (1 ml) for 1 h. Then the stir bar was dried with paper and left *in vacuo* overnight.

Synthesis of triazoles. DMSO was saturated with acetylene at room temperature. Catalytic stir bar, pre-saturated DMSO (1 ml), triethylamine (0.2 mmol, 28 μl) and corresponding azide (0.5 mmol) were added into the screw-capped tube. The tube was immediately closed and heated at 30 °C for 24 hours. After the reaction, the mixture was diluted with a deuterated solvent, and the yield was measured by ^{1}H NMR using TMSPh as an internal standard. Then, the solvent was evaporated on a rotary evaporator and the product was purified by flash chromatography on silica gel 60 (0.015-0.40 mm) with hexane/ethyl acetate gradient elution. The organic layer was dried over Na_2SO_4. The solvent was evaporated *in vacuo*.

In case of purification of products **1** and **5**, the solvent was evaporated. Obtained mixture was dissolved in methylene chloride, filtered, and washed with disodium EDTA water solution. Then obtained solution was dried over Na_2SO_4. After solvent evaporation *in vacuo* , the pure products were obtained.

SEM/EDX studies. Target-oriented approach was utilized for the optimization of the analytic measurements. Before measurements, the samples were mounted on a 32 mm aluminum specimen stub and fixed by a carbon conductive plasticine. The samples was coated with a thin film (30 nm) of carbon. The observations were carried out using a Hitachi Regulus 8230 field-emission scanning electron microscope (FE-SEM). Images were acquired in a secondary electron mode at a 3 kV accelerating voltage and at a working distance of 8-10 mm. EDX-SEM

studies were carried out using an Bruker Quantax 400 system with detector XFlash 6|60 at a 20 kV accelerating voltage and at a working distance of 15 mm.

NMR-spectroscopy. NMR spectra were recorded on Bruker Fourier 300 HD (Bruker BioSpin AG, Switzerland) at 300.1 MHz for ^{1}H and 75.5 MHz for ^{13}C. Chemical shifts δ are given in ppm using residual protons of deuterated solvent as internal standards: acetone-d_6 (^{1}H, δ = 2.05 ppm; ^{13}C, δ = 29.84 ppm), $CDCl_3$ (^{1}H, δ = 7.26 ppm; ^{13}C, δ = 77.16 ppm).

Mass-spectrometry. High-resolution mass spectra were recorded on Bruker maXis Q-TOF instrument (Bruker Daltonik GmbH, Bremen, Germany) equipped with electrospray ionization (ESI) ion source in positive ion mode (HV capillary at 4.5 kV with spray shield offset at -0.5 kV) with scan range of m/z 50–1500. External calibration of the mass spectrometer was performed using low-concentration tuning mix solution (Agilent Technologies). Direct syringe injection was applied for the analyzed solutions in MeCN (flow rate: 5 μL/min). Nitrogen was used as both nebulizing gas (0.4 bar) and dry gas (4.0 L /min, 200 °C). All spectra were recorded at 1 Hz frequency and processed using Bruker Data Analysis 4.0 software.

GC-MS analysis. GC-MS experiments were carried out with an Agilent 7890A GC system, equipped with an Agilent 5975C mass-selective detector (electron impact, 70 eV) and a HP-5MS column (30 m × 0.25 mm × 0.25 mm) using He as carrier gas at a flow of 1.0 mL min^{-1}.

Characterization of obtained compounds. 1-(Phenylmethyl)-1*H*-1,2,3-triazole (**1**). White solid. ^{1}H NMR (300.1 MHz, acetone-d_6) δ 7.97 (d, *J* = 0.7 Hz, 1H), 7.67 (s, 1H), 7.52 – 7.19 (m, 5H), 5.65 (s, 2H). ^{13}C NMR (75.5 MHz, acetone-d_6) δ 136.34, 133.42, 128.76, 128.13, 127.88, 124.06, 53.04 137.22, 134.30, 129.65, 129.02, 128.76, 124.94, 53.92. HRMS (ESI-TOF): *m/z* calculated for [M+nH]$^{+}$: 160.0869, found 160.0869 (Δ = 0 ppm).

1-[[4-*tert*-Butylphenyl]methyl]-1*H*-1,2,3-triazole (**2**). White solid. ^{1}H NMR (300.1 MHz, acetone-d_6) δ 7.95 (d, *J* = 1.0 Hz, 1H), 7.66 (d, *J* = 1.0 Hz, 1H), 7.51 – 7.33 (m, 2H), 7.32 – 7.22 (m, 2H), 5.61 (s, 2H), 1.29 (s, 9H). ^{13}C NMR (75.5 MHz, acetone-d_6) δ 151.91, 134.24, 128.58, 126.50, 124.83, 53.63, 35.08, 31.54. HRMS (ESI-TOF): *m/z* calculated for [M+nH]$^{+}$: 216.1495, found 216.1499 (Δ = 1,85 ppm).

1-[(2-Bromophenyl)methyl]-1*H*-1,2,3-triazole (**3**). White solid. ^{1}H NMR (300.1 MHz, acetone-d_6) δ 8.01 (s, 1H), 7.71 (s, 1H), 7.68 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.35 (dtd, *J* = 26.8, 7.5, 1.6 Hz, 2H), 7.12 (dd, *J* = 7.6, 1.9 Hz, 1H), 5.76 (s, 2H). ^{13}C NMR (75.5 MHz, acetone-d_6) δ 136.29, 134.21, 133.88, 131.09, 131.01, 129.09, 125.48, 123.71, 53.88. HRMS (ESI-TOF): *m/z* calculated for [M+nH]$^{+}$: 237.9974, found 237.9980 (Δ = 2,52 ppm).

1-Octyl-1*H*-1,2,3-triazole (**4**). Yellow oil. ^{1}H NMR (300.1 MHz, chloroform-*d*) δ 7.69 (s, 1H), 7.52 (s, 1H), 4.37 (t, *J* = 7.2 Hz, 2H), 1.99 – 1.84 (m, 2H), 1.61 – 1.12 (m, 10H), 0.86 (t, *J* = 6.5 Hz, 3H). ^{13}C NMR (75.5 MHz, chloroform-*d*) δ 133.88, 123.21, 50.32, 31.81, 30.46, 29.16, 29.07, 26.59, 22.71, 14.18. HRMS (ESI-TOF): *m/z* calculated for [M+nH]$^{+}$: 182.1652, found 182.1656 (Δ = 2,20 ppm).

Ethyl 1*H*-1,2,3-triazole-1-butanoate (**5**). Brown oil. ^{1}H NMR (300.1 MHz, chloroform-d) δ 7.69 (d, J = 1.0 Hz, 1H), 7.56 (d, J = 1.0 Hz, 1H), 4.46 (t, J = 6.7 Hz, 2H), 4.12 (q, J = 7.1 Hz, 2H), 2.39 – 2.29 (m, 2H), 2.24 (q, J = 6.5 Hz, 2H), 1.24 (t, J = 7.2 Hz, 3H). ^{13}C NMR (75.5 MHz, $CDCl_3$) δ 172.45, 134.02, 123.60, 60.85, 49.18, 30.79, 25.62, 14.29. HRMS (ESI-TOF): *m/z* calculated for [M+nH]$^{+}$: 184.1081, found 184.1080 (Δ = 0,54 ppm).

1,1′-[(1,3-Phenylene)bis(methylene)]bis[1*H*-1,2,3-triazole] (**6**). Yellow solid. ^{1}H NMR (300.1 MHz, acetone-d_6) δ 7.97 (d, *J* = 1.0 Hz, 2H), 7.66 (d, *J* = 1.0 Hz, 2H), 7.45 – 7.23 (m, 4H), 5.66 (s, 4H). ^{13}C NMR (75.5 MHz,

acetone) δ 137.92, 134.33, 130.21, 128.60, 128.34, 125.03, 53.66. HRMS (ESI-TOF): *m/z* calculated for $[M+nH]^+$: 241.1196, found 241.1204. (Δ = 3,32 ppm).

1,1′-(1,8-Octanediyl)bis[1*H*-1,2,3-triazole] (**7**). White solid. ^{1}H NMR (300.1 MHz, chloroform-*d*) δ 7.61 (d, J = 1.0 Hz, 2H), 7.51 (d, J = 1.0 Hz, 2H), 4.30 (t, J = 7.2 Hz, 4H), 1.93 – 1.63 (m, 4H), 1.33 – 1.05 (m, 8H). ^{13}C NMR (75.5 MHz, chloroform-*d*) δ 133.68, 123.24,49.99, 30.13, 28.57, 26.15. HRMS (ESI-TOF): *m/z* calculated for [M+nH]+: 249.1822, found 249.1826 (Δ = 1,61 ppm).

Mass-spectra of solvents after sleeve immersion

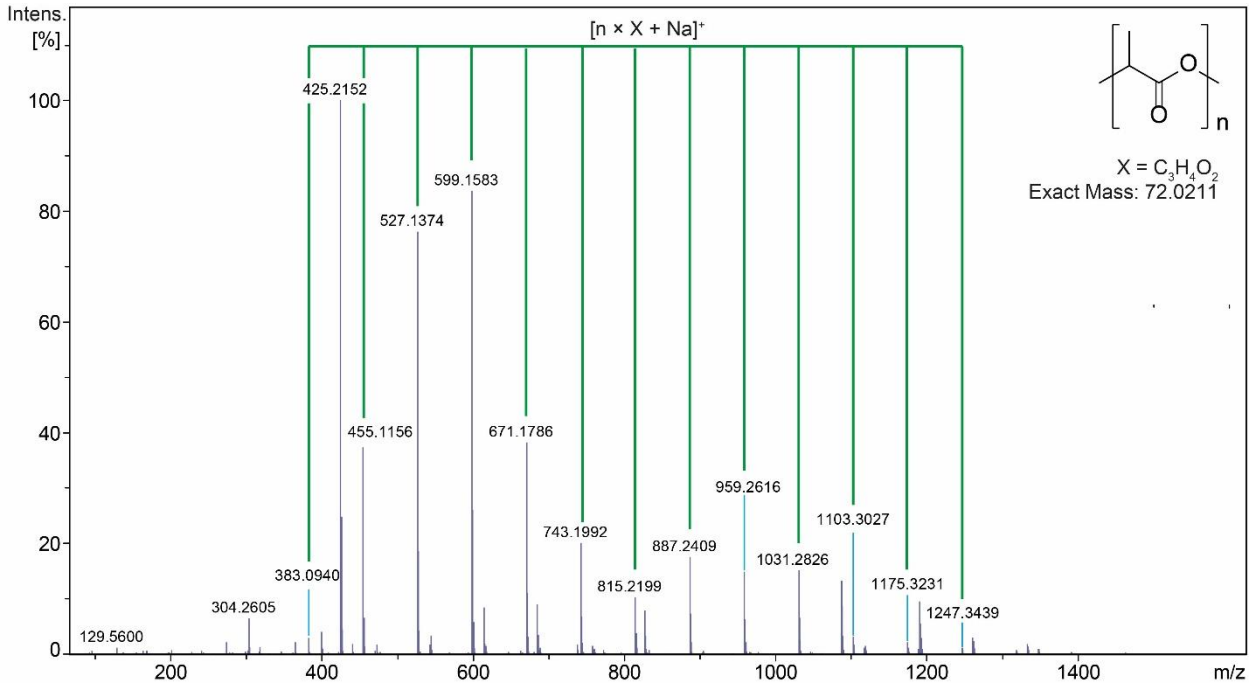

Figure S1. ESI-MS spectra of DMF after PLA immersion for 1 h.

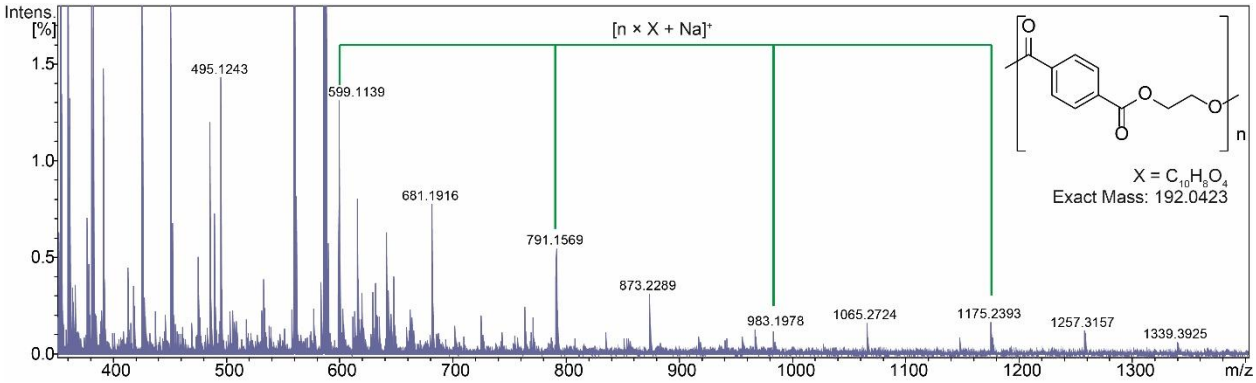

Figure S2. ESI-MS spectra of DMF after PETG immersion for 1 h.

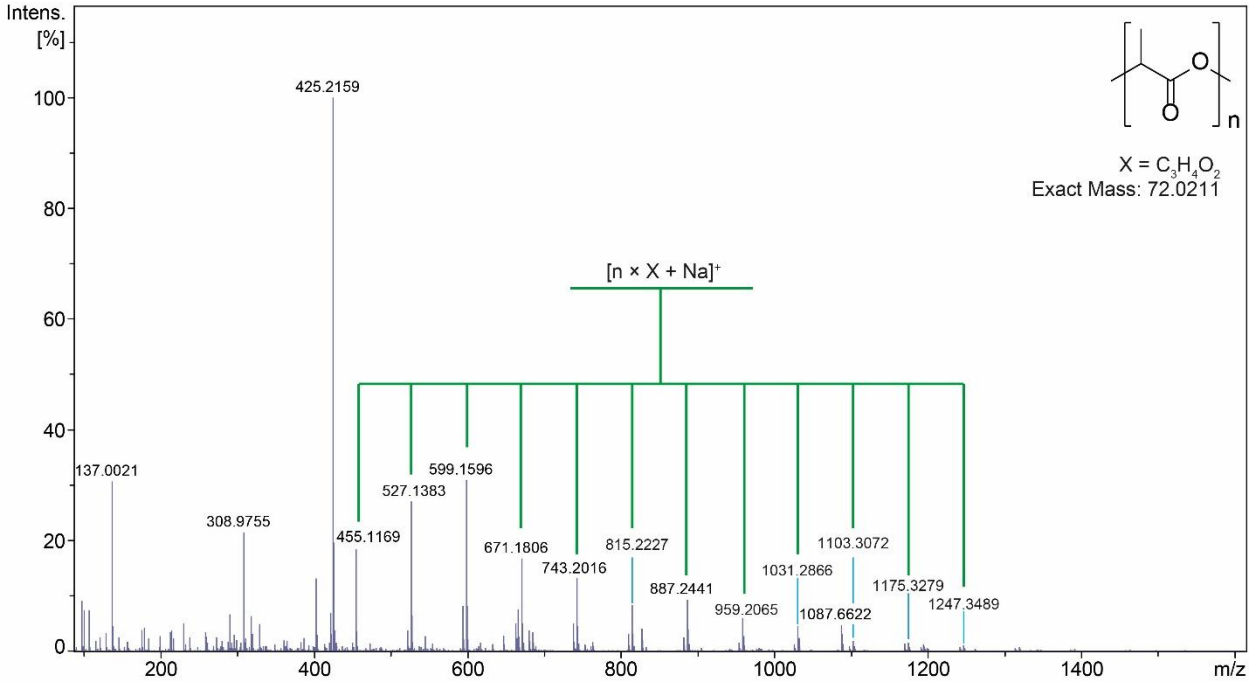

Figure S3. ESI-MS spectra of DMSO after PLA immersion for 1 h.

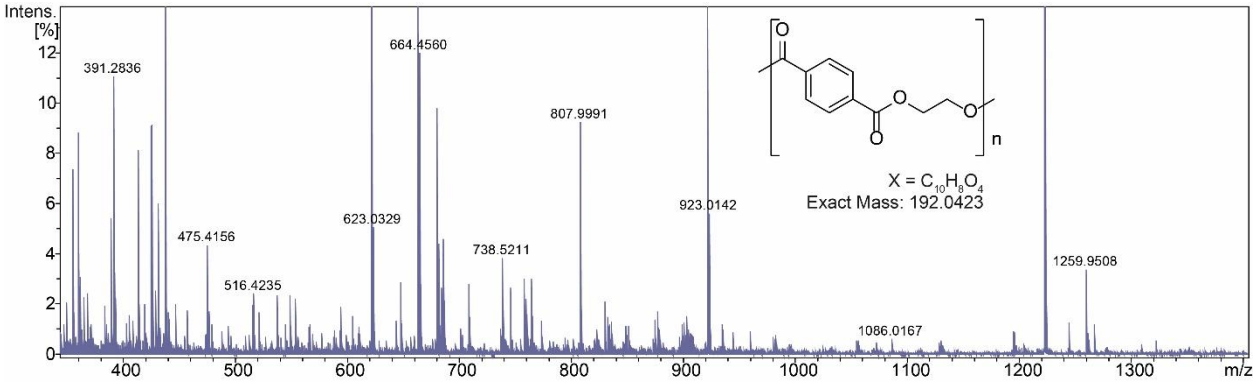

Figure S4. ESI-MS spectra of DMSO after PETG immersion for 1 h.

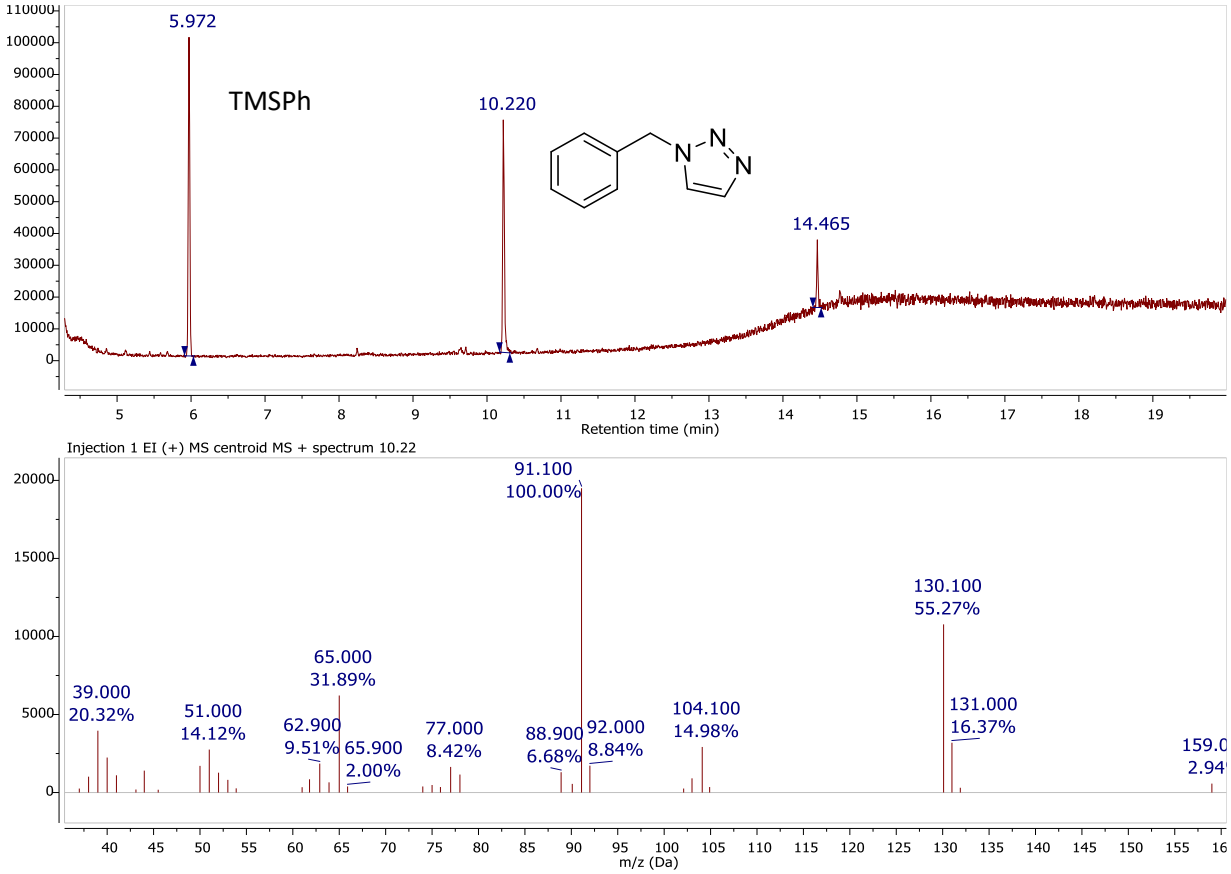

Figure S5. GC-MS of solution of catalytic stir bar after the 1'st cycle of click-reaction.

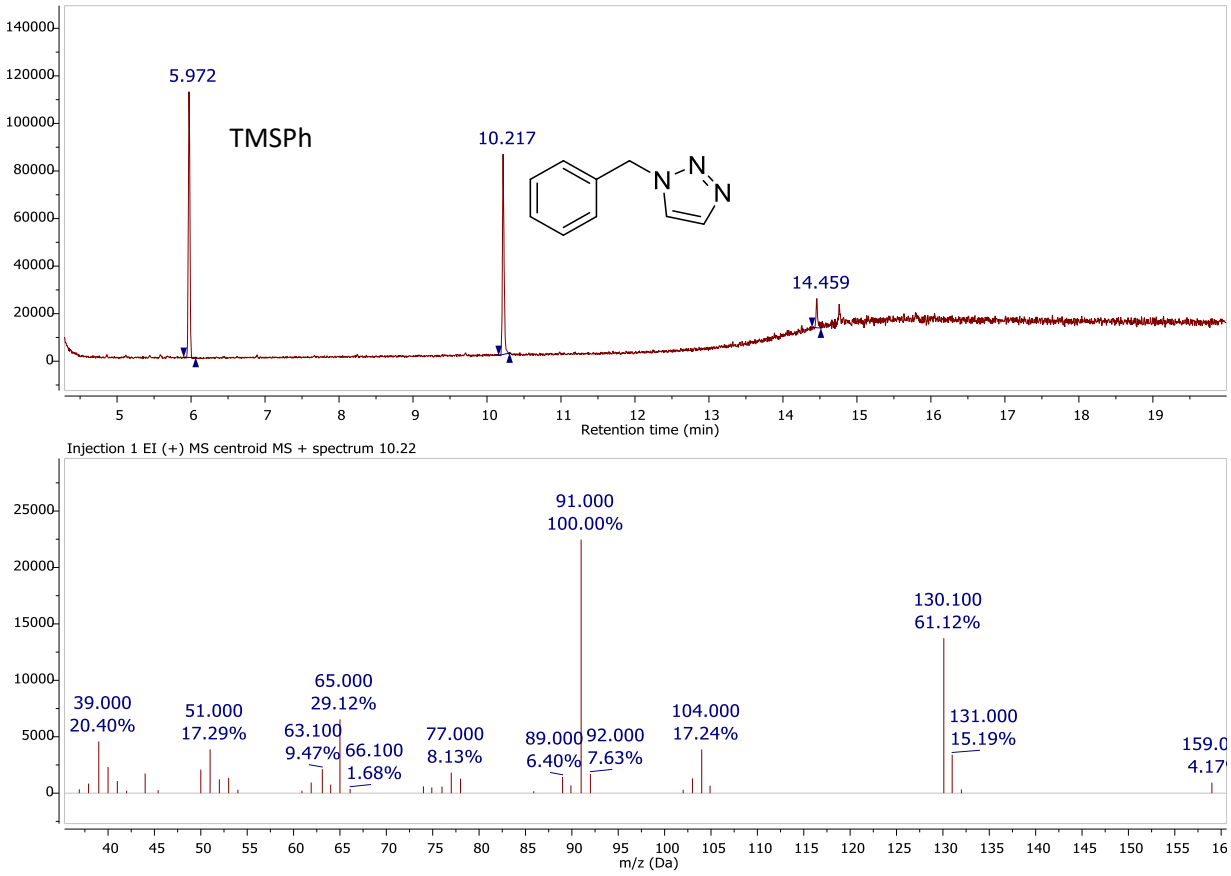

Figure S6. GC-MS of solution of catalytic stir bar after the 2'nd cycle of click-reaction.

EDX analysis of the sleeves

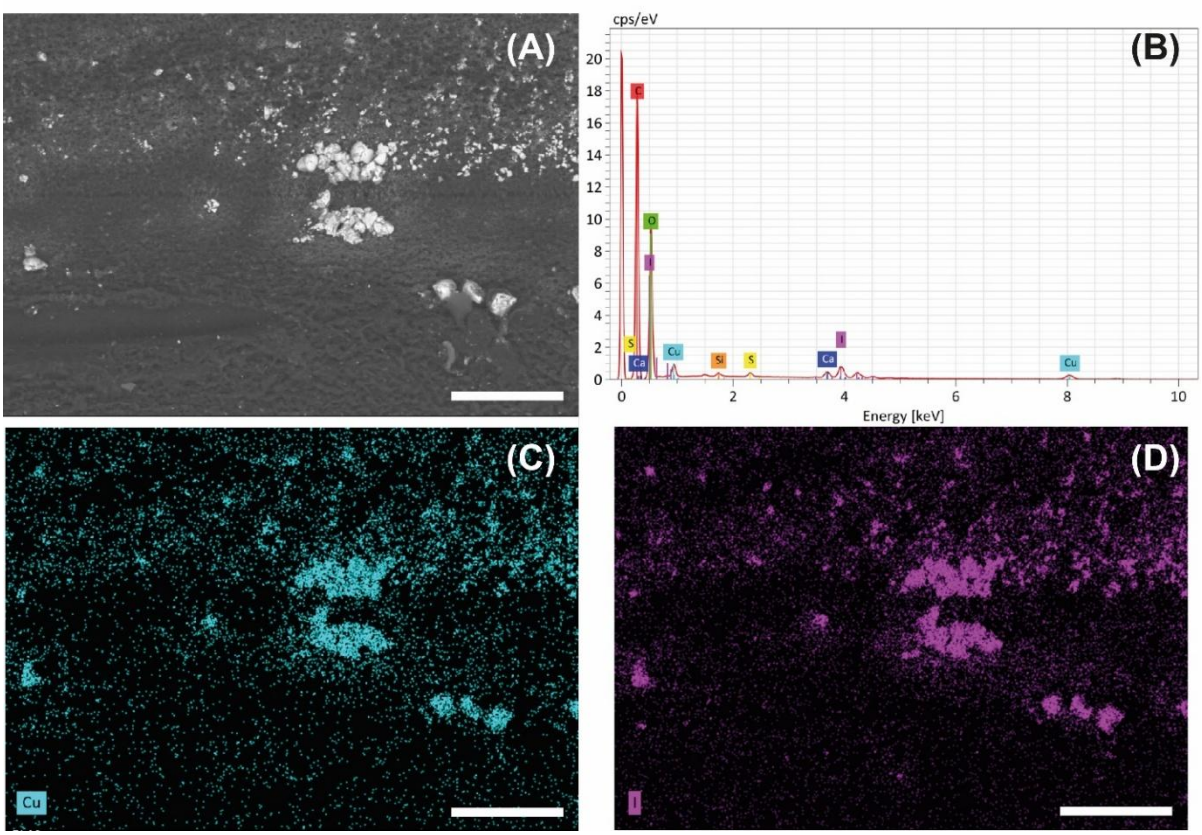

Figure S7. EDX analysis of CuI-PLA 3D printed sleeve: A – SEM image; B – EDX spectrum; C and D – distribution maps for Cu and I, respectively. Scale bar corresponds to 100 µm.

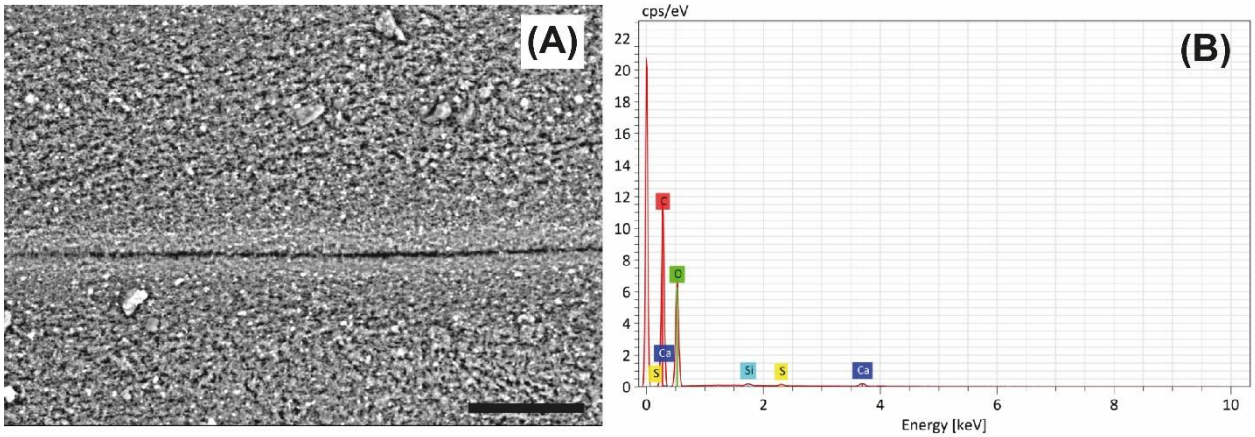

Figure S8. EDX analysis of CuI-PLA 3D printed sleeve after the reaction: A – SEM image; B – EDX spectrum. Scale bar corresponds to 100 µm.

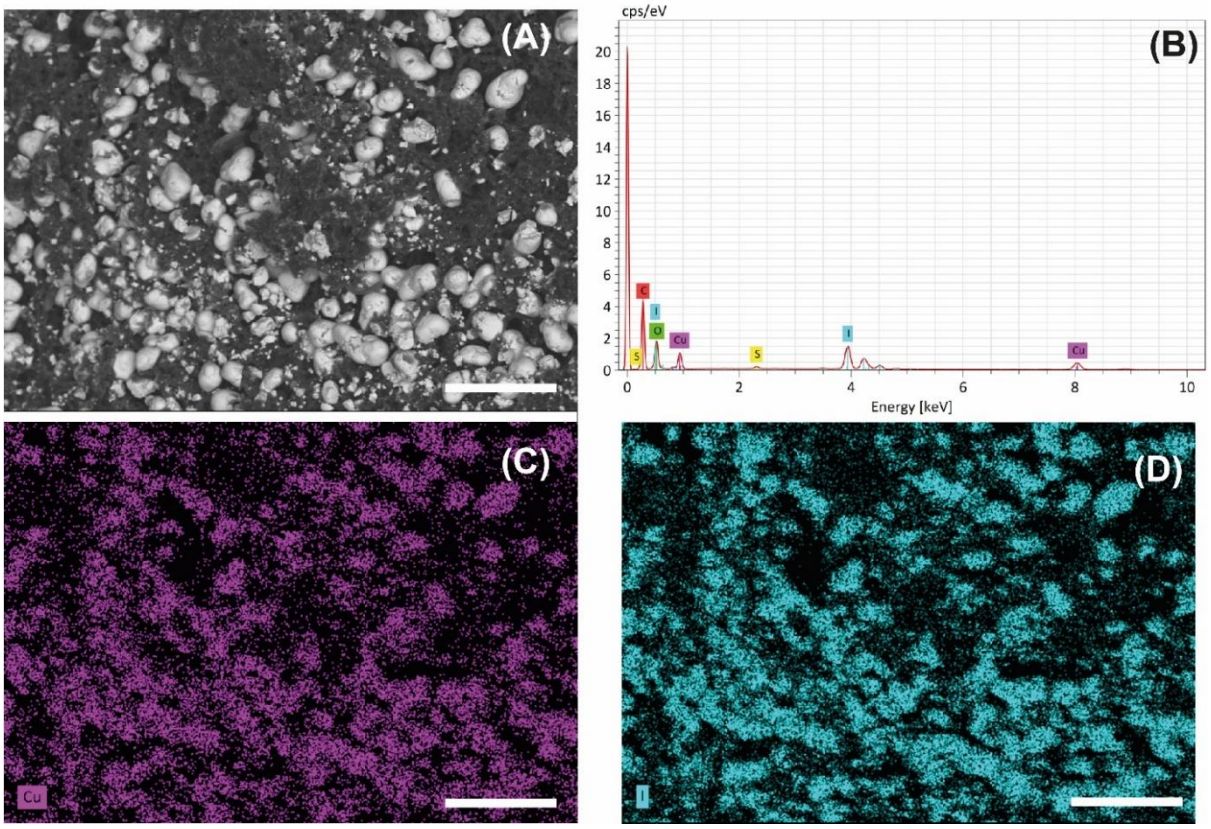

Figure S9. EDX analysis of CuI-PETG 3D printed sleeve: A – SEM image; B – EDX spectrum; C and D – distribution maps for Cu and I, respectively. Scale bar corresponds to 100 μm.

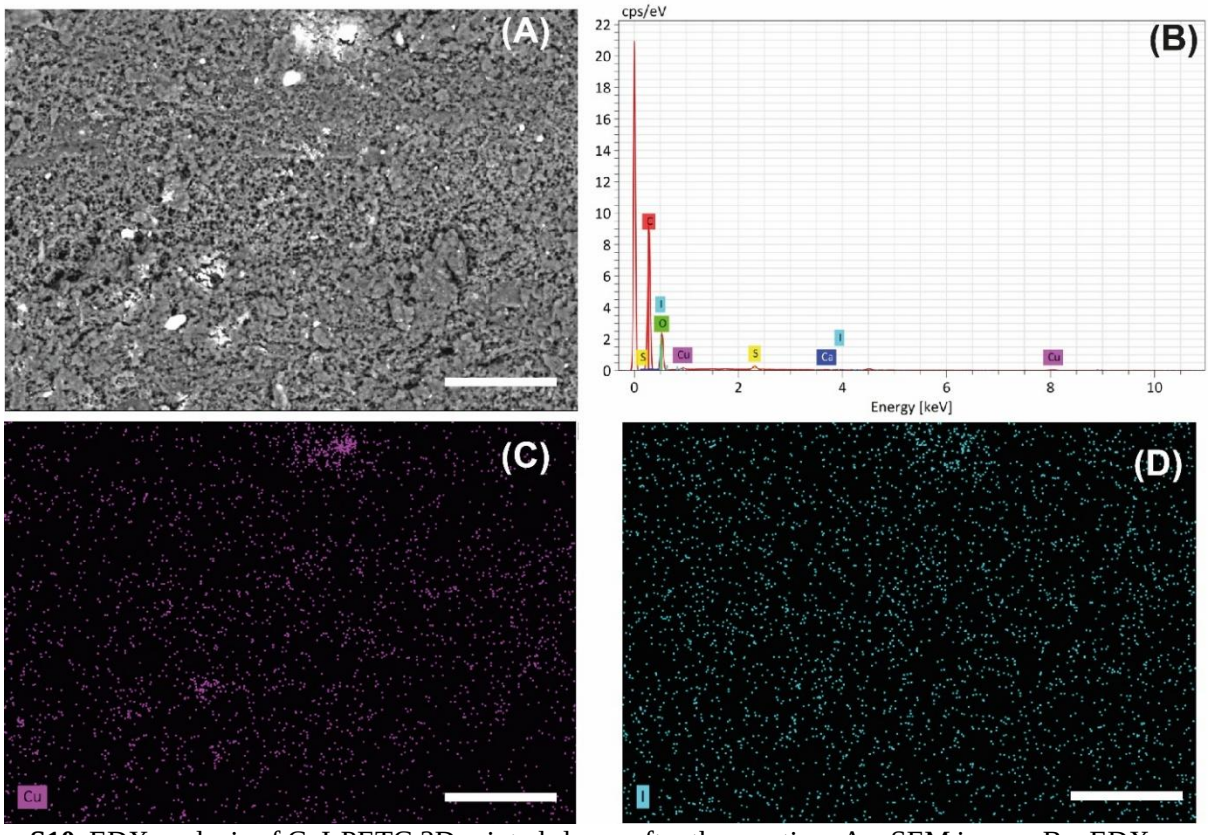

Figure S10. EDX analysis of CuI-PETG 3D printed sleeve after the reaction: A – SEM image; B – EDX spectrum; C and D – distribution maps for Cu and I, respectively. Scale bar corresponds to 100 μm.

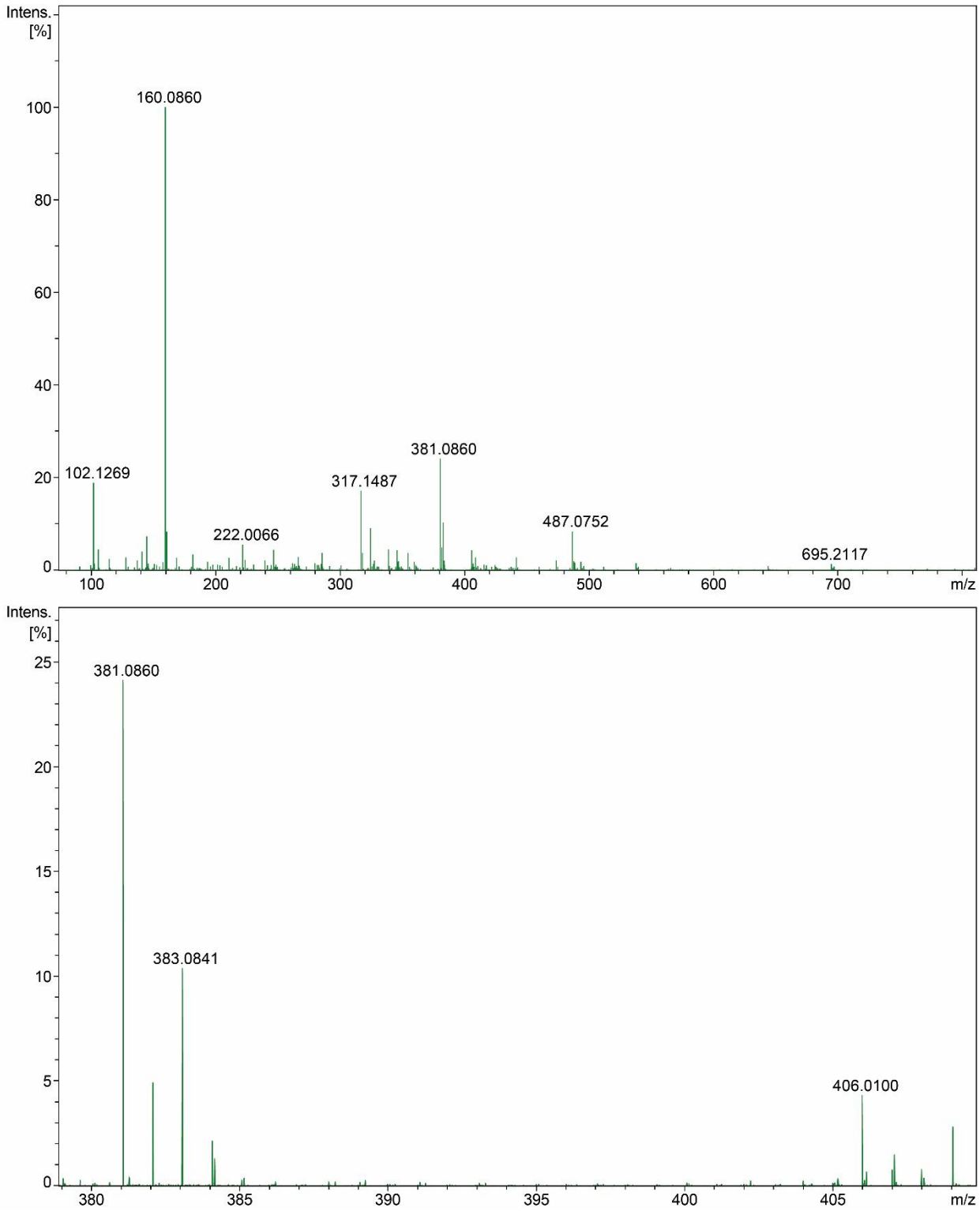

Figure S11. ESI-MS spectrum of reaction solution after the 1'st cycle. Cu containing compound is observed.

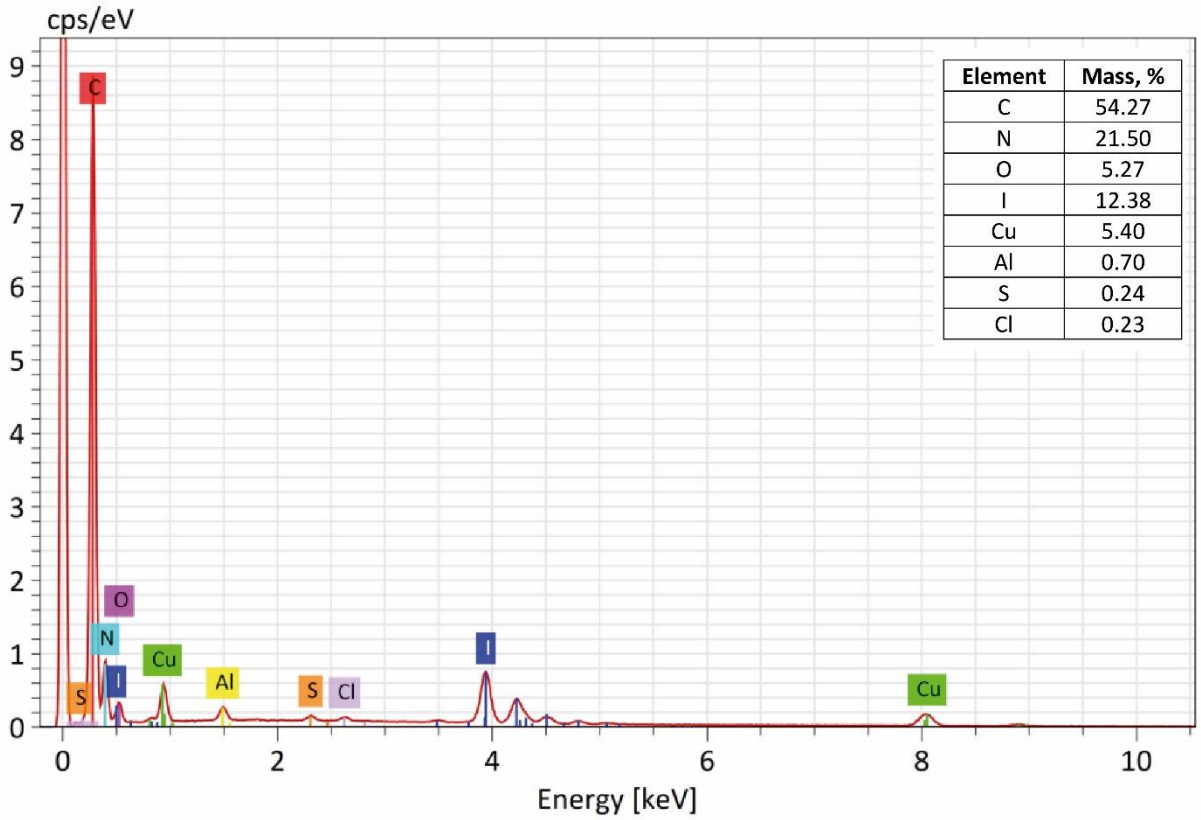

Figure S12. EDX spectrum of reaction mixture after the 1'st cycle after the solvent evaporation.

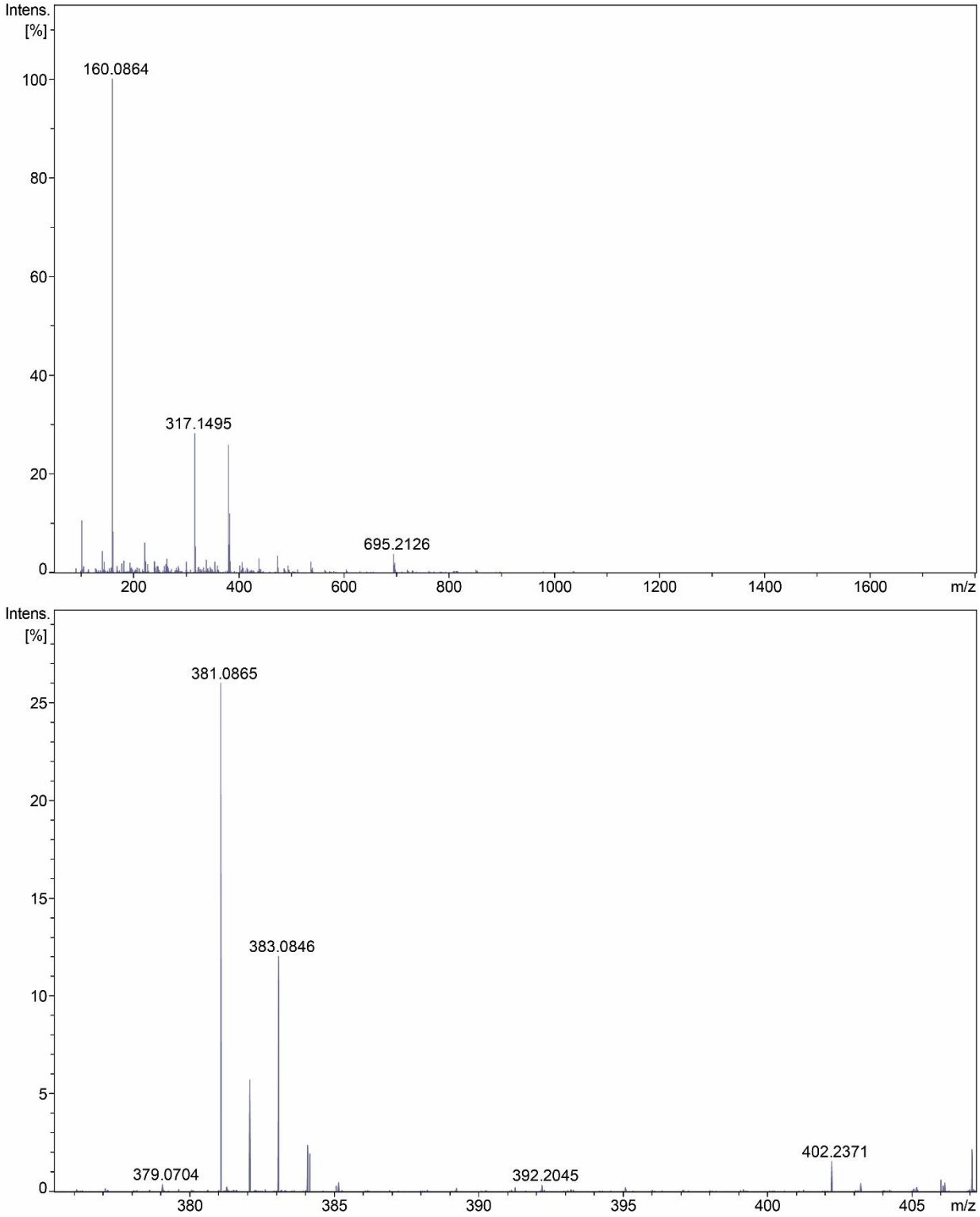

Figure S13. ESI-MS spectrum of reaction solution after the 2'nd cycle. Cu containing compound is observed.

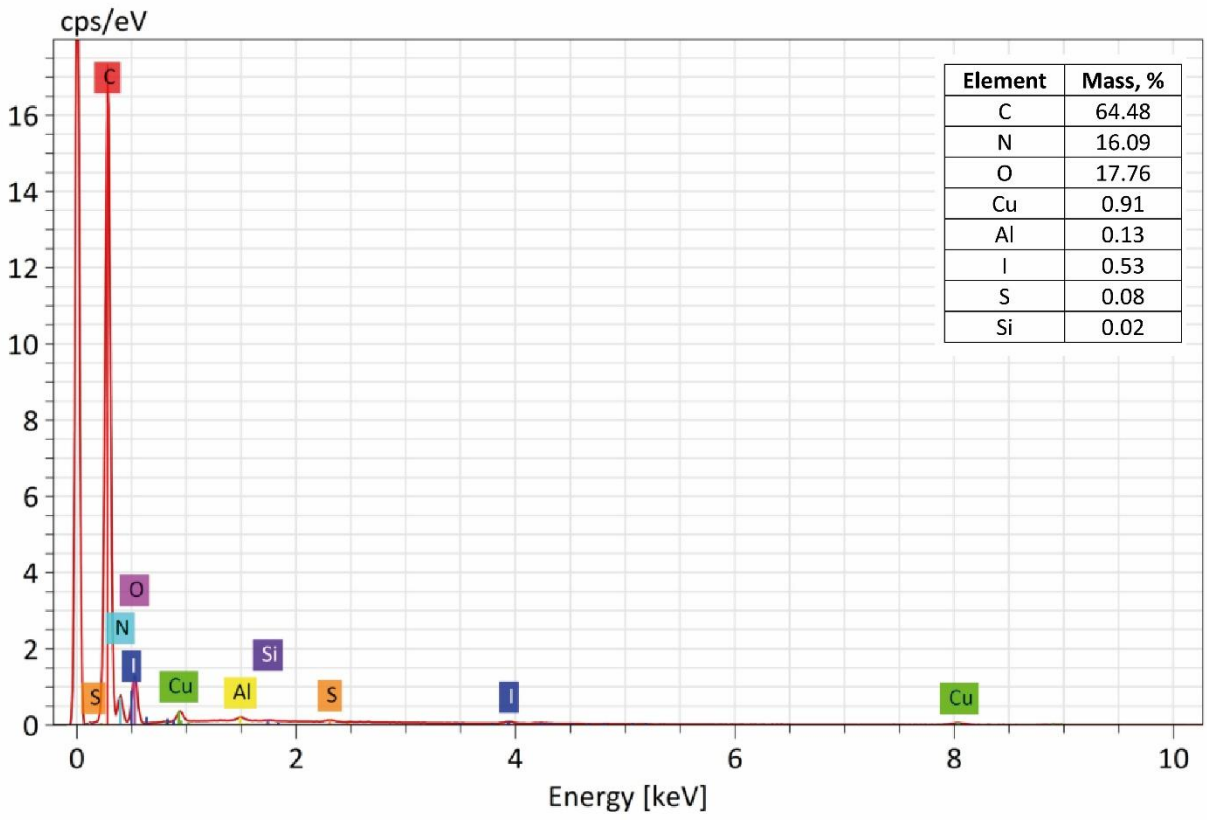

Figure S14. EDX spectrum of reaction mixture after the 2'nd cycle after the solvent evaporation.

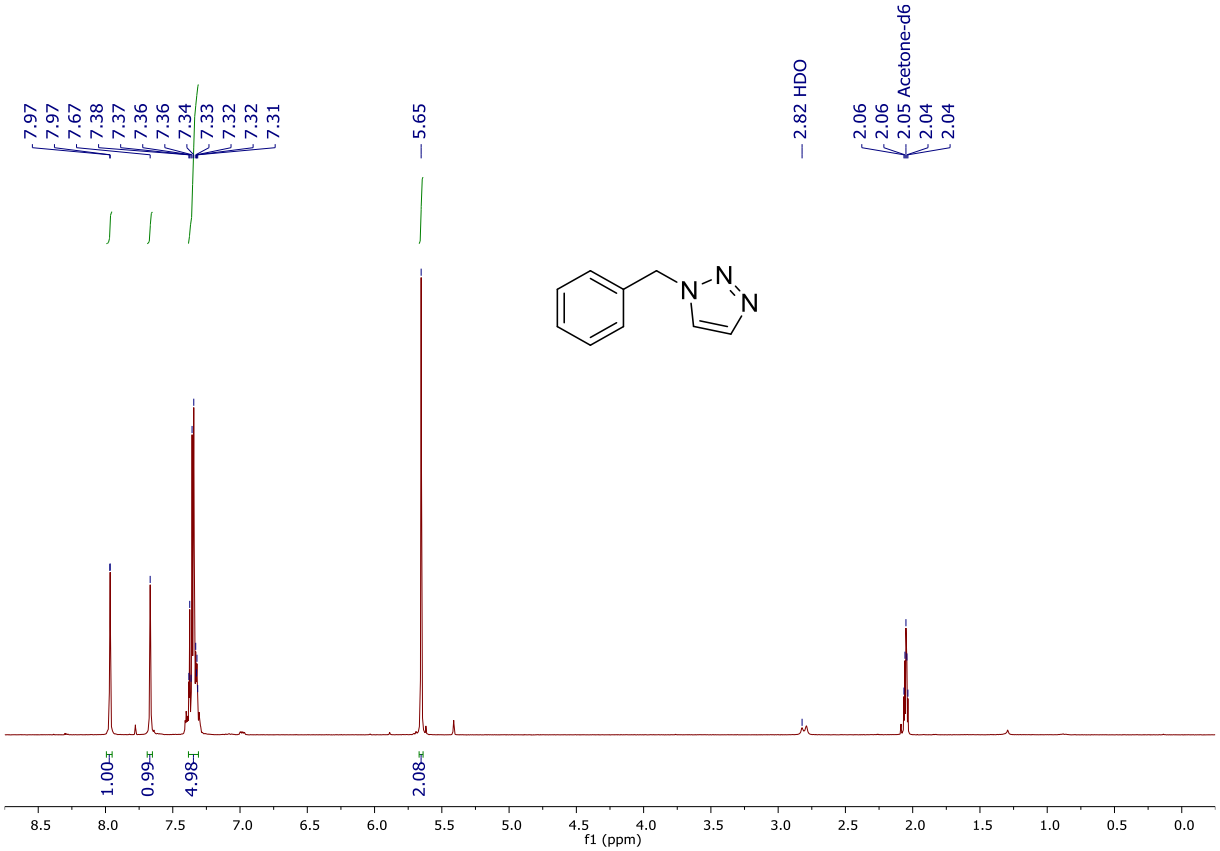

Figure S15. ^{1}H NMR spectrum of **1**.

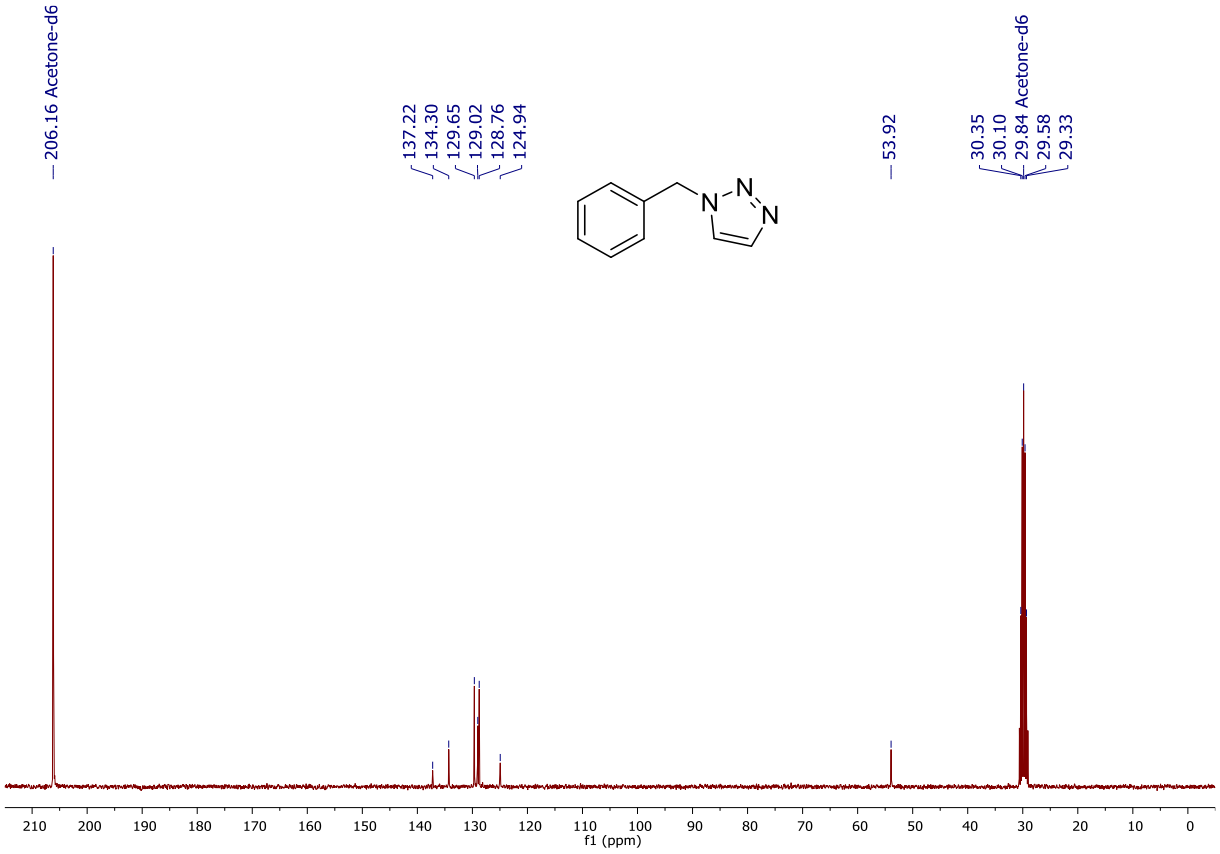

Figure S16. ^{13}C {^{1}H} NMR spectrum of **1**.

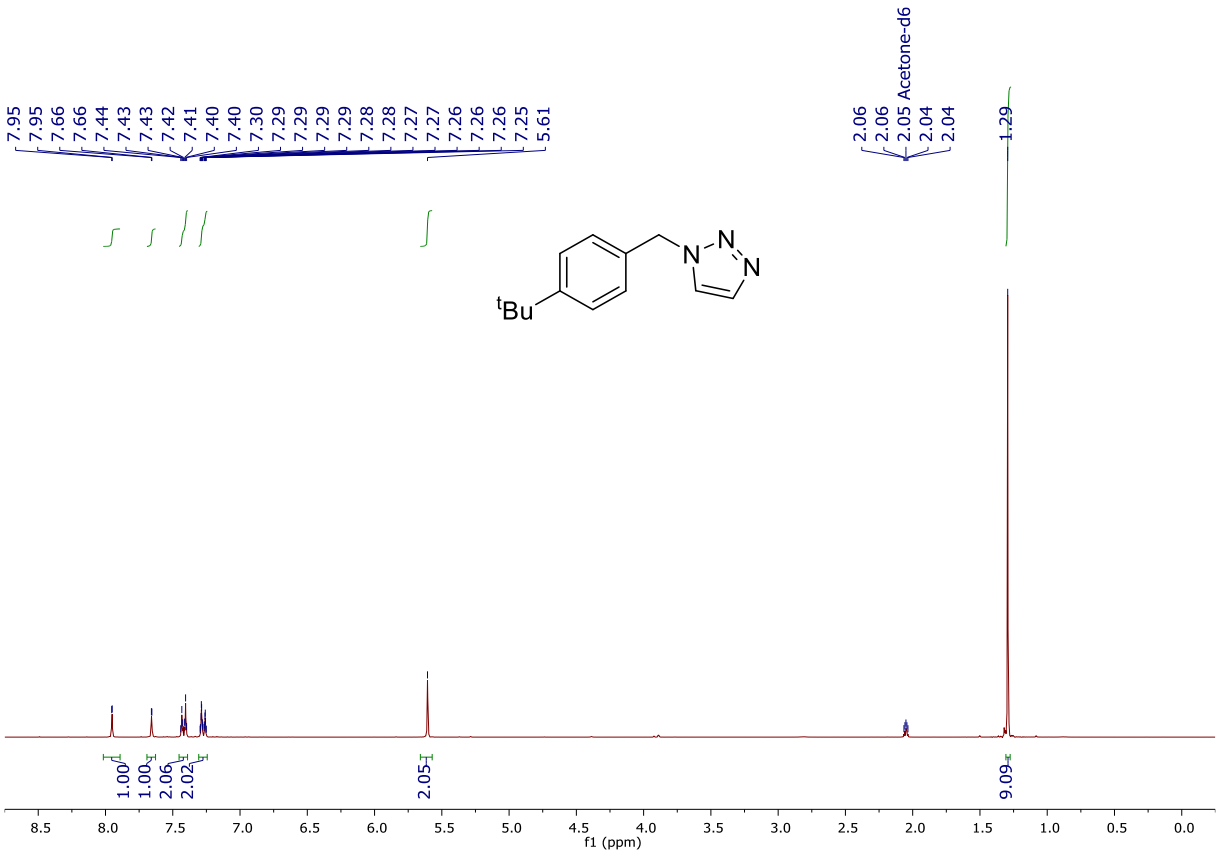

Figure S17. ^{1}H NMR spectrum of **2**.

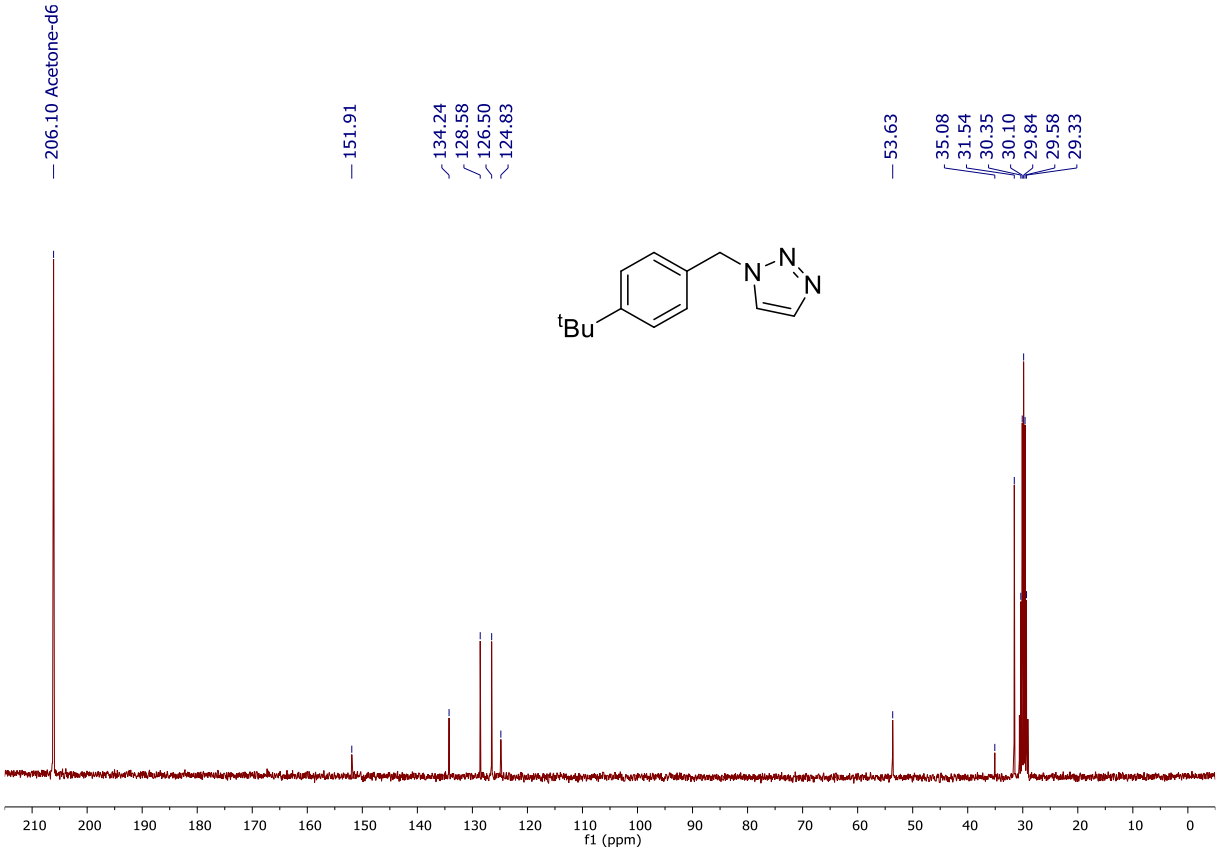

Figure S18. ^{13}C {^{1}H} NMR spectrum of **2**.

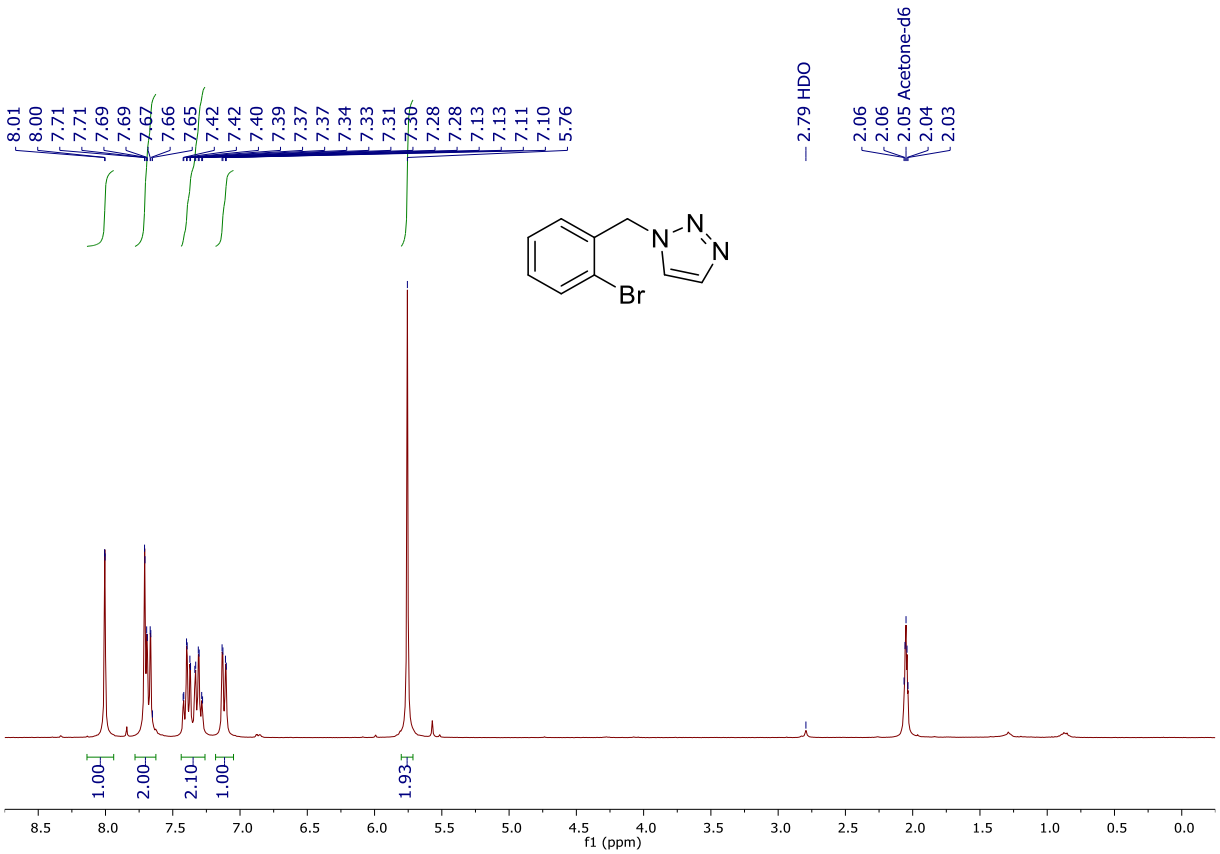

Figure S19. ^{1}H NMR spectrum of **3**.

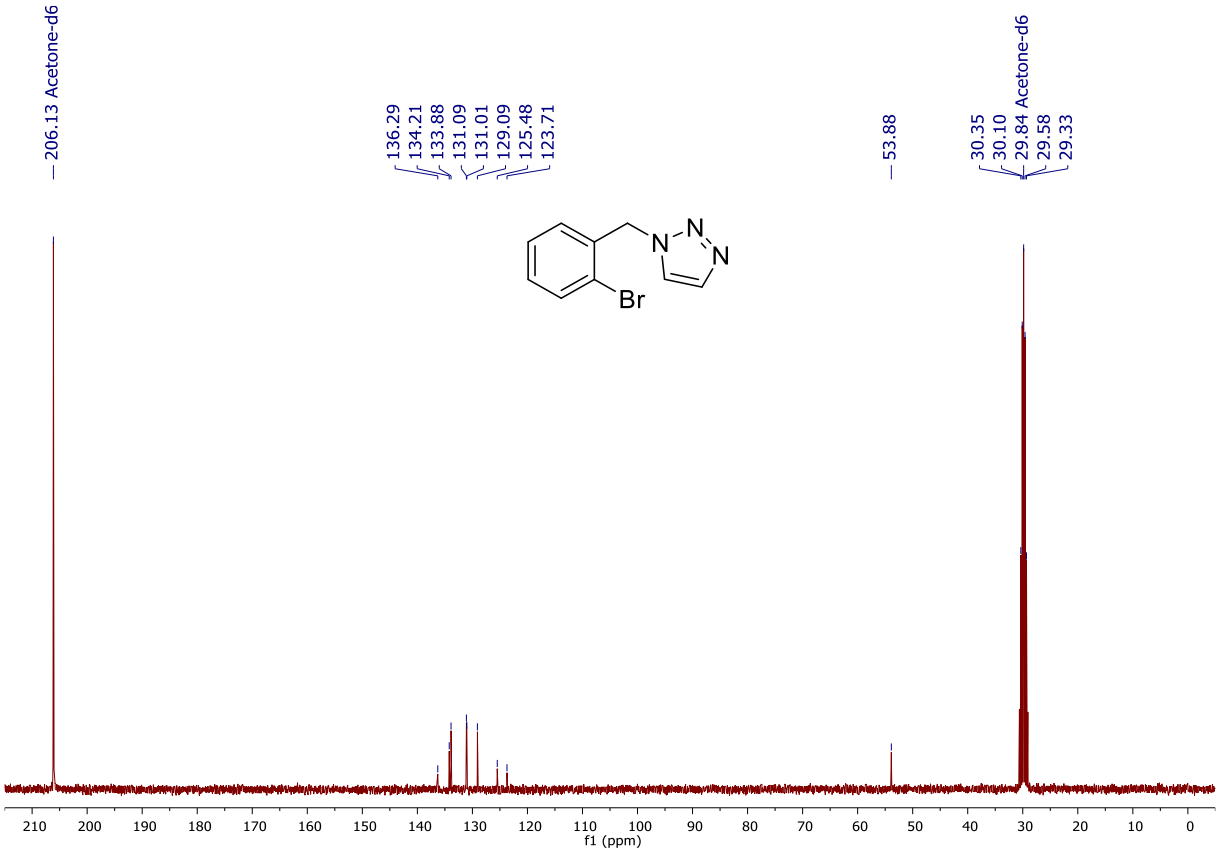

Figure S20. ^{13}C {^{1}H} NMR spectrum of **3**.

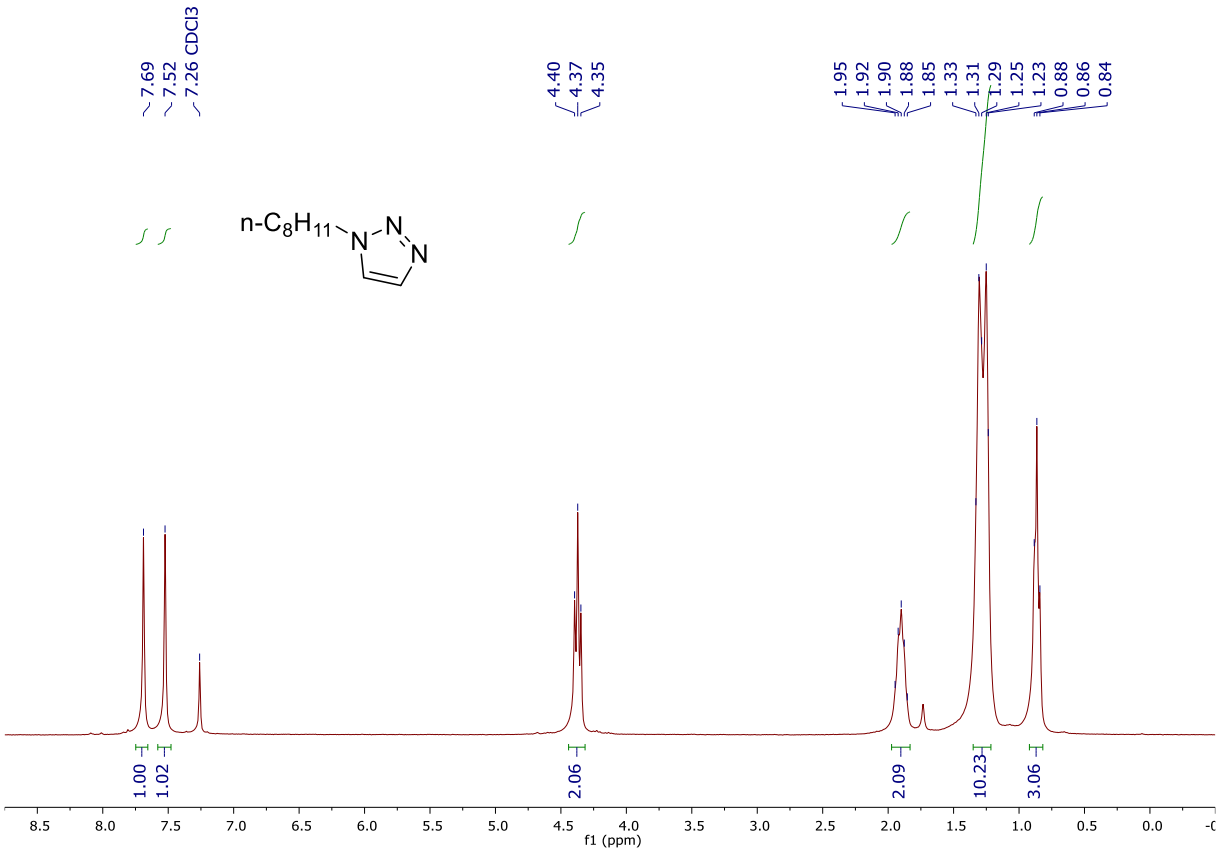

Figure S21. ^{1}H NMR spectrum of **4**.

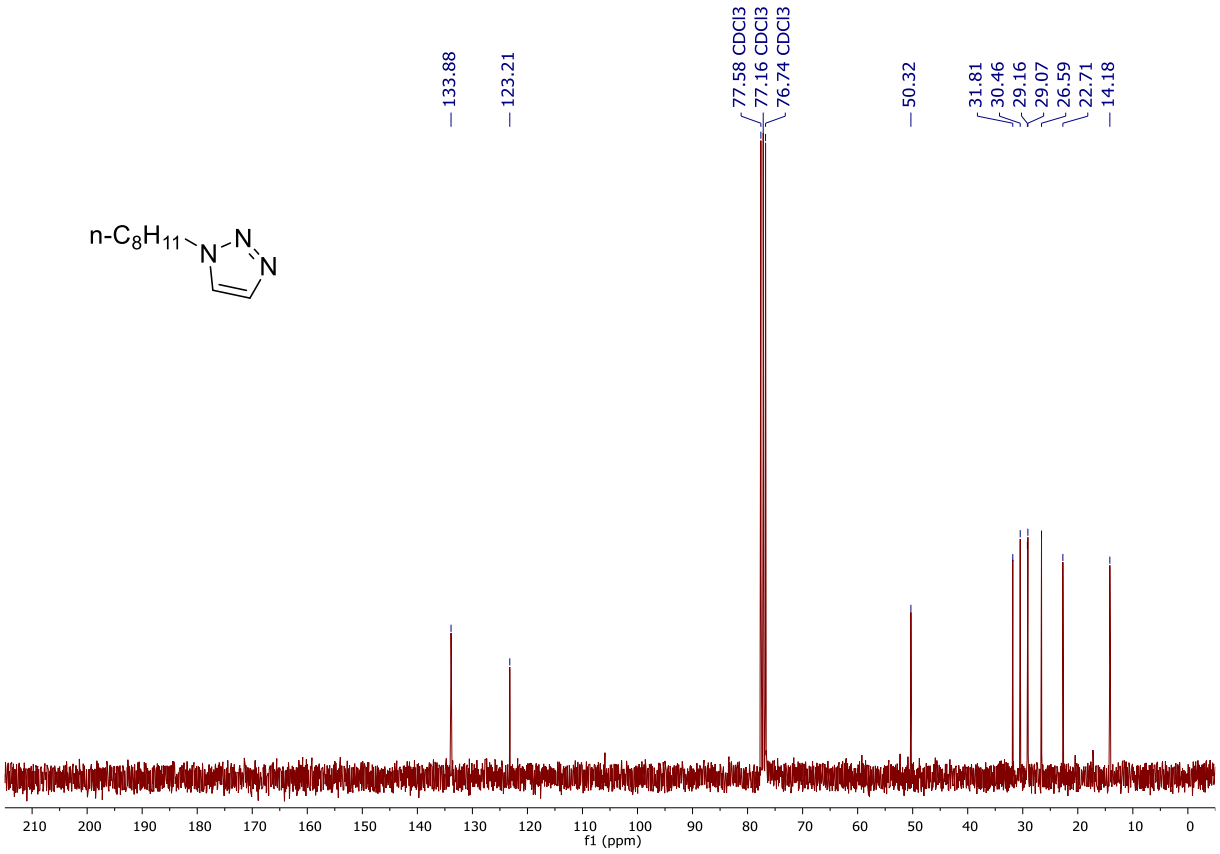

Figure S22. ^{13}C {^{1}H} NMR spectrum of **4**.

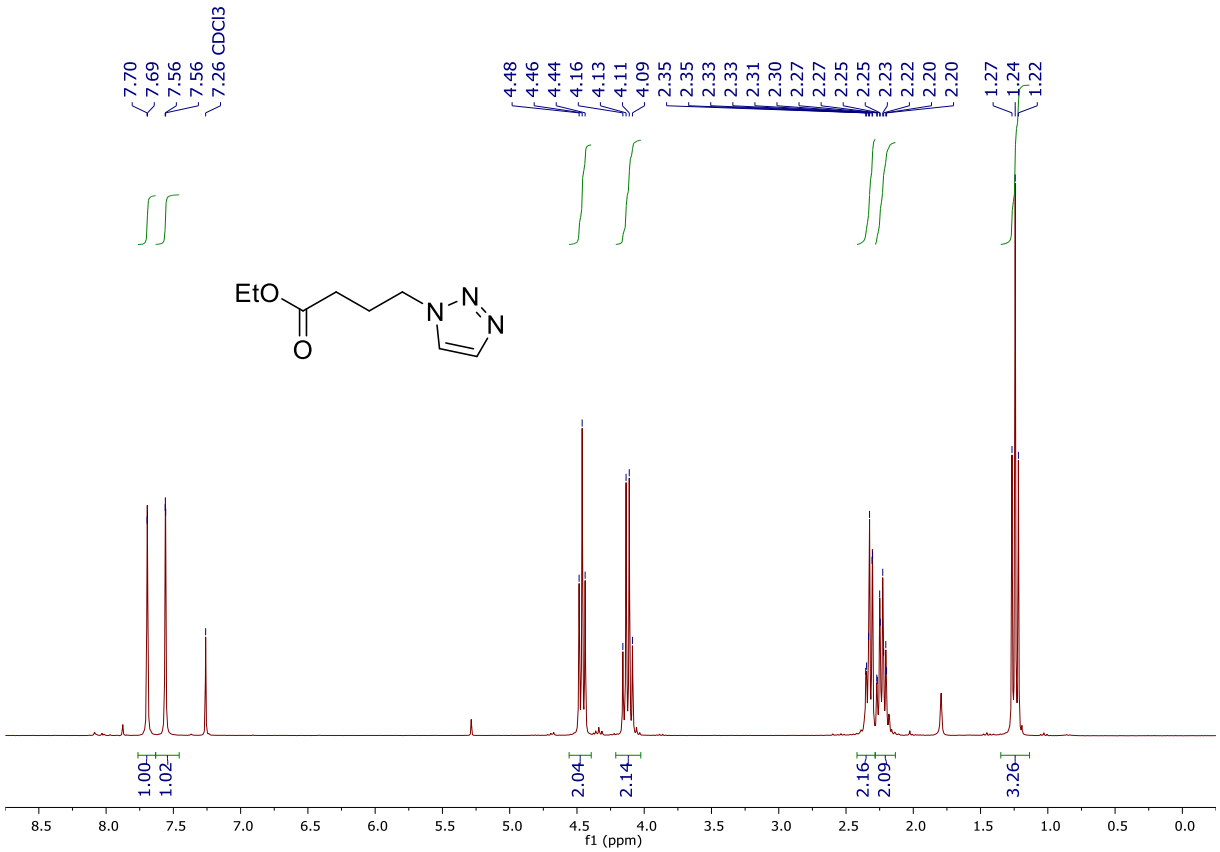

Figure S23. ^{1}H NMR spectrum of **5**.

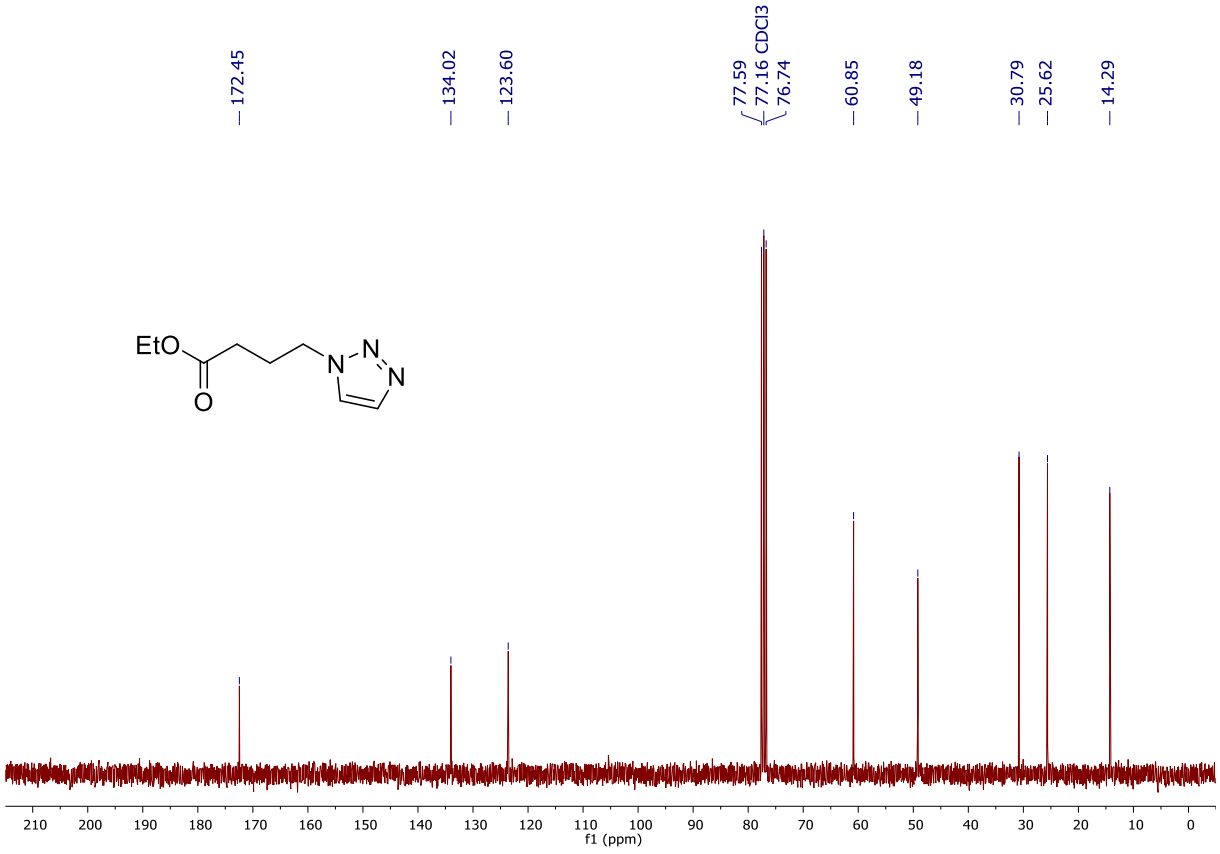

Figure S24. ^{13}C {^{1}H} NMR spectrum of **5**.

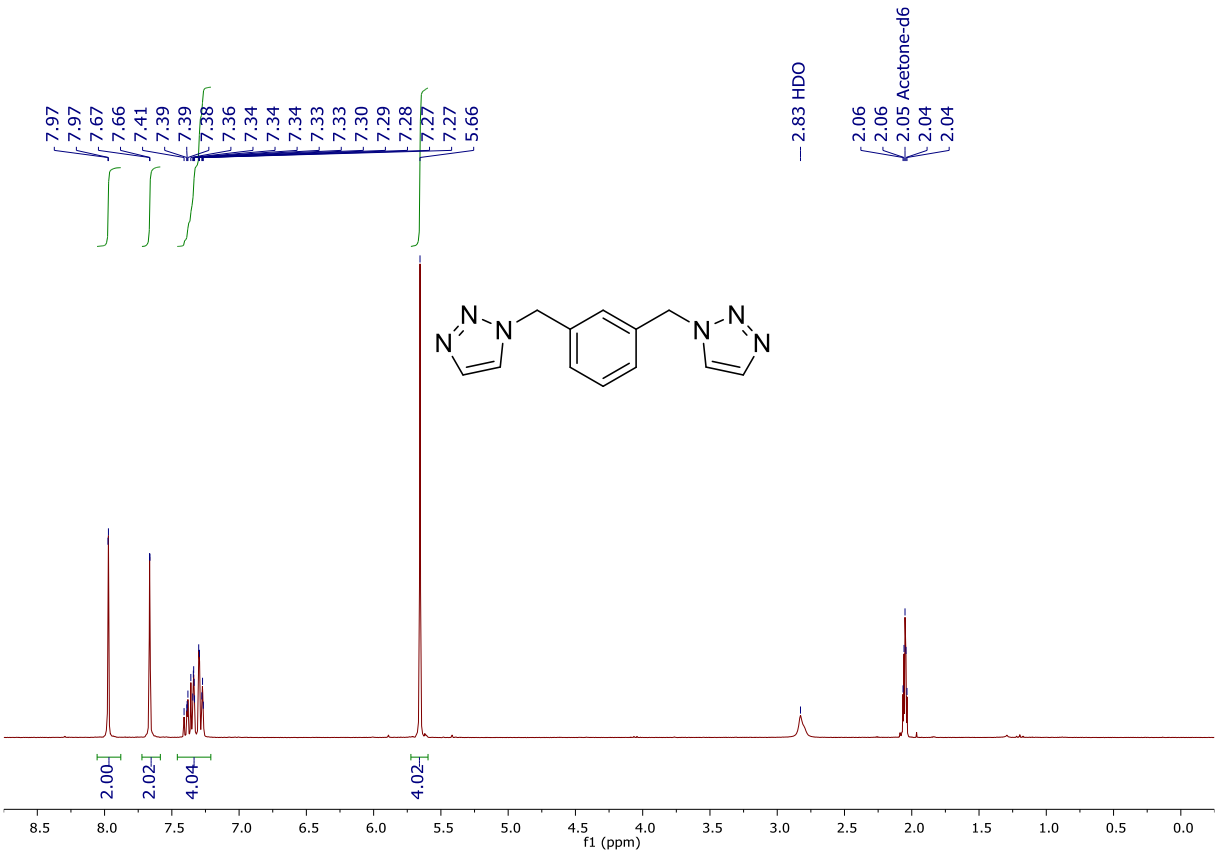

Figure S25. ^{1}H NMR spectrum of **6**.

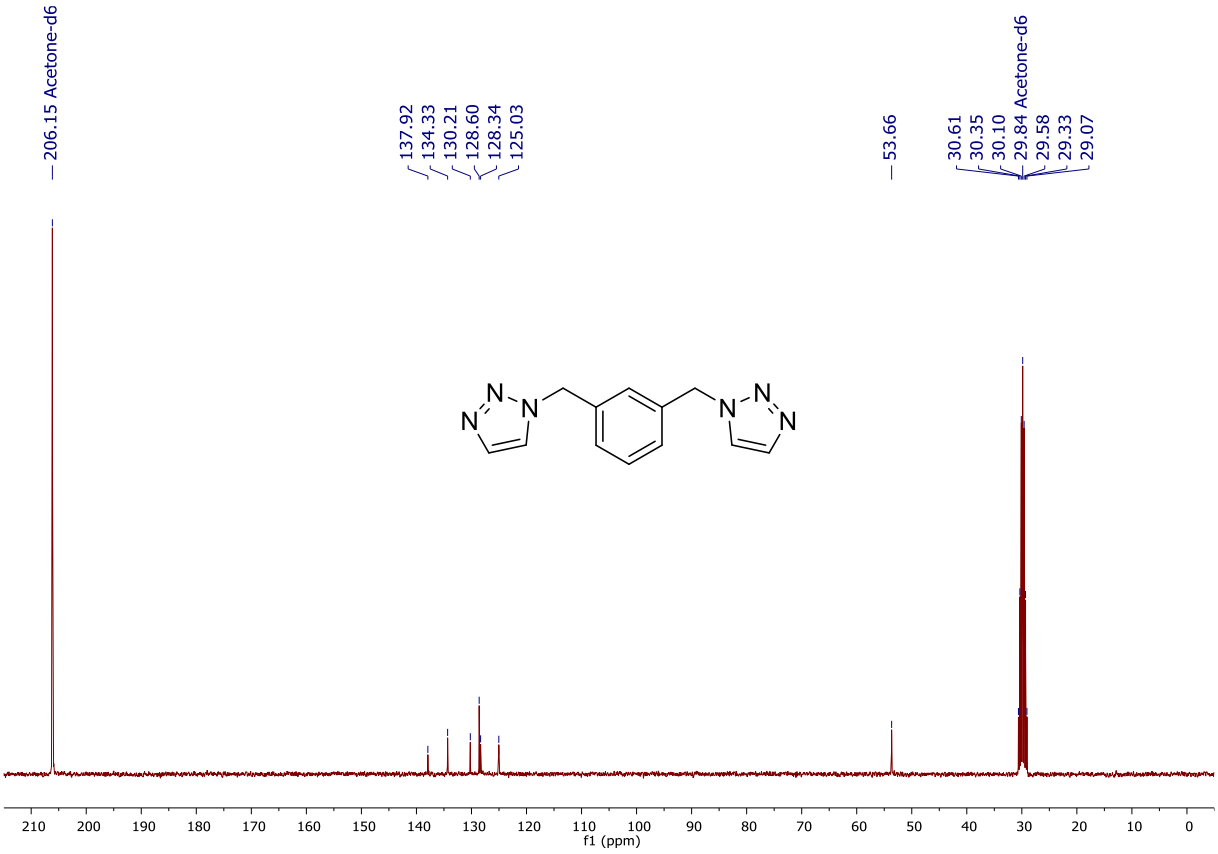

Figure S26. ^{13}C {^{1}H} NMR spectrum of **6**.

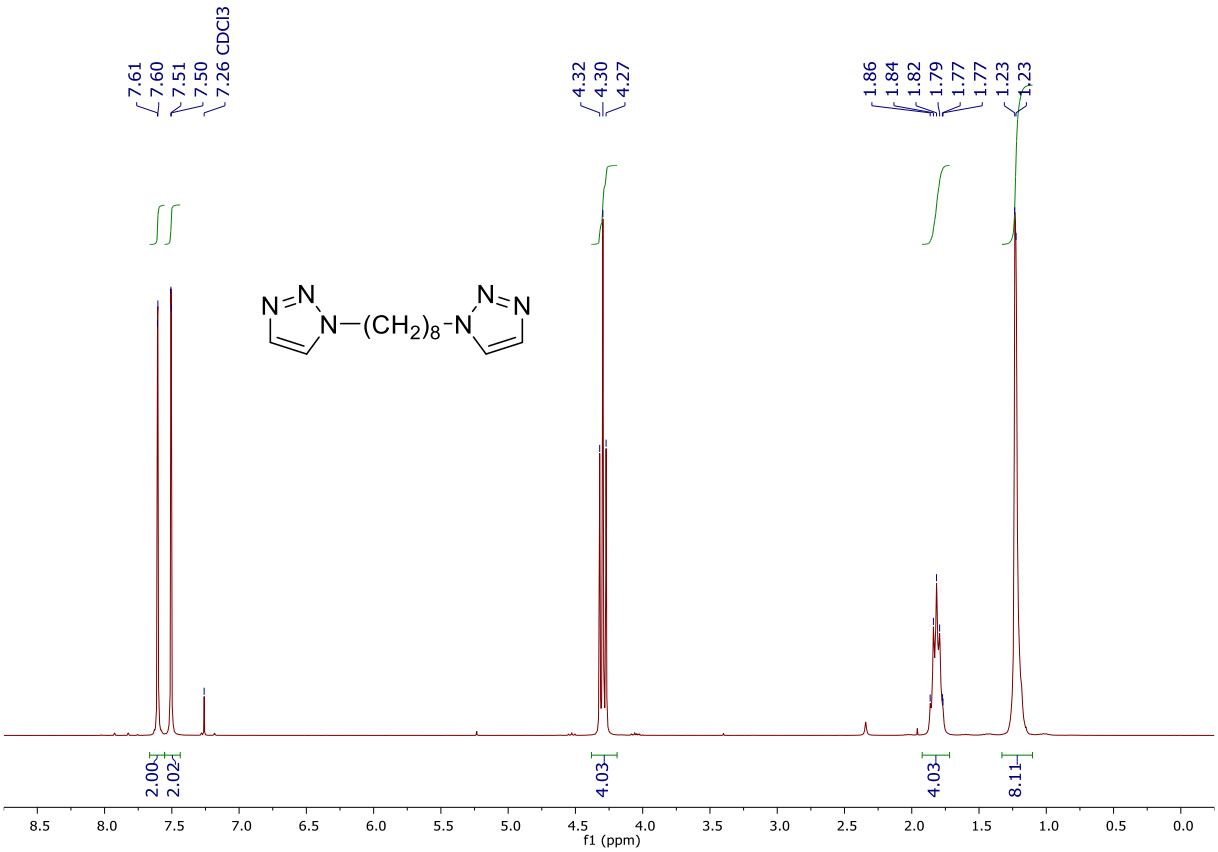

Figure S27. ^{1}H NMR spectrum of **7**.

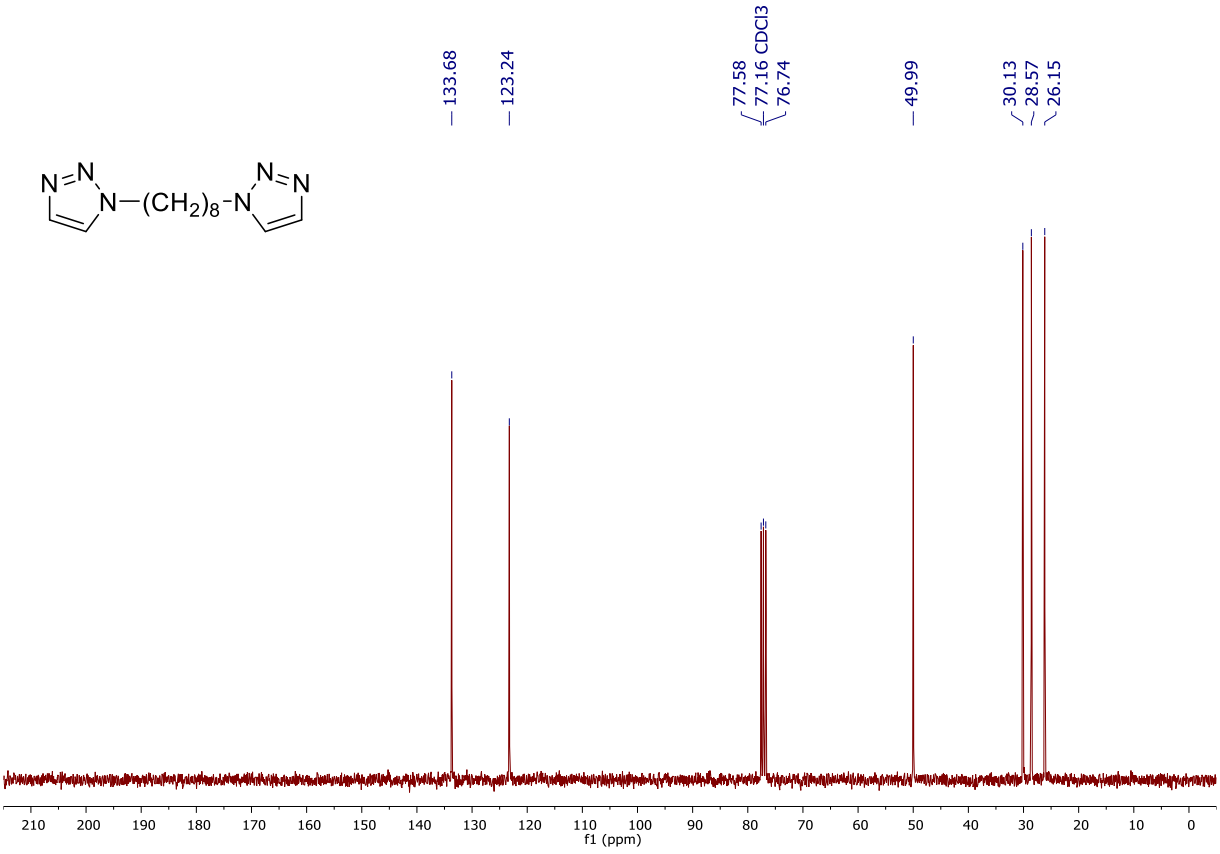

Figure S28. ^{13}C {^{1}H} NMR spectrum of **7**.

Mass-spectra of obtained products

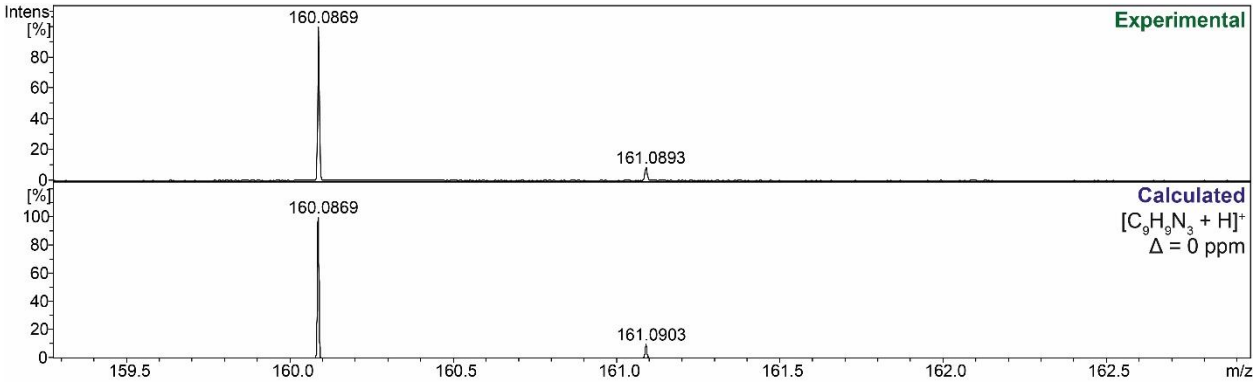

Figure S29. ESI-HRMS of **1**.

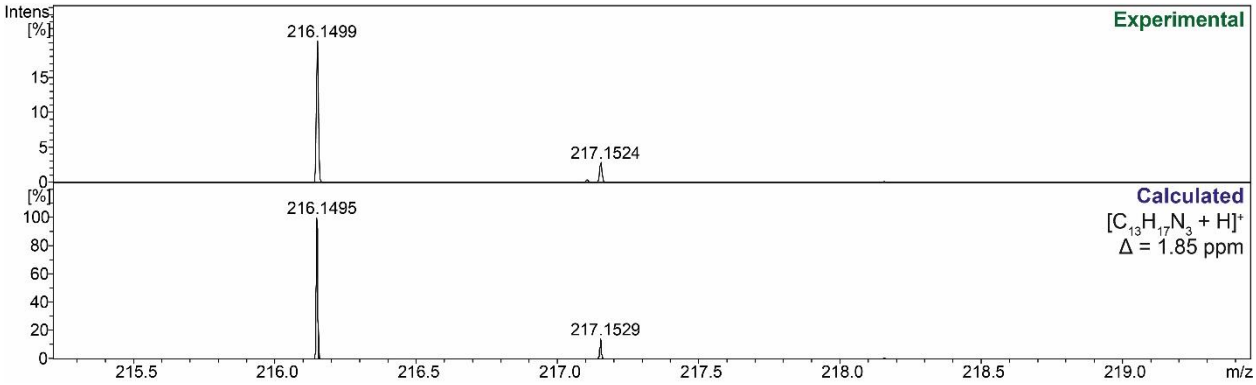

Figure S30. ESI-HRMS of **2**.

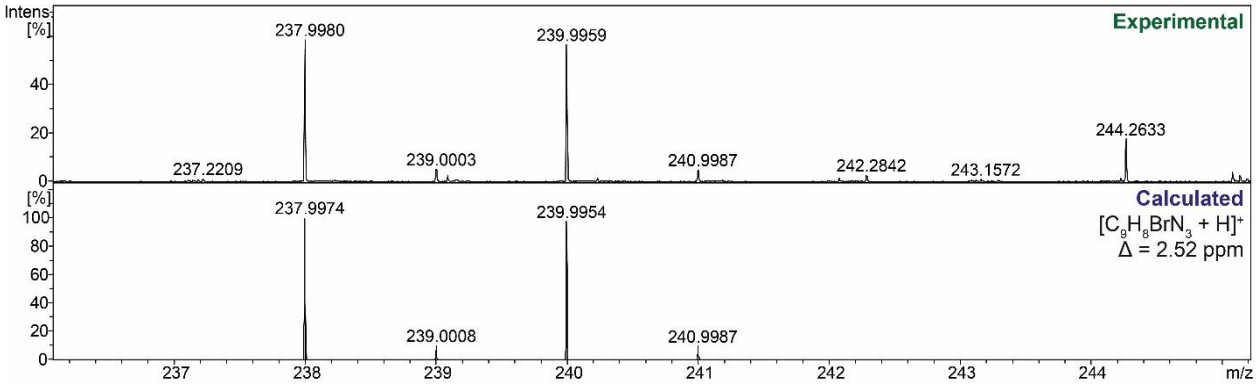

Figure S31. ESI-HRMS of **3**.

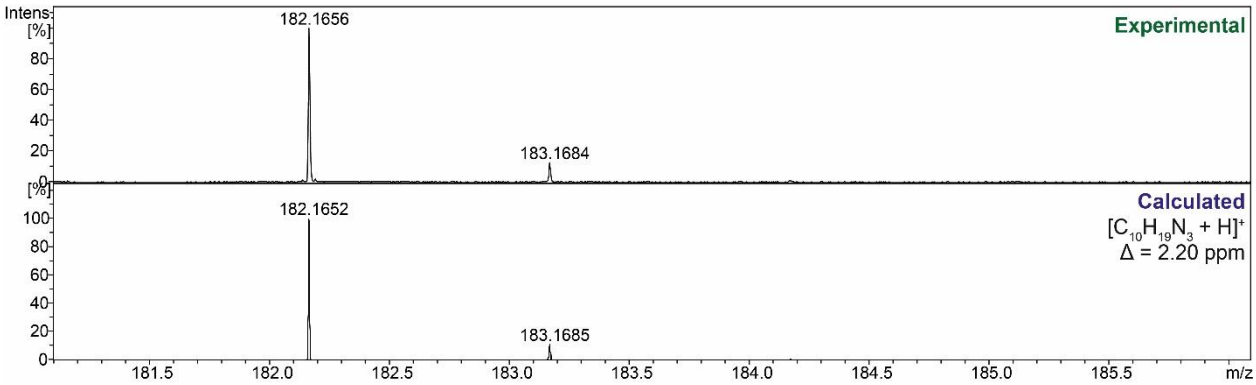

Figure S32. ESI-HRMS of **4**.

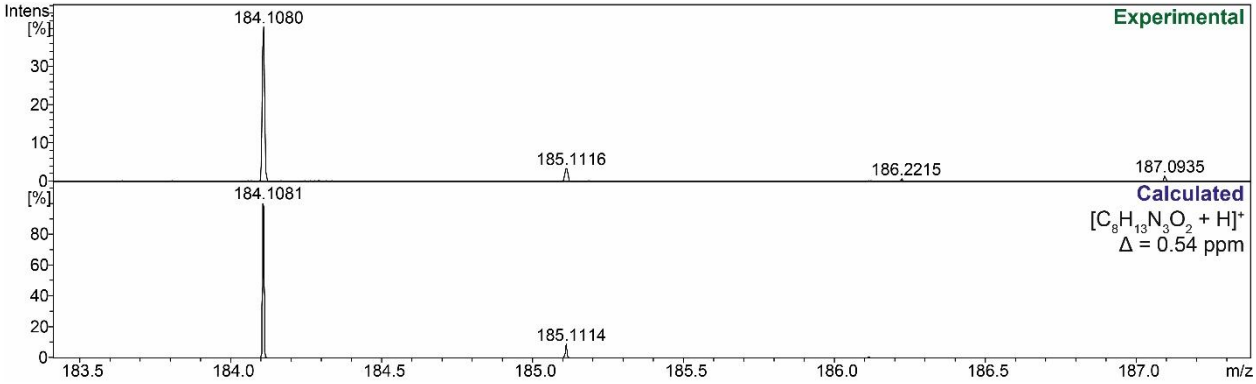

Figure S33. ESI-HRMS of **5**.

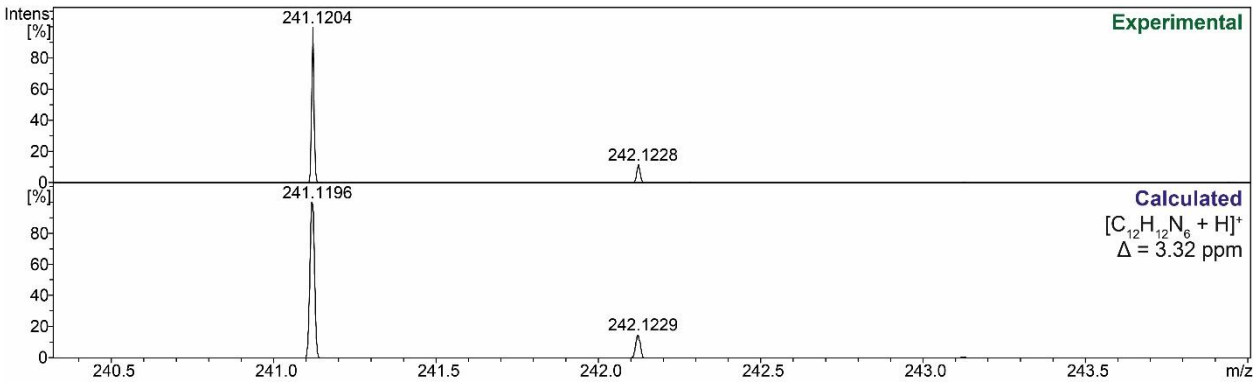

Figure S34. ESI-HRMS of **6**.

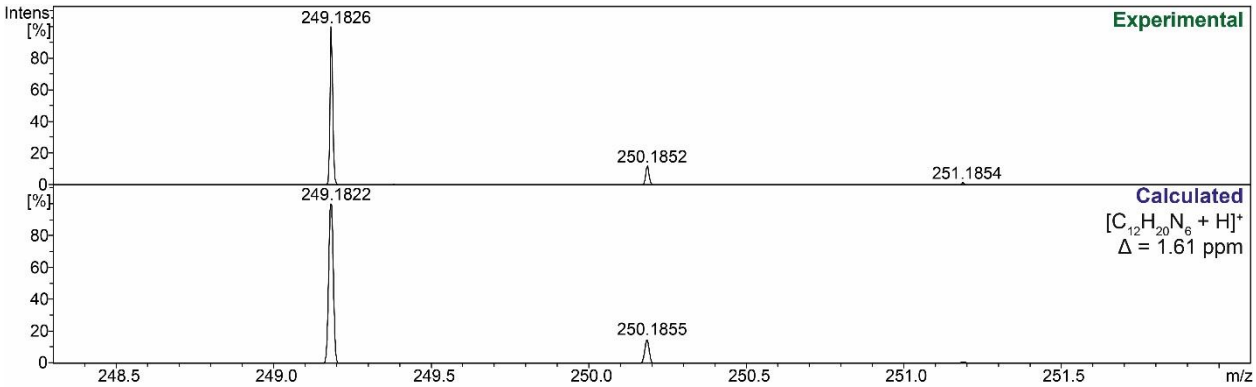

Figure S35. ESI-HRMS of **7**.

X-Ray crystallographic data and refinement details

X-ray diffraction data were collected at 100K on a four-circle Rigaku Synergy S diffractometer equipped with a HyPix6000HE area-detector (kappa geometry, shutterless ω-scan technique), using monochromatized Cu K_α-radiation. The intensity data were integrated and corrected for absorption and decay by the CrysAlisPro program.[S2] The structure was solved by direct methods using SHELXT[S3] and refined on F^2 using SHELXL-2018[S4] in the OLEX2 program. [S5] All non-hydrogen atoms were refined with individual anisotropic displacement parameters. All hydrogen atoms were placed in ideal calculated positions and refined as riding atoms with relative isotropic displacement parameters.

All atoms of both molecules are disordered over two positions with the contribution of main component of 0.9243(9).

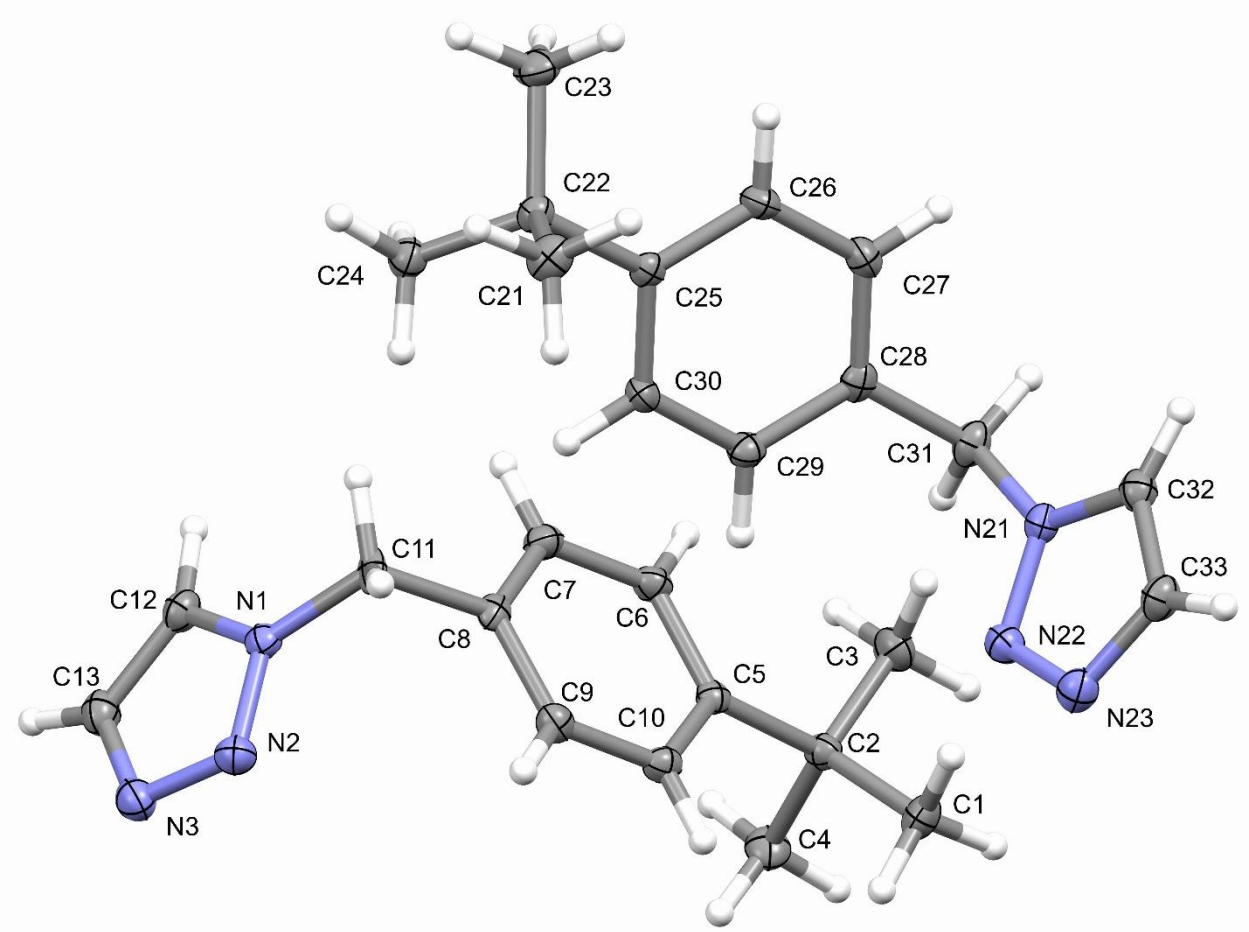

Figure S36. X-ray crystallographic images of 1-[[4-*tert*-butylphenyl]methyl]-1*H*-1,2,3-triazole (**2**)

CCDC number	2444362	
Empirical formula	C13 H17 N3	
Formula weight	215.29	
Temperature	99.97(16) K	
Wavelength	1.54184 Å	
Crystal system	Orthorhombic	
Space group	$Pca2_1$	
Unit cell dimensions	a = 20.18697(13) Å	α= 90°.
	b = 5.78964(3) Å	β= 90°.
	c = 20.16168(12) Å	γ = 90°.
Volume	2356.40(2) $Å^3$	
Z	8	
Density (calculated)	1.214 g/cm^3	
Absorption coefficient	0.577 mm^{-1}	
F(000)	928	
Crystal size	0.36 x 0.16 x 0.14 mm^3	
Theta range for data collection	4.380 to 80.706°.	
Index ranges	-25<=h<=25, -5<=k<=7, -25<=l<=25	
Reflections collected	28053	
Independent reflections	5066 [R(int) = 0.0320]	
Observed reflections	5001	
Completeness to theta = 67.684°	100.0 %	
Absorption correction	Gaussian	
Max. and min. transmission	1.000 and 0.575	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5066 / 45 / 396	
Goodness-of-fit on F^2	1.057	
Final R indices [I>2sigma(I)]	R1 = 0.0338, wR2 = 0.0908	
R indices (all data)	R1 = 0.0342, wR2 = 0.0912	
Absolute structure parameter	0.2(5)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.252 and -0.271 e.$Å^{-3}$	

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for 1-[[4-*tert*-butylphenyl]methyl]-1*H*-1,2,3-triazole. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	1974(1)	3809(3)	5870(1)	16(1)
N(1A)	2009(9)	6270(30)	5862(13)	16(1)
N(2)	2048(1)	1501(3)	5921(1)	20(1)
N(2A)	1351(9)	5890(30)	5877(13)	20(1)
N(3)	1450(1)	591(3)	5943(1)	22(1)
N(3A)	987(10)	7760(30)	5892(14)	22(1)
C(1)	4028(1)	4549(4)	2878(1)	22(1)
C(1A)	3967(14)	5440(60)	2880(20)	22(1)
C(2)	3342(1)	5627(3)	3010(1)	16(1)
C(2A)	3285(11)	4360(40)	2991(12)	16(1)
C(3)	3346(1)	8050(4)	2705(1)	24(1)
C(3A)	2750(14)	5730(50)	2639(15)	24(1)
C(4)	2800(1)	4196(4)	2668(1)	23(1)
C(4A)	3352(14)	1910(40)	2711(15)	23(1)
C(5)	3186(1)	5667(3)	3753(1)	14(1)
C(5A)	3196(12)	4320(40)	3758(12)	14(1)
C(6)	2827(1)	7458(3)	4048(1)	17(1)
C(6A)	3362(12)	6220(40)	4158(14)	17(1)
C(7)	2628(1)	7364(3)	4712(1)	18(1)
C(7A)	3199(12)	6430(40)	4827(13)	18(1)
C(8)	2796(1)	5457(4)	5102(1)	15(1)
C(8A)	2874(13)	4470(40)	5008(11)	15(1)
C(9)	3166(1)	3684(3)	4822(1)	17(1)
C(9A)	2581(12)	2640(30)	4707(12)	17(1)
C(10)	3355(1)	3788(3)	4162(1)	16(1)
C(10A)	2837(11)	2550(30)	4065(13)	16(1)
C(11)	2554(1)	5274(4)	5820(1)	17(1)
C(11A)	2617(13)	5420(60)	5621(13)	17(1)
C(12)	1328(1)	4394(4)	5856(1)	19(1)
C(12A)	2069(11)	8560(30)	5916(17)	19(1)
C(13)	997(1)	2331(4)	5900(1)	22(1)
C(13A)	1452(11)	9380(50)	5948(17)	22(1)
N(21)	5508(1)	8650(3)	4100(1)	16(1)
N(21A)	5530(8)	11300(30)	4093(14)	16(1)
N(22)	5442(1)	6345(3)	4064(1)	20(1)

N(22A)	6171(10)	10650(30)	4143(14)	20(1)
N(23)	6043(1)	5458(4)	4062(1)	21(1)
N(23A)	6479(11)	12620(30)	4093(14)	21(1)
C(21)	4684(1)	9379(4)	7325(1)	23(1)
C(21A)	4155(14)	6780(40)	7231(15)	23(1)
C(22)	4140(1)	10727(3)	6960(1)	16(1)
C(22A)	4136(11)	9200(40)	6951(13)	16(1)
C(23)	4136(1)	13198(4)	7231(1)	24(1)
C(23A)	4661(14)	10720(50)	7284(15)	24(1)
C(24)	3463(1)	9638(4)	7103(1)	20(1)
C(24A)	3474(16)	10410(60)	7070(20)	20(1)
C(25)	4311(1)	10661(3)	6216(1)	14(1)
C(25A)	4327(12)	9350(40)	6176(14)	14(1)
C(26)	4676(1)	12419(3)	5912(1)	18(1)
C(26A)	4147(13)	11270(40)	5824(14)	18(1)
C(27)	4862(1)	12255(3)	5248(1)	18(1)
C(27A)	4339(12)	11340(40)	5163(14)	18(1)
C(28)	4695(1)	10343(3)	4869(1)	16(1)
C(28A)	4739(18)	9640(40)	4879(12)	16(1)
C(29)	4322(1)	8596(3)	5165(1)	17(1)
C(29A)	4846(12)	7660(30)	5253(12)	17(1)
C(30)	4134(1)	8760(3)	5829(1)	16(1)
C(30A)	4704(11)	7550(30)	5927(13)	16(1)
C(31)	4918(1)	10111(3)	4159(1)	20(1)
C(31A)	4918(1)	10111(3)	4159(1)	20(1)
C(32)	6152(1)	9279(3)	4129(1)	18(1)
C(32A)	5450(11)	13580(30)	4063(17)	18(1)
C(33)	6487(1)	7221(4)	4100(1)	21(1)
C(33A)	6080(11)	14400(50)	4081(18)	21(1)

Table S3. Bond lengths [Å] and angles [°] for 1-[[4-*tert*-butylphenyl]methyl]-1*H*-1,2,3-triazole.

N(1)-N(2)	1.349(2)
N(1)-C(11)	1.449(3)
N(1)-C(12)	1.346(3)
N(1A)-N(2A)	1.35(2)
N(1A)-C(11A)	1.41(2)
N(1A)-C(12A)	1.33(2)
N(2)-N(3)	1.317(3)
N(2A)-N(3A)	1.31(2)
N(3)-C(13)	1.364(3)
N(3A)-C(13A)	1.33(2)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(1)-C(2)	1.542(3)
C(1A)-H(1D)	0.9800
C(1A)-H(1E)	0.9800
C(1A)-H(1F)	0.9800
C(1A)-C(2A)	1.53(2)
C(2)-C(3)	1.532(3)
C(2)-C(4)	1.537(3)
C(2)-C(5)	1.531(3)
C(2A)-C(3A)	1.51(2)
C(2A)-C(4A)	1.53(2)
C(2A)-C(5A)	1.56(2)
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(3A)-H(3D)	0.9800
C(3A)-H(3E)	0.9800
C(3A)-H(3F)	0.9800
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(4A)-H(4D)	0.9800
C(4A)-H(4E)	0.9800
C(4A)-H(4F)	0.9800
C(5)-C(6)	1.397(3)
C(5)-C(10)	1.407(3)

C(5A)-C(6A)	1.40(2)
C(5A)-C(10A)	1.40(2)
C(6)-H(6)	0.9500
C(6)-C(7)	1.399(3)
C(6A)-H(6A)	0.9500
C(6A)-C(7A)	1.39(2)
C(7)-H(7)	0.9500
C(7)-C(8)	1.397(3)
C(7A)-H(7A)	0.9500
C(7A)-C(8A)	1.36(2)
C(8)-C(9)	1.389(3)
C(8)-C(11)	1.532(3)
C(8A)-C(9A)	1.36(2)
C(8A)-C(11A)	1.45(2)
C(9)-H(9)	0.9500
C(9)-C(10)	1.386(3)
C(9A)-H(9A)	0.9500
C(9A)-C(10A)	1.39(2)
C(10)-H(10)	0.9500
C(10A)-H(10A)	0.9500
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(11A)-H(11C)	0.9900
C(11A)-H(11D)	0.9900
C(12)-H(12)	0.9500
C(12)-C(13)	1.373(3)
C(12A)-H(12A)	0.9500
C(12A)-C(13A)	1.34(2)
C(13)-H(13)	0.9500
C(13A)-H(13A)	0.9500
N(21)-N(22)	1.343(2)
N(21)-C(31)	1.467(3)
N(21)-C(32)	1.351(3)
N(21A)-N(22A)	1.35(2)
N(21A)-C(31A)	1.421(16)
N(21A)-C(32A)	1.33(2)
N(22)-N(23)	1.317(3)
N(22A)-N(23A)	1.31(2)
N(23)-C(33)	1.361(3)
N(23A)-C(33A)	1.31(2)

C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(21)-C(22)	1.536(3)
C(21A)-H(21D)	0.9800
C(21A)-H(21E)	0.9800
C(21A)-H(21F)	0.9800
C(21A)-C(22A)	1.51(2)
C(22)-C(23)	1.532(3)
C(22)-C(24)	1.531(3)
C(22)-C(25)	1.539(3)
C(22A)-C(23A)	1.53(2)
C(22A)-C(24A)	1.53(2)
C(22A)-C(25A)	1.61(3)
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(23A)-H(23D)	0.9800
C(23A)-H(23E)	0.9800
C(23A)-H(23F)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(24A)-H(24D)	0.9800
C(24A)-H(24E)	0.9800
C(24A)-H(24F)	0.9800
C(25)-C(26)	1.399(3)
C(25)-C(30)	1.396(3)
C(25A)-C(26A)	1.36(2)
C(25A)-C(30A)	1.39(2)
C(26)-H(26)	0.9500
C(26)-C(27)	1.393(3)
C(26A)-H(26A)	0.9500
C(26A)-C(27A)	1.39(2)
C(27)-H(27)	0.9500
C(27)-C(28)	1.387(3)
C(27A)-H(27A)	0.9500
C(27A)-C(28A)	1.39(2)
C(28)-C(29)	1.394(3)
C(28)-C(31)	1.506(3)

C(28A)-C(29A)	1.39(2)
C(28A)-C(31A)	1.52(2)
C(29)-H(29)	0.9500
C(29)-C(30)	1.395(3)
C(29A)-H(29A)	0.9500
C(29A)-C(30A)	1.39(2)
C(30)-H(30)	0.9500
C(30A)-H(30A)	0.9500
C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(31A)-H(31C)	0.9900
C(31A)-H(31D)	0.9900
C(32)-H(32)	0.9500
C(32)-C(33)	1.371(3)
C(32A)-H(32A)	0.9500
C(32A)-C(33A)	1.36(2)
C(33)-H(33)	0.9500
C(33A)-H(33A)	0.9500

N(2)-N(1)-C(11)	119.72(18)
C(12)-N(1)-N(2)	110.97(16)
C(12)-N(1)-C(11)	129.29(18)
N(2A)-N(1A)-C(11A)	144(2)
C(12A)-N(1A)-N(2A)	104.5(17)
C(12A)-N(1A)-C(11A)	107(2)
N(3)-N(2)-N(1)	107.33(16)
N(3A)-N(2A)-N(1A)	114.7(19)
N(2)-N(3)-C(13)	108.48(17)
N(2A)-N(3A)-C(13A)	101(2)
H(1A)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(2)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1C)	109.5
H(1D)-C(1A)-H(1E)	109.5
H(1D)-C(1A)-H(1F)	109.5
H(1E)-C(1A)-H(1F)	109.5
C(2A)-C(1A)-H(1D)	109.5
C(2A)-C(1A)-H(1E)	109.5

C(2A)-C(1A)-H(1F)	109.5
C(3)-C(2)-C(1)	107.26(18)
C(3)-C(2)-C(4)	108.45(18)
C(4)-C(2)-C(1)	110.09(18)
C(5)-C(2)-C(1)	111.16(18)
C(5)-C(2)-C(3)	112.35(17)
C(5)-C(2)-C(4)	107.50(17)
C(1A)-C(2A)-C(4A)	104(2)
C(1A)-C(2A)-C(5A)	105(2)
C(3A)-C(2A)-C(1A)	111(2)
C(3A)-C(2A)-C(4A)	112(2)
C(3A)-C(2A)-C(5A)	113(2)
C(4A)-C(2A)-C(5A)	111.2(18)
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(2A)-C(3A)-H(3D)	109.5
C(2A)-C(3A)-H(3E)	109.5
C(2A)-C(3A)-H(3F)	109.5
H(3D)-C(3A)-H(3E)	109.5
H(3D)-C(3A)-H(3F)	109.5
H(3E)-C(3A)-H(3F)	109.5
C(2)-C(4)-H(4A)	109.5
C(2)-C(4)-H(4B)	109.5
C(2)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(2A)-C(4A)-H(4D)	109.5
C(2A)-C(4A)-H(4E)	109.5
C(2A)-C(4A)-H(4F)	109.5
H(4D)-C(4A)-H(4E)	109.5
H(4D)-C(4A)-H(4F)	109.5
H(4E)-C(4A)-H(4F)	109.5
C(6)-C(5)-C(2)	122.29(18)
C(6)-C(5)-C(10)	116.8(2)
C(10)-C(5)-C(2)	120.72(18)

C(6A)-C(5A)-C(2A)	122.2(19)
C(6A)-C(5A)-C(10A)	116(2)
C(10A)-C(5A)-C(2A)	120.5(19)
C(5)-C(6)-H(6)	119.1
C(5)-C(6)-C(7)	121.81(18)
C(7)-C(6)-H(6)	119.1
C(5A)-C(6A)-H(6A)	117.6
C(7A)-C(6A)-C(5A)	125(2)
C(7A)-C(6A)-H(6A)	117.6
C(6)-C(7)-H(7)	120.0
C(8)-C(7)-C(6)	119.98(18)
C(8)-C(7)-H(7)	120.0
C(6A)-C(7A)-H(7A)	126.3
C(8A)-C(7A)-C(6A)	107(2)
C(8A)-C(7A)-H(7A)	126.3
C(7)-C(8)-C(11)	120.6(2)
C(9)-C(8)-C(7)	119.1(2)
C(9)-C(8)-C(11)	120.3(2)
C(7A)-C(8A)-C(11A)	95(2)
C(9A)-C(8A)-C(7A)	138(2)
C(9A)-C(8A)-C(11A)	121(2)
C(8)-C(9)-H(9)	119.8
C(10)-C(9)-C(8)	120.41(18)
C(10)-C(9)-H(9)	119.8
C(8A)-C(9A)-H(9A)	126.7
C(8A)-C(9A)-C(10A)	107(2)
C(10A)-C(9A)-H(9A)	126.7
C(5)-C(10)-H(10)	119.0
C(9)-C(10)-C(5)	121.92(18)
C(9)-C(10)-H(10)	119.0
C(5A)-C(10A)-H(10A)	117.6
C(9A)-C(10A)-C(5A)	125(2)
C(9A)-C(10A)-H(10A)	117.6
N(1)-C(11)-C(8)	111.28(19)
N(1)-C(11)-H(11A)	109.4
N(1)-C(11)-H(11B)	109.4
C(8)-C(11)-H(11A)	109.4
C(8)-C(11)-H(11B)	109.4
H(11A)-C(11)-H(11B)	108.0
N(1A)-C(11A)-C(8A)	138(3)

N(1A)-C(11A)-H(11C)	102.7
N(1A)-C(11A)-H(11D)	102.7
C(8A)-C(11A)-H(11C)	102.7
C(8A)-C(11A)-H(11D)	102.7
H(11C)-C(11A)-H(11D)	105.0
N(1)-C(12)-H(12)	127.7
N(1)-C(12)-C(13)	104.59(18)
C(13)-C(12)-H(12)	127.7
N(1A)-C(12A)-H(12A)	127.1
N(1A)-C(12A)-C(13A)	106(2)
C(13A)-C(12A)-H(12A)	127.1
N(3)-C(13)-C(12)	108.63(18)
N(3)-C(13)-H(13)	125.7
C(12)-C(13)-H(13)	125.7
N(3A)-C(13A)-C(12A)	114(2)
N(3A)-C(13A)-H(13A)	123.2
C(12A)-C(13A)-H(13A)	123.2
N(22)-N(21)-C(31)	119.78(17)
N(22)-N(21)-C(32)	111.43(16)
C(32)-N(21)-C(31)	128.55(17)
N(22A)-N(21A)-C(31A)	133.6(16)
C(32A)-N(21A)-N(22A)	113.3(17)
C(32A)-N(21A)-C(31A)	112.3(15)
N(23)-N(22)-N(21)	107.25(16)
N(23A)-N(22A)-N(21A)	101.9(18)
N(22)-N(23)-C(33)	108.27(18)
N(22A)-N(23A)-C(33A)	113(2)
H(21A)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(22)-C(21)-H(21A)	109.5
C(22)-C(21)-H(21B)	109.5
C(22)-C(21)-H(21C)	109.5
H(21D)-C(21A)-H(21E)	109.5
H(21D)-C(21A)-H(21F)	109.5
H(21E)-C(21A)-H(21F)	109.5
C(22A)-C(21A)-H(21D)	109.5
C(22A)-C(21A)-H(21E)	109.5
C(22A)-C(21A)-H(21F)	109.5
C(21)-C(22)-C(25)	107.10(17)

C(23)-C(22)-C(21)	107.85(17)
C(23)-C(22)-C(25)	111.87(17)
C(24)-C(22)-C(21)	109.76(18)
C(24)-C(22)-C(23)	108.20(17)
C(24)-C(22)-C(25)	111.97(18)
C(21A)-C(22A)-C(23A)	111(2)
C(21A)-C(22A)-C(24A)	113(2)
C(21A)-C(22A)-C(25A)	114.1(19)
C(23A)-C(22A)-C(25A)	103(2)
C(24A)-C(22A)-C(23A)	106(2)
C(24A)-C(22A)-C(25A)	110(2)
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(22A)-C(23A)-H(23D)	109.5
C(22A)-C(23A)-H(23E)	109.5
C(22A)-C(23A)-H(23F)	109.5
H(23D)-C(23A)-H(23E)	109.5
H(23D)-C(23A)-H(23F)	109.5
H(23E)-C(23A)-H(23F)	109.5
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(22A)-C(24A)-H(24D)	109.5
C(22A)-C(24A)-H(24E)	109.5
C(22A)-C(24A)-H(24F)	109.5
H(24D)-C(24A)-H(24E)	109.5
H(24D)-C(24A)-H(24F)	109.5
H(24E)-C(24A)-H(24F)	109.5
C(26)-C(25)-C(22)	121.84(18)
C(30)-C(25)-C(22)	120.50(18)
C(30)-C(25)-C(26)	117.6(2)
C(26A)-C(25A)-C(22A)	119(2)
C(26A)-C(25A)-C(30A)	125(2)

C(30A)-C(25A)-C(22A)	116.1(19)
C(25)-C(26)-H(26)	119.6
C(27)-C(26)-C(25)	120.88(18)
C(27)-C(26)-H(26)	119.6
C(25A)-C(26A)-H(26A)	121.7
C(25A)-C(26A)-C(27A)	117(2)
C(27A)-C(26A)-H(26A)	121.7
C(26)-C(27)-H(27)	119.4
C(28)-C(27)-C(26)	121.26(18)
C(28)-C(27)-H(27)	119.4
C(26A)-C(27A)-H(27A)	118.9
C(26A)-C(27A)-C(28A)	122(2)
C(28A)-C(27A)-H(27A)	118.9
C(27)-C(28)-C(29)	118.3(2)
C(27)-C(28)-C(31)	121.49(19)
C(29)-C(28)-C(31)	120.2(2)
C(27A)-C(28A)-C(31A)	113.8(18)
C(29A)-C(28A)-C(27A)	117(2)
C(29A)-C(28A)-C(31A)	128.9(19)
C(28)-C(29)-H(29)	119.7
C(28)-C(29)-C(30)	120.51(18)
C(30)-C(29)-H(29)	119.7
C(28A)-C(29A)-H(29A)	118.8
C(30A)-C(29A)-C(28A)	122(2)
C(30A)-C(29A)-H(29A)	118.8
C(25)-C(30)-H(30)	119.3
C(29)-C(30)-C(25)	121.43(18)
C(29)-C(30)-H(30)	119.3
C(25A)-C(30A)-C(29A)	116(2)
C(25A)-C(30A)-H(30A)	122.2
C(29A)-C(30A)-H(30A)	122.2
N(21)-C(31)-C(28)	111.82(19)
N(21)-C(31)-H(31A)	109.3
N(21)-C(31)-H(31B)	109.3
C(28)-C(31)-H(31A)	109.3
C(28)-C(31)-H(31B)	109.3
H(31A)-C(31)-H(31B)	107.9
N(21A)-C(31A)-C(28A)	112.5(19)
N(21A)-C(31A)-H(31C)	109.1
N(21A)-C(31A)-H(31D)	109.1

C(28A)-C(31A)-H(31C)	109.1
C(28A)-C(31A)-H(31D)	109.1
H(31C)-C(31A)-H(31D)	107.8
N(21)-C(32)-H(32)	128.1
N(21)-C(32)-C(33)	103.80(17)
C(33)-C(32)-H(32)	128.1
N(21A)-C(32A)-H(32A)	128.4
N(21A)-C(32A)-C(33A)	103(2)
C(33A)-C(32A)-H(32A)	128.4
N(23)-C(33)-C(32)	109.24(18)
N(23)-C(33)-H(33)	125.4
C(32)-C(33)-H(33)	125.4
N(23A)-C(33A)-C(32A)	108(2)
N(23A)-C(33A)-H(33A)	126.1
C(32A)-C(33A)-H(33A)	126.1

Table S4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for 1-[[4-*tert*-butylphenyl]methyl]-1*H*-1,2,3-triazole. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	17(1)	16(1)	14(1)	-1(1)	1(1)	-1(1)
N(1A)	17(1)	16(1)	14(1)	-1(1)	1(1)	-1(1)
N(2)	21(1)	18(1)	22(1)	0(1)	1(1)	1(1)
N(2A)	21(1)	18(1)	22(1)	0(1)	1(1)	1(1)
N(3)	23(1)	22(1)	22(1)	1(1)	2(1)	-4(1)
N(3A)	23(1)	22(1)	22(1)	1(1)	2(1)	-4(1)
C(1)	20(1)	25(1)	20(1)	-1(1)	4(1)	5(1)
C(1A)	20(1)	25(1)	20(1)	-1(1)	4(1)	5(1)
C(2)	19(1)	14(1)	17(1)	1(1)	0(1)	0(1)
C(2A)	19(1)	14(1)	17(1)	1(1)	0(1)	0(1)
C(3)	29(1)	20(1)	22(1)	5(1)	3(1)	-1(1)
C(3A)	29(1)	20(1)	22(1)	5(1)	3(1)	-1(1)
C(4)	22(1)	26(1)	20(1)	-4(1)	-4(1)	-5(1)
C(4A)	22(1)	26(1)	20(1)	-4(1)	-4(1)	-5(1)
C(5)	12(1)	14(1)	15(1)	-1(1)	-2(1)	-2(1)
C(5A)	12(1)	14(1)	15(1)	-1(1)	-2(1)	-2(1)
C(6)	18(1)	14(1)	21(1)	1(1)	-1(1)	1(1)
C(6A)	18(1)	14(1)	21(1)	1(1)	-1(1)	1(1)
C(7)	17(1)	16(1)	21(1)	-4(1)	1(1)	1(1)
C(7A)	17(1)	16(1)	21(1)	-4(1)	1(1)	1(1)
C(8)	10(1)	20(1)	15(1)	-4(1)	-1(1)	-3(1)
C(8A)	10(1)	20(1)	15(1)	-4(1)	-1(1)	-3(1)
C(9)	14(1)	16(1)	20(1)	3(1)	-2(1)	1(1)
C(9A)	14(1)	16(1)	20(1)	3(1)	-2(1)	1(1)
C(10)	14(1)	15(1)	20(1)	-1(1)	-1(1)	2(1)
C(10A)	14(1)	15(1)	20(1)	-1(1)	-1(1)	2(1)
C(11)	16(1)	28(1)	8(1)	-1(1)	2(1)	-6(1)
C(11A)	16(1)	28(1)	8(1)	-1(1)	2(1)	-6(1)
C(12)	15(1)	24(1)	19(1)	-1(1)	0(1)	2(1)
C(12A)	15(1)	24(1)	19(1)	-1(1)	0(1)	2(1)
C(13)	18(1)	27(1)	21(1)	-2(1)	1(1)	-4(1)
C(13A)	18(1)	27(1)	21(1)	-2(1)	1(1)	-4(1)
N(21)	14(1)	18(1)	14(1)	1(1)	2(1)	1(1)
N(21A)	14(1)	18(1)	14(1)	1(1)	2(1)	1(1)
N(22)	20(1)	18(1)	22(1)	1(1)	1(1)	-1(1)

N(22A)	20(1)	18(1)	22(1)	1(1)	1(1)	-1(1)
N(23)	22(1)	21(1)	21(1)	4(1)	2(1)	4(1)
N(23A)	22(1)	21(1)	21(1)	4(1)	2(1)	4(1)
C(21)	22(1)	27(1)	19(1)	0(1)	-2(1)	4(1)
C(21A)	22(1)	27(1)	19(1)	0(1)	-2(1)	4(1)
C(22)	15(1)	17(1)	16(1)	0(1)	0(1)	2(1)
C(22A)	15(1)	17(1)	16(1)	0(1)	0(1)	2(1)
C(23)	31(1)	19(1)	21(1)	-5(1)	1(1)	0(1)
C(23A)	31(1)	19(1)	21(1)	-5(1)	1(1)	0(1)
C(24)	20(1)	21(1)	18(1)	0(1)	3(1)	0(1)
C(24A)	20(1)	21(1)	18(1)	0(1)	3(1)	0(1)
C(25)	11(1)	14(1)	17(1)	1(1)	-1(1)	2(1)
C(25A)	11(1)	14(1)	17(1)	1(1)	-1(1)	2(1)
C(26)	19(1)	13(1)	21(1)	-1(1)	-1(1)	-2(1)
C(26A)	19(1)	13(1)	21(1)	-1(1)	-1(1)	-2(1)
C(27)	17(1)	17(1)	21(1)	4(1)	1(1)	-2(1)
C(27A)	17(1)	17(1)	21(1)	4(1)	1(1)	-2(1)
C(28)	13(1)	18(1)	16(1)	3(1)	0(1)	5(1)
C(28A)	13(1)	18(1)	16(1)	3(1)	0(1)	5(1)
C(29)	16(1)	17(1)	18(1)	-3(1)	-1(1)	-1(1)
C(29A)	16(1)	17(1)	18(1)	-3(1)	-1(1)	-1(1)
C(30)	15(1)	14(1)	19(1)	-1(1)	2(1)	-3(1)
C(30A)	15(1)	14(1)	19(1)	-1(1)	2(1)	-3(1)
C(31)	17(1)	25(1)	18(1)	1(1)	0(1)	4(1)
C(31A)	17(1)	25(1)	18(1)	1(1)	0(1)	4(1)
C(32)	16(1)	21(1)	18(1)	0(1)	0(1)	-1(1)
C(32A)	16(1)	21(1)	18(1)	0(1)	0(1)	-1(1)
C(33)	17(1)	25(1)	21(1)	1(1)	1(1)	3(1)
C(33A)	17(1)	25(1)	21(1)	1(1)	1(1)	3(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2× 10^3) for 1-[[4-*tert*-butylphenyl]methyl]-1*H*-1,2,3-triazole.

	x	y	z	U(eq)
H(1A)	4128	4632	2403	33
H(1B)	4027	2930	3020	33
H(1C)	4366	5400	3127	33
H(1D)	3944	7104	2964	33
H(1E)	4106	5171	2420	33
H(1F)	4287	4731	3182	33
H(3A)	3663	9025	2944	36
H(3B)	2902	8726	2739	36
H(3C)	3475	7950	2237	36
H(3D)	2321	5432	2850	36
H(3E)	2732	5270	2172	36
H(3F)	2852	7386	2668	36
H(4A)	2903	4051	2195	34
H(4B)	2371	4969	2722	34
H(4C)	2780	2657	2869	34
H(4D)	3757	1198	2884	34
H(4E)	3376	1982	2226	34
H(4F)	2967	990	2844	34
H(6)	2715	8775	3790	21
H(6A)	3604	7443	3959	21
H(7)	2378	8596	4897	22
H(7A)	3297	7709	5106	22
H(9)	3289	2391	5084	20
H(9A)	2264	1629	4896	20
H(10)	3607	2556	3980	20
H(10A)	2762	1175	3817	20
H(11A)	2912	4632	6100	21
H(11B)	2445	6835	5989	21
H(11C)	2731	4209	5949	21
H(11D)	2926	6704	5714	21
H(12)	1144	5900	5824	23
H(12A)	2469	9424	5929	23
H(13)	529	2145	5901	26
H(13A)	1353	10976	6006	26

H(21A)	5109	10168	7267	34
H(21B)	4713	7814	7143	34
H(21C)	4576	9296	7799	34
H(21D)	4022	5679	6888	34
H(21E)	3850	6676	7608	34
H(21F)	4606	6427	7380	34
H(23A)	3971	13189	7689	36
H(23B)	3846	14163	6956	36
H(23C)	4587	13822	7223	36
H(23D)	5075	9851	7329	36
H(23E)	4504	11193	7723	36
H(23F)	4739	12097	7011	36
H(24A)	3472	8002	6979	30
H(24B)	3122	10437	6846	30
H(24C)	3364	9779	7577	30
H(24D)	3507	12026	6937	30
H(24E)	3365	10326	7547	30
H(24F)	3126	9639	6816	30
H(26)	4799	13744	6161	21
H(26A)	3903	12488	6022	21
H(27)	5108	13475	5052	22
H(27A)	4192	12585	4894	22
H(29)	4195	7284	4912	20
H(29A)	5022	6328	5040	20
H(30)	3880	7552	6021	19
H(30A)	4854	6314	6199	19
H(31A)	4554	9434	3893	24
H(31B)	5016	11663	3978	24
H(31C)	4945	8625	3918	24
H(31D)	4562	11042	3953	24
H(32)	6331	10792	4161	22
H(32A)	5048	14437	4037	22
H(33)	6955	7053	4106	25
H(33A)	6207	15978	4083	25

Table S6. Torsion angles [°] for 1-[[4-*tert*-butylphenyl]methyl]-1*H*-1,2,3-triazole.

N(1)-N(2)-N(3)-C(13)	0.4(2)
N(1)-C(12)-C(13)-N(3)	0.4(3)
N(1A)-N(2A)-N(3A)-C(13A)	-6(3)
N(1A)-C(12A)-C(13A)-N(3A)	-2(3)
N(2)-N(1)-C(11)-C(8)	84.8(3)
N(2)-N(1)-C(12)-C(13)	-0.2(3)
N(2)-N(3)-C(13)-C(12)	-0.5(3)
N(2A)-N(1A)-C(11A)-C(8A)	44(7)
N(2A)-N(1A)-C(12A)-C(13A)	-1(3)
N(2A)-N(3A)-C(13A)-C(12A)	5(3)
C(1)-C(2)-C(5)-C(6)	145.07(19)
C(1)-C(2)-C(5)-C(10)	-39.9(3)
C(1A)-C(2A)-C(5A)-C(6A)	44(3)
C(1A)-C(2A)-C(5A)-C(10A)	-147(2)
C(2)-C(5)-C(6)-C(7)	173.3(2)
C(2)-C(5)-C(10)-C(9)	-173.91(19)
C(2A)-C(5A)-C(6A)-C(7A)	169(2)
C(2A)-C(5A)-C(10A)-C(9A)	-162(2)
C(3)-C(2)-C(5)-C(6)	24.9(3)
C(3)-C(2)-C(5)-C(10)	-160.15(19)
C(3A)-C(2A)-C(5A)-C(6A)	-77(3)
C(3A)-C(2A)-C(5A)-C(10A)	92(3)
C(4)-C(2)-C(5)-C(6)	-94.4(2)
C(4)-C(2)-C(5)-C(10)	80.6(2)
C(4A)-C(2A)-C(5A)-C(6A)	156(2)
C(4A)-C(2A)-C(5A)-C(10A)	-35(3)
C(5)-C(6)-C(7)-C(8)	1.0(3)
C(5A)-C(6A)-C(7A)-C(8A)	2(4)
C(6)-C(5)-C(10)-C(9)	1.3(3)
C(6)-C(7)-C(8)-C(9)	0.5(3)
C(6)-C(7)-C(8)-C(11)	-177.1(2)
C(6A)-C(5A)-C(10A)-C(9A)	7(4)
C(6A)-C(7A)-C(8A)-C(9A)	-14(5)
C(6A)-C(7A)-C(8A)-C(11A)	-165(2)
C(7)-C(8)-C(9)-C(10)	-1.1(3)
C(7)-C(8)-C(11)-N(1)	98.6(2)
C(7A)-C(8A)-C(9A)-C(10A)	20(5)
C(7A)-C(8A)-C(11A)-N(1A)	103(4)

C(8)-C(9)-C(10)-C(5)	0.1(3)
C(8A)-C(9A)-C(10A)-C(5A)	-14(3)
C(9)-C(8)-C(11)-N(1)	-79.0(3)
C(9A)-C(8A)-C(11A)-N(1A)	-54(6)
C(10)-C(5)-C(6)-C(7)	-1.9(3)
C(10A)-C(5A)-C(6A)-C(7A)	0(4)
C(11)-N(1)-N(2)-N(3)	-178.6(2)
C(11)-N(1)-C(12)-C(13)	178.1(2)
C(11)-C(8)-C(9)-C(10)	176.6(2)
C(11A)-N(1A)-N(2A)-N(3A)	-147(4)
C(11A)-N(1A)-C(12A)-C(13A)	162(3)
C(11A)-C(8A)-C(9A)-C(10A)	165(3)
C(12)-N(1)-N(2)-N(3)	-0.1(3)
C(12)-N(1)-C(11)-C(8)	-93.4(3)
C(12A)-N(1A)-N(2A)-N(3A)	4(3)
C(12A)-N(1A)-C(11A)-C(8A)	-107(4)
N(21)-N(22)-N(23)-C(33)	0.2(3)
N(21)-C(32)-C(33)-N(23)	-0.6(3)
N(21A)-N(22A)-N(23A)-C(33A)	6(3)
N(21A)-C(32A)-C(33A)-N(23A)	2(3)
N(22)-N(21)-C(31)-C(28)	84.7(2)
N(22)-N(21)-C(32)-C(33)	0.7(3)
N(22)-N(23)-C(33)-C(32)	0.2(3)
N(22A)-N(21A)-C(31A)-C(28A)	76(3)
N(22A)-N(21A)-C(32A)-C(33A)	1(3)
N(22A)-N(23A)-C(33A)-C(32A)	-6(4)
C(21)-C(22)-C(25)-C(26)	-93.4(2)
C(21)-C(22)-C(25)-C(30)	83.1(2)
C(21A)-C(22A)-C(25A)-C(26A)	161(2)
C(21A)-C(22A)-C(25A)-C(30A)	-23(3)
C(22)-C(25)-C(26)-C(27)	175.85(19)
C(22)-C(25)-C(30)-C(29)	-175.72(19)
C(22A)-C(25A)-C(26A)-C(27A)	178(2)
C(22A)-C(25A)-C(30A)-C(29A)	178(2)
C(23)-C(22)-C(25)-C(26)	24.6(3)
C(23)-C(22)-C(25)-C(30)	-158.89(19)
C(23A)-C(22A)-C(25A)-C(26A)	-79(3)
C(23A)-C(22A)-C(25A)-C(30A)	98(3)
C(24)-C(22)-C(25)-C(26)	146.28(19)
C(24)-C(22)-C(25)-C(30)	-37.2(3)

C(24A)-C(22A)-C(25A)-C(26A)	33(3)
C(24A)-C(22A)-C(25A)-C(30A)	-150(2)
C(25)-C(26)-C(27)-C(28)	-0.4(3)
C(25A)-C(26A)-C(27A)-C(28A)	-5(4)
C(26)-C(25)-C(30)-C(29)	0.9(3)
C(26)-C(27)-C(28)-C(29)	1.3(3)
C(26)-C(27)-C(28)-C(31)	-177.5(2)
C(26A)-C(25A)-C(30A)-C(29A)	-6(4)
C(26A)-C(27A)-C(28A)-C(29A)	11(5)
C(26A)-C(27A)-C(28A)-C(31A)	-177(2)
C(27)-C(28)-C(29)-C(30)	-1.1(3)
C(27)-C(28)-C(31)-N(21)	98.2(2)
C(27A)-C(28A)-C(29A)-C(30A)	-15(5)
C(27A)-C(28A)-C(31A)-N(21A)	93(3)
C(28)-C(29)-C(30)-C(25)	0.0(3)
C(28A)-C(29A)-C(30A)-C(25A)	13(4)
C(29)-C(28)-C(31)-N(21)	-80.6(3)
C(29A)-C(28A)-C(31A)-N(21A)	-96(4)
C(30)-C(25)-C(26)-C(27)	-0.7(3)
C(30A)-C(25A)-C(26A)-C(27A)	2(4)
C(31)-N(21)-N(22)-N(23)	-175.6(2)
C(31)-N(21)-C(32)-C(33)	175.1(2)
C(31)-C(28)-C(29)-C(30)	177.7(2)
C(31A)-N(21A)-N(22A)-N(23A)	-174(2)
C(31A)-N(21A)-C(32A)-C(33A)	173(2)
C(31A)-C(28A)-C(29A)-C(30A)	175(3)
C(32)-N(21)-N(22)-N(23)	-0.6(3)
C(32)-N(21)-C(31)-C(28)	-89.3(3)
C(32A)-N(21A)-N(22A)-N(23A)	-5(3)
C(32A)-N(21A)-C(31A)-C(28A)	-93(2)

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