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Supporting information for article:

Solid-state structure and antimicrobial and cytotoxicity studies of a cucurbit[6]uril-like Cu6*L*4 constructed from 3,5-bis[(1*H*-tetrazol-5-yl)methyl]-4*H*-1,2,4-triazol-4-amine

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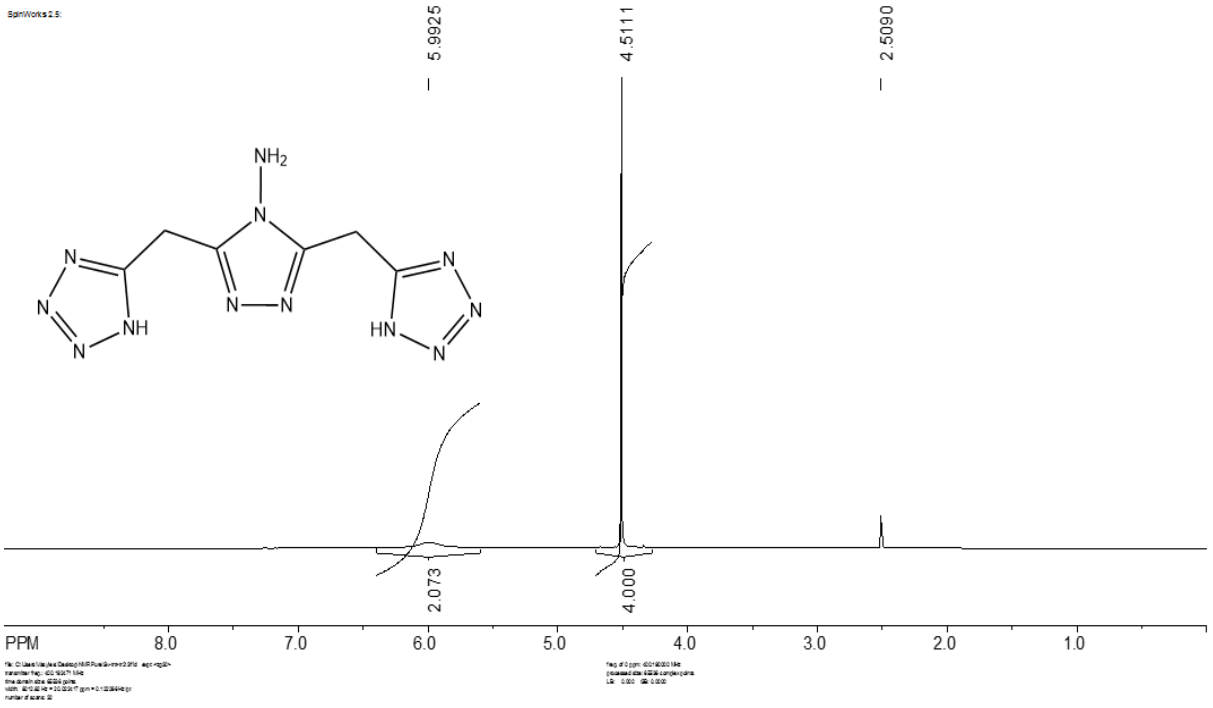

Figure S1 ^{1}H-NMR spectrum in d_6-DMSO of **L**.

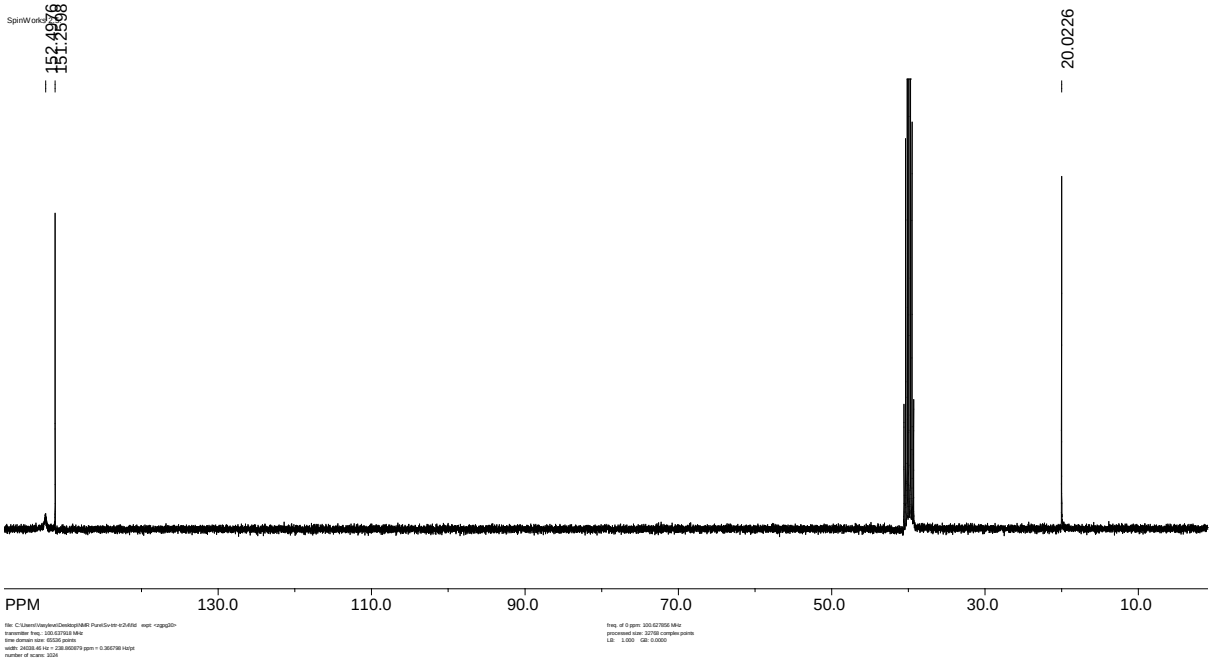

Figure S2 ^{13}C-NMR spectrum in d_6-DMSO of **L**.

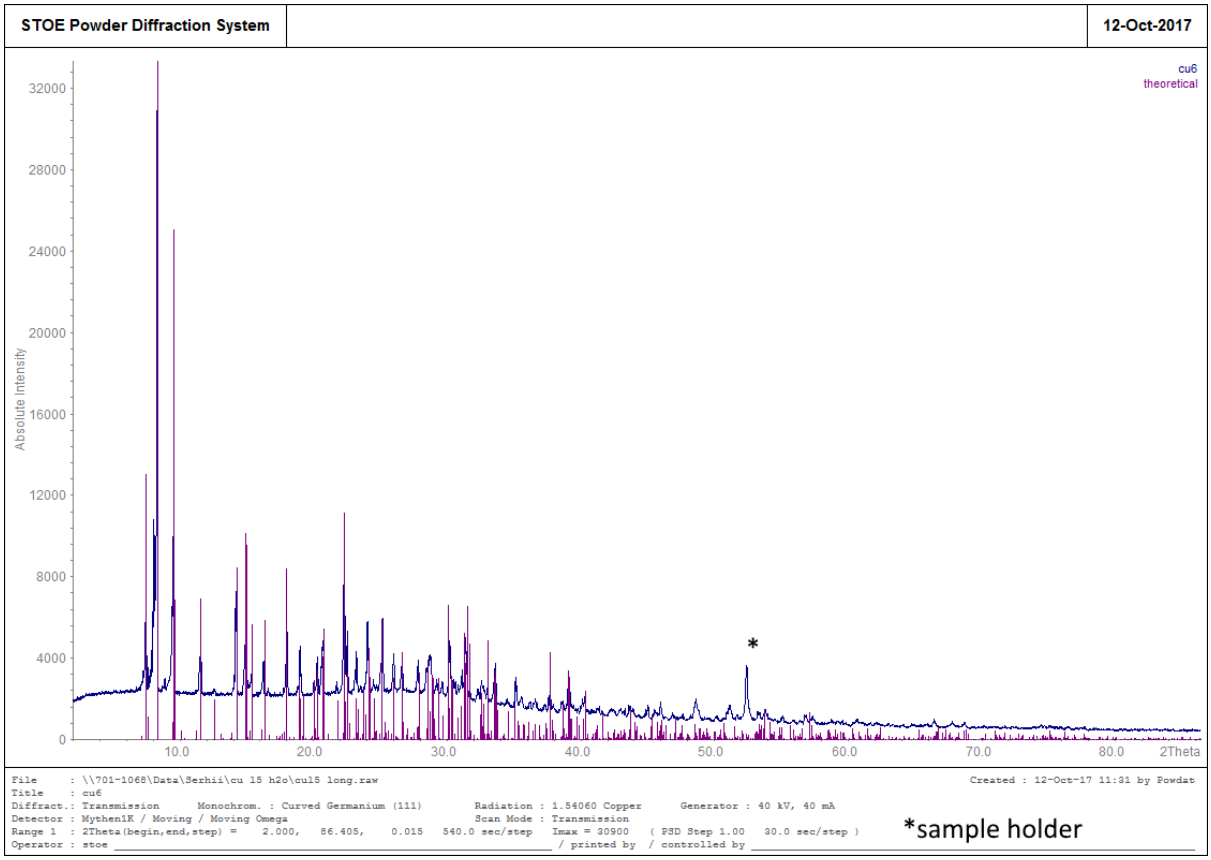

Figure S3 XPRD of Cu_6-complex (**1**): magenta-simulated; blue-obtained.

Table S1 Selected geometric parameters (Å)

Cu1—N1	1.977 (4)	Cu4—N16	1.990 (3)
Cu1—N2	1.992 (3)	Cu4—N14	1.993 (3)
Cu1—N3	1.995 (3)	Cu4—N13	1.994 (4)
Cu1—N4	2.006 (3)	Cu4—N15	2.003 (3)
Cu1—O2A	2.231 (11)	Cu4—O4B	2.246 (4)
Cu1—O2B	2.360 (4)	Cu4—O3A	2.346 (12)
Cu2—N6	1.977 (3)	Cu5—N18	1.980 (3)
Cu2—N8	1.983 (3)	Cu5—N19	1.984 (4)
Cu2—N7	1.988 (3)	Cu5—N20	1.991 (3)
Cu2—N5	1.999 (4)	Cu5—N17	2.000 (3)
Cu2—O4A	2.258 (11)	Cu5—O3B	2.233 (4)
Cu2—O2B	2.305 (4)	Cu5—O3A	2.387 (12)
Cu3—N12	1.997 (4)	Cu6—N24	2.003 (4)

Cu3—N10	2.012 (3)	Cu6—N21	2.017 (3)
Cu3—N9	2.025 (3)	Cu6—N23	2.018 (4)
Cu3—N11	2.040 (4)	Cu6—N22	2.022 (4)
Cu3—O3	2.165 (3)	Cu6—O6	2.182 (3)

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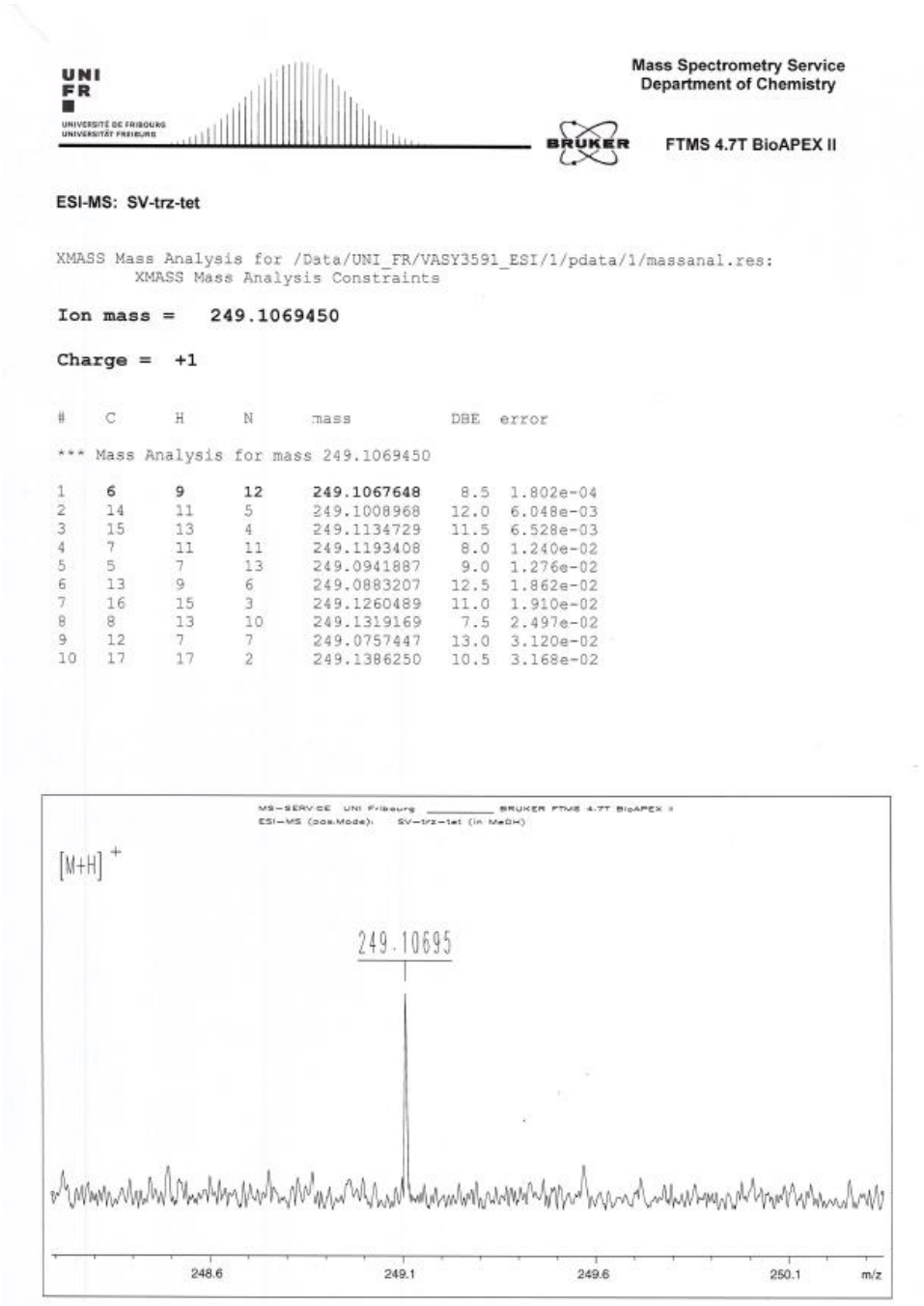

Figure S4 HR-MS of the **L** performed in MeOH solution.

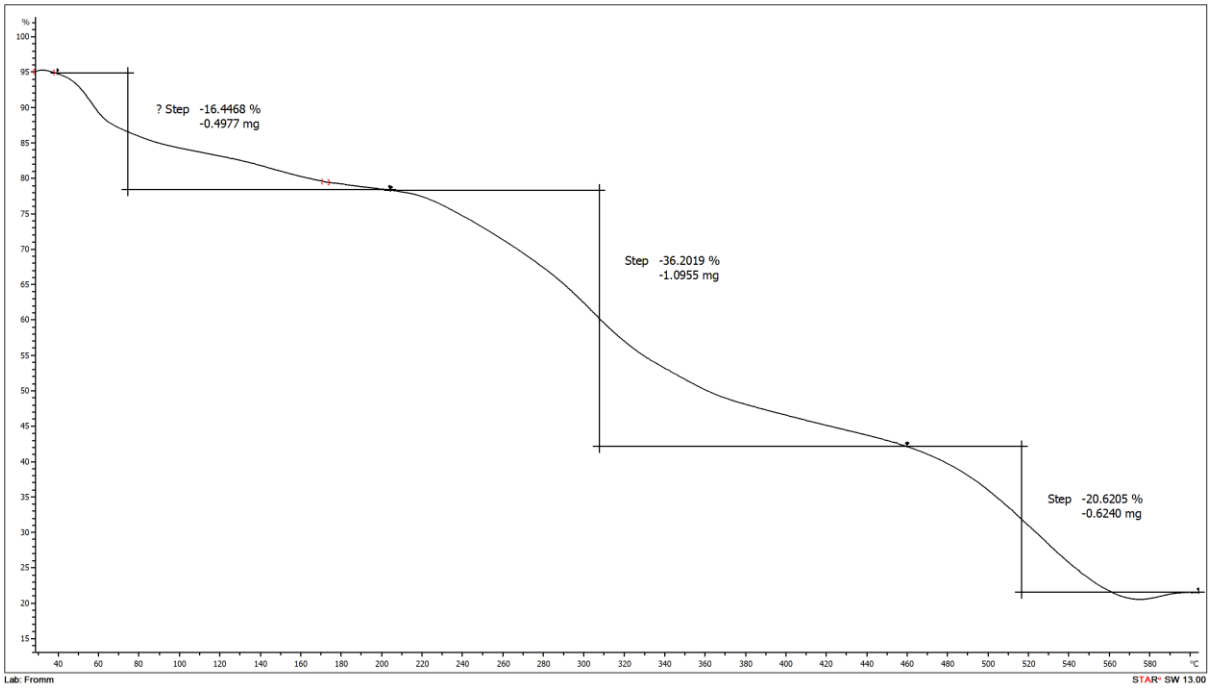

Figure S5 TGA of the complex, recorded in range 298 to 873 K.

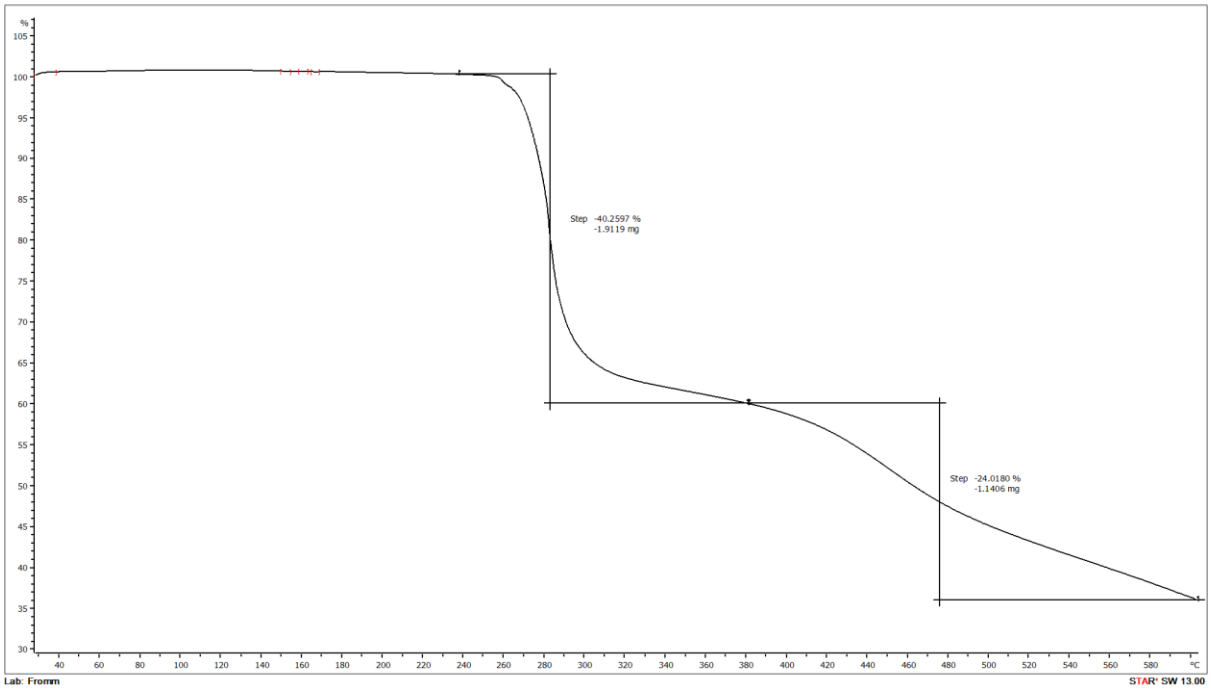

Figure S6 TGA of the ligand performed in range of 298 to 873 K.

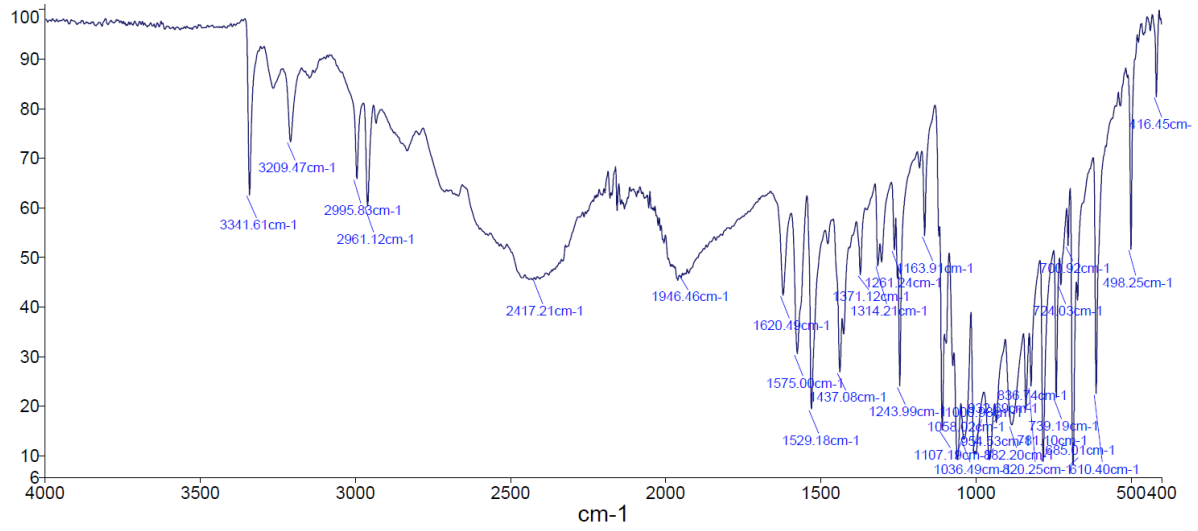

Figure S7 FT-IR of the ligand recorded in range 4000 – 400 cm^{-1}.

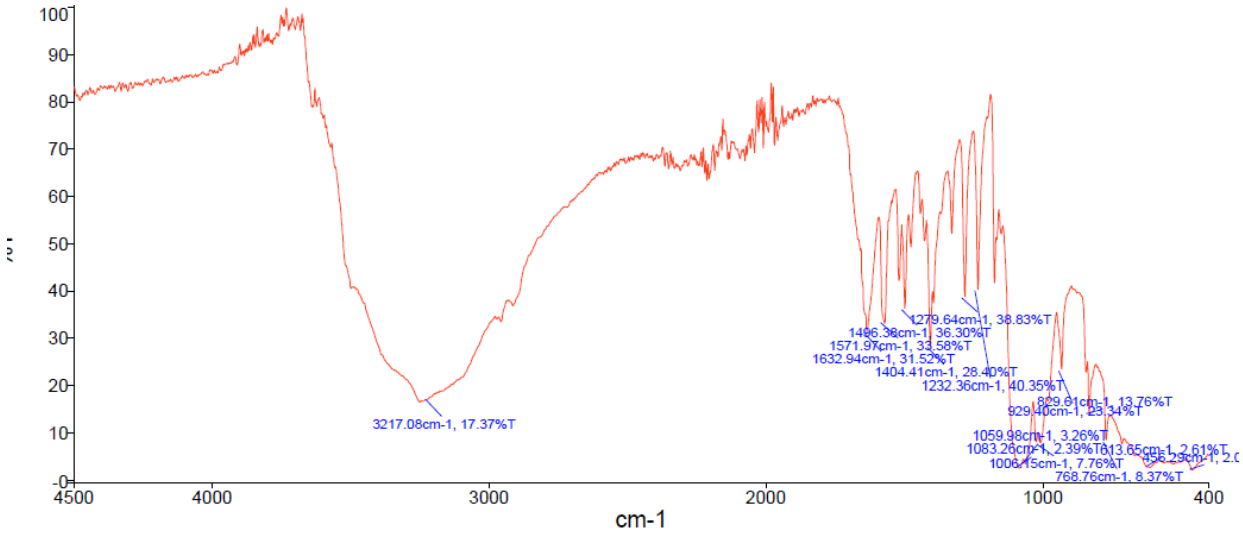

Figure S8 FT-IR of the complex recorded from 4500 – 400 cm^{-1} range.

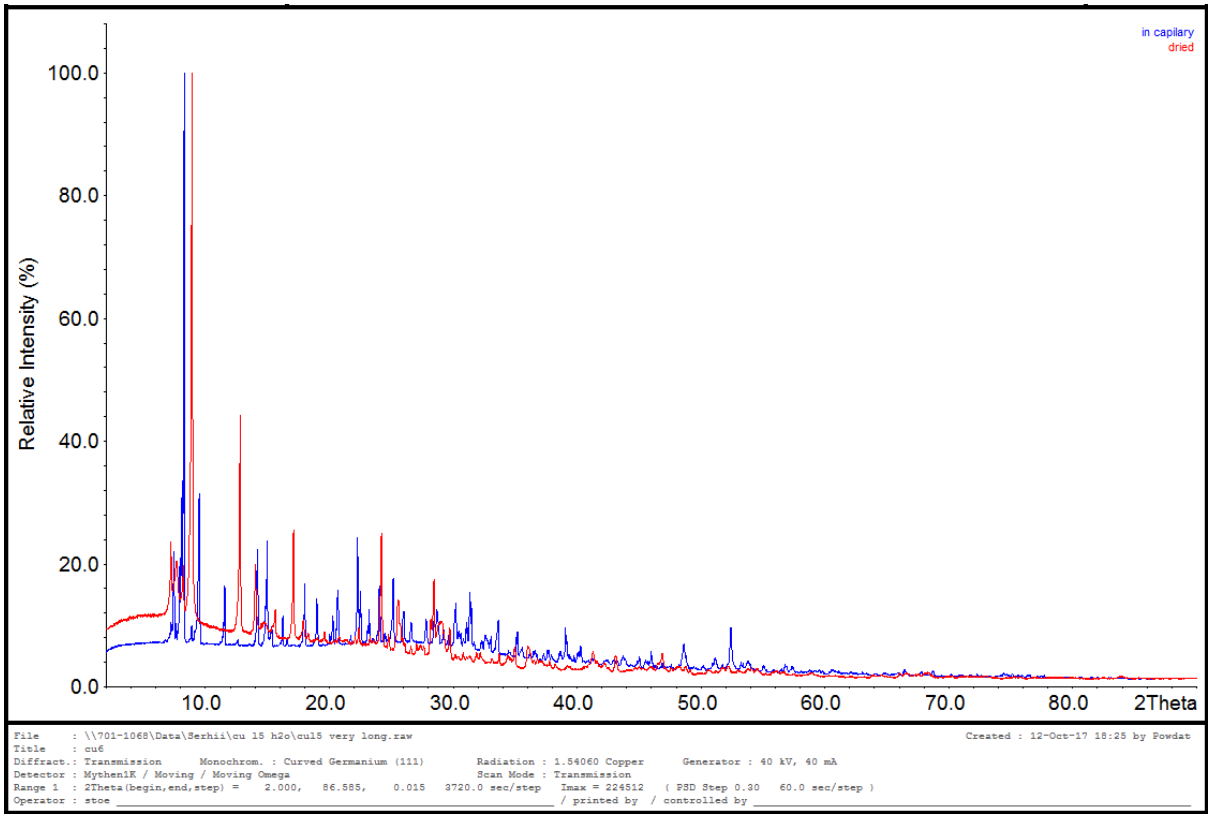

Figure S9 Comparison of complex in a non-dried and dried forms. Blue – measured in glass capillary with mother liquor, and red – dried crystals measured in range 2θ = 2 to 86.9°.

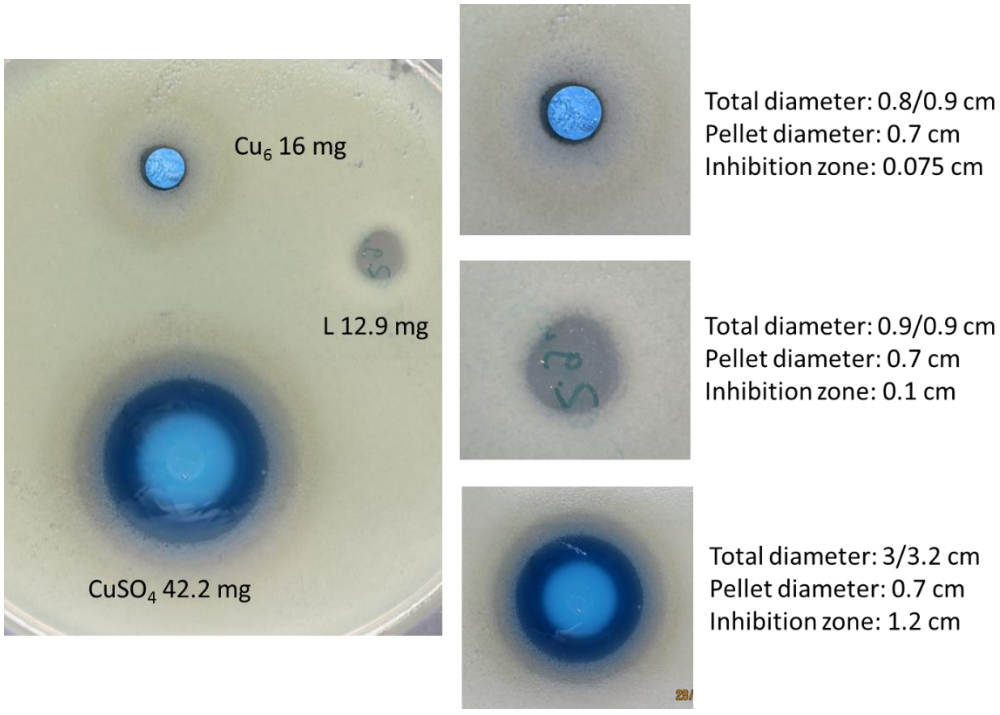

Figure S10. Kirby Bauer test of the Cu6-complex; L –ligand; and blank $CuSO_4$ against bacteria *E. coli*.

Table S2 Overview of the amount of substance used and the ZOI`s for the triplicates

	$CuSO_4 \cdot 5H_2O$			L			Cu_6		
Amount of substance [mmol]	0.17	0.29	0.16	0.05	0.04	0.04	0.05	0.03	0.02
ZOI [mm]	12	13	13	1	1.3	1.	0.8	0.5	0.5

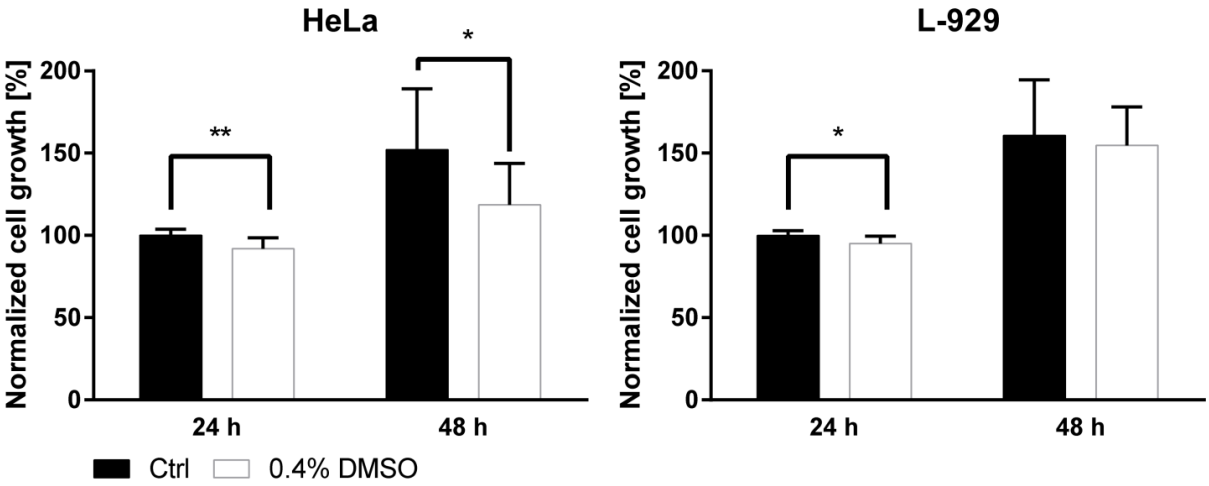

Figure S11. The effect of 0.4% DMSO on the HeLa and L-929 cell growth; cell growth was normalized to the 24 h Ctrl (in %); the bar chart represents the mean ± SD cell growth of 3 experiments (in triplicates) after 24 h and 48 h of 0.4% DMSO incubation time, statistical significance was determined via the multiple t-test (*$p < 0.05$, **$p < 0.01$, ***$p < 0.001$)

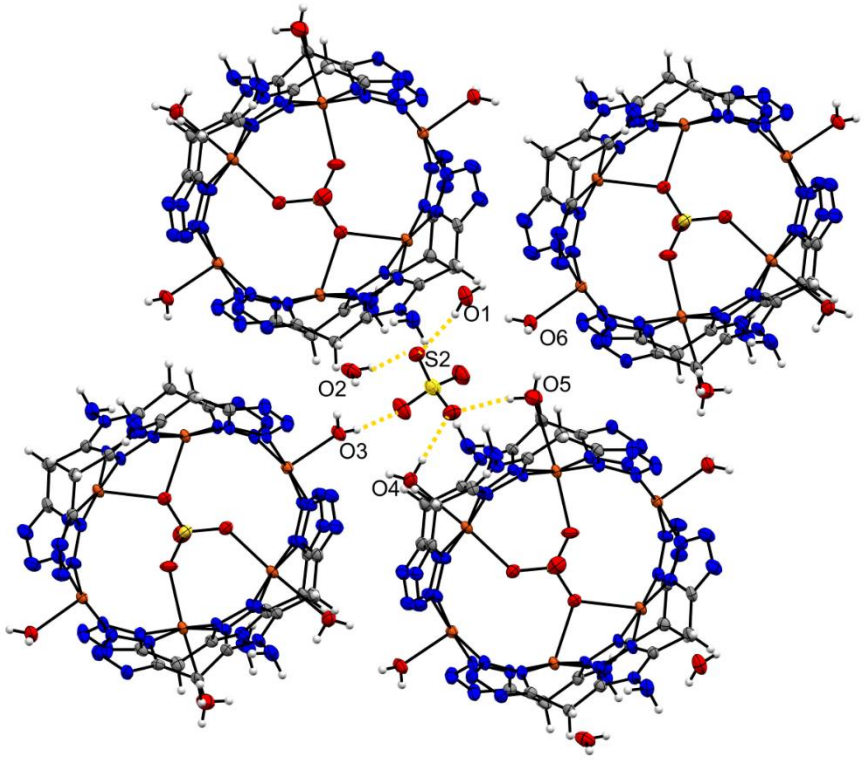

Figure S12. Formation of intermolecular hydrogen bonds between coordinated water molecules, O1 – O6 to uncoordinated SO_4^{2-}.