Electronic Supplementary Information (ESI)

Ternary coordination compounds of Cu(II) with glycine and 2,2'-bipyridine: Synthesis, structural characterization, magnetic and biological properties

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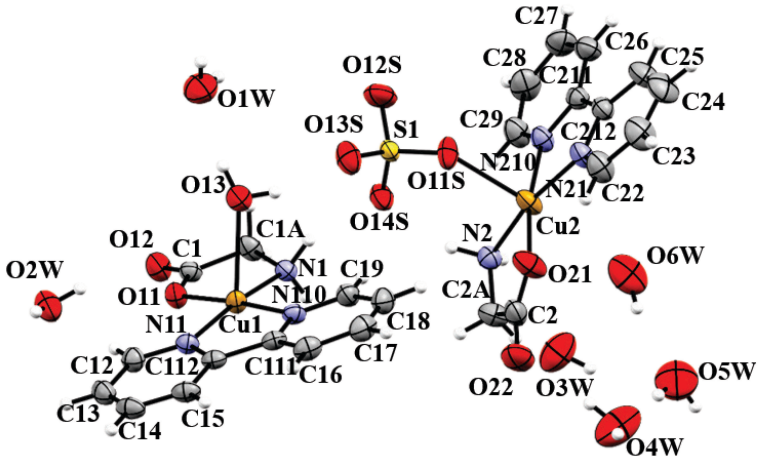
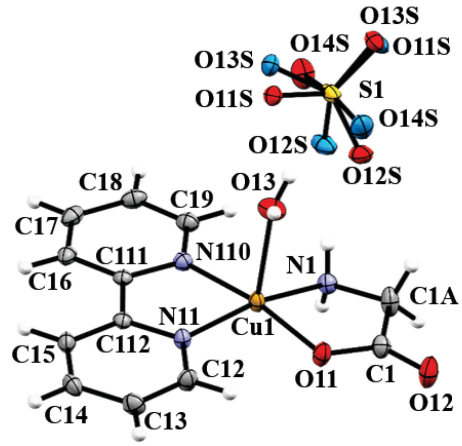
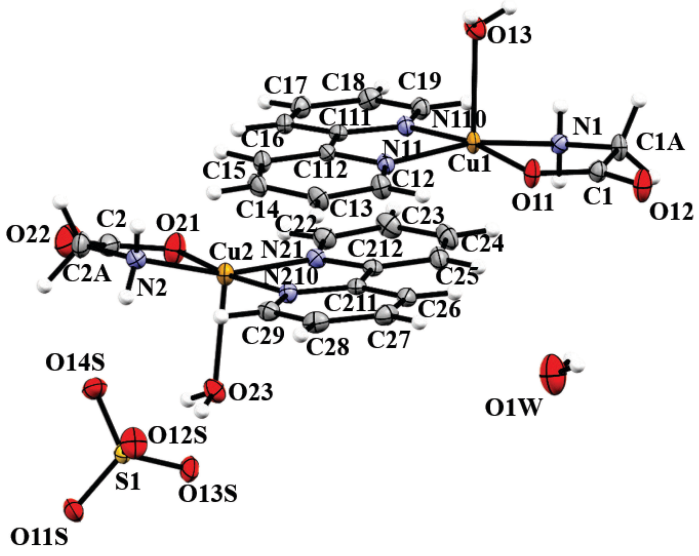


1a·6H₂O



1b



1b·H₂O

Figure S1. Asymmetric unit of **1a·6H₂O**, **1b** and **1b·H₂O**. Displacement ellipsoids of non-hydrogen atoms are drawn at the 50% probability level. Oxygen atoms of one disordered part of sulfate ions are shown in blue colour.

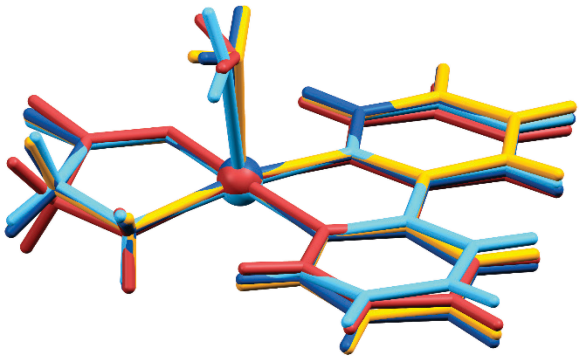


Figure S2. Overlapped complex cations of **1a·6H₂O** (light blue), **1b** (dark blue) and **1b·H₂O** (yellow and red).

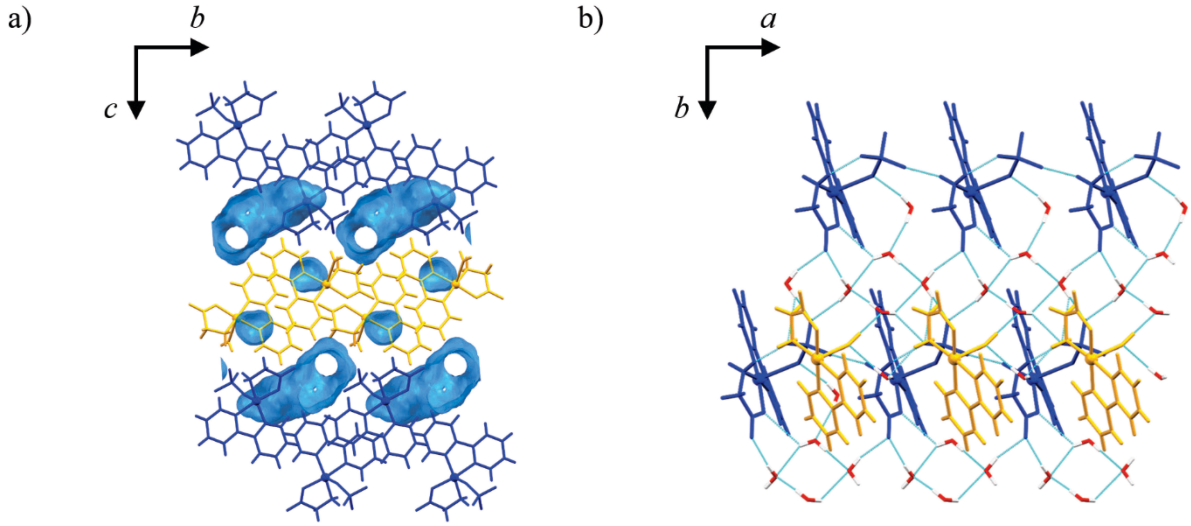


Figure S3. Packing of complex anions (blue) and cations (yellow) in **1a·6H₂O** a) in *b*-*c* plane and b) *a*-*b* plane. Blue surfaces in a) show contact surface around water molecules. Hydrogen bonds in b) are shown as cyan lines.

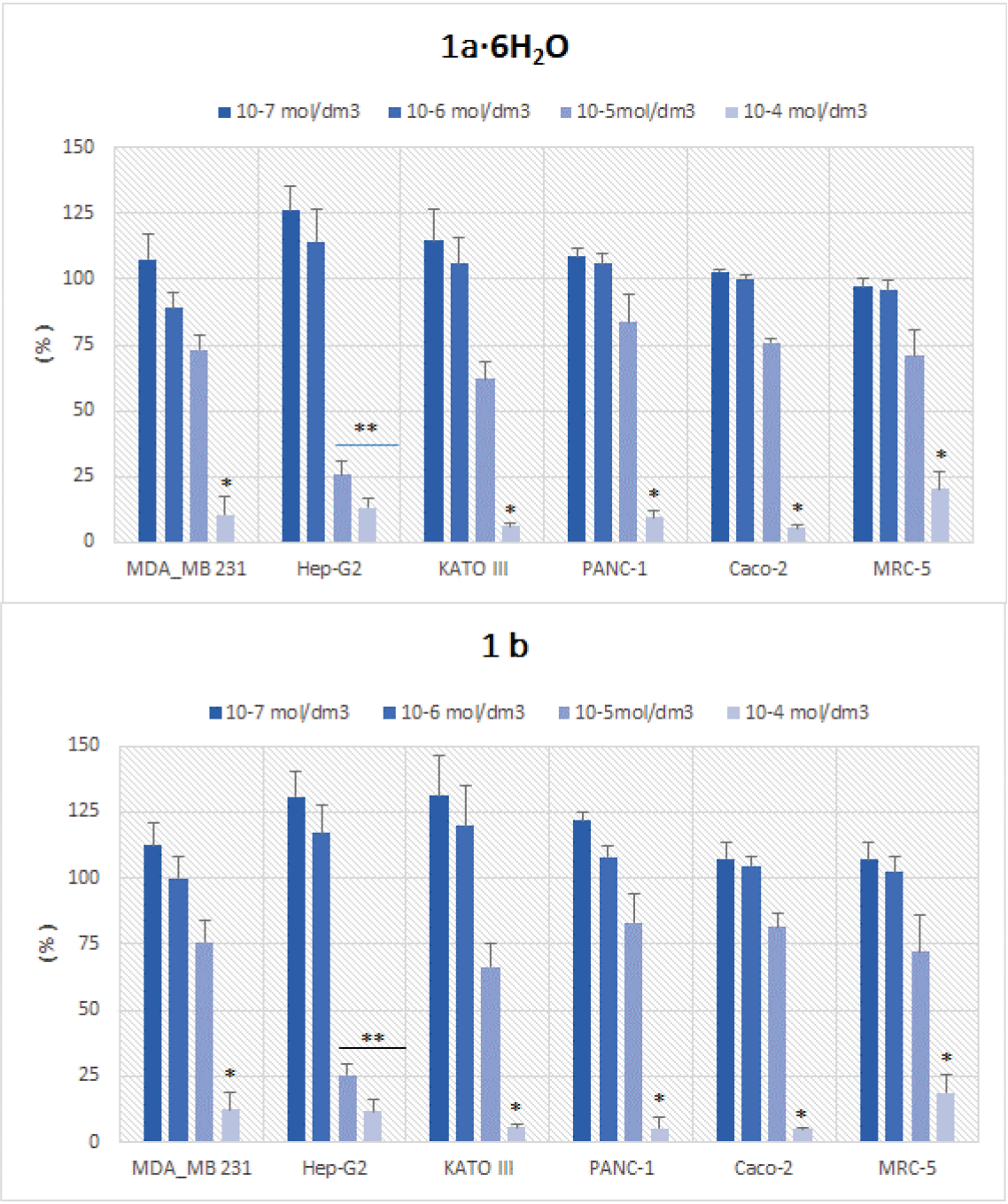


Figure S4. Antiproliferative effect of compounds **1a** and **1b**. Data are presented as mean (SD) of cell viability (%) obtained from three independent experiments done in triplicate. (*) statistically significant ($P < 0.05$) in respect to control group determined by Mann-Whitney U – test.

Table S1. Crystallographic data for coordination compounds **1a·6H₂O**, **1b** and **1b·H₂O**

Compound	**1a·6H₂O**	**1b**	**1b·H₂O**
Formula	$C_{24}H_{38}Cu_2N_6O_{15}S$	$C_{24}H_{28}Cu_2N_6O_{10}S$	$C_{24}H_{30}Cu_2N_6O_{11}S$
Formula weight	809.74	719.66	737.68
Space group	$P\bar{1}$	$C\,2/c$	$P\,2_1/c$
a/Å	7.3674(3)	21.6670(12)	20.1814(9)
b/Å	10.6440(5)	6.7922(3)	6.7748(3)
c/Å	21.6080(8)	21.0213(11)	20.9225(8)
α/°	85.638(3)	90	90
β/°	87.793(3)	121.389(7)	106.977(4)
γ/°	71.320(4)	90	90
V/Å^3	1600.38(12)	2640.9(3)	2736.0(2)
D_{calc}/g cm^{-3}	1.680	1.810	1.791
μ/mm^{-1}	1.474	1.761	1.705
F(000)	836	1472	1512
θ range/°	4.3–30.0	4.2–27.0	4.2–27.0
T/K	293	150	150
Radiation wavelength	0.71073	0.71073	0.71073
Range of h, k, l	-9–9, -13–14, -28–28	-27–27, -8–8, -26–26	-25–23, -8–8, -26–26
Reflections collected	30616	21309	31716
Independent reflections	7685	2875	5961
Observed reflections ($I \geq 2\sigma$)	6622	2489	5172
R_{int}	0.041	0.051	0.040
R^a, $wR^b[I \geq 2\sigma(I)]$	0.0389, 0.0992	0.0280, 0.0669	0.0316, 0.0751
Goodness-of-fit, S^c	1.05	1.05	1.05
No. of parameters	521	237	453
$\Delta\rho_{min}$, $\Delta\rho_{max}$ (e Å^{-3})	-0.89, 0.61	-0.27, 0.40	-0.57, 0.40
CCDC no.	2217106	2217105	2217107

[a] $R = \Sigma \left| \left| F_o \right| - \left| F_c \right| \right| / \Sigma \left| F_o \right|$; [b] $wR = [\Sigma(F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2]^{1/2}$; [c] $S = \Sigma[w(F_o^2 - F_c^2)^2 / (N_{obs} - N_{param})]^{1/2}$

Table S2. Selected bond lengths (Å) and angles (°) for compounds **1a·6H$_2$O**, **1b** and **1b·H$_2$O.**

	1a·6H$_2$O	**1b**	**1b·H$_2$O**
Cu1–O11	1.9423(15)	1.9469(19)	1.9473(16)
Cu1–O13	2.608(2)	2.2429(15)	2.2535(14)
Cu1–N1	1.981(2)	1.9860(19)	1.989(2)
Cu1–N11	1.9898(17)	1.9949(17)	1.9955(19)
Cu1–N110	1.9982(17)	2.017(2)	2.0140(19)
Cu2–O11S	2.3589(17)	-	-
Cu2–O21	1.9526(18)	-	1.9222(18)
Cu2–O23	-	-	2.2809(14)
Cu2–N2	1.978(2)	-	1.998(2)
Cu2–N21	1.988(2)	-	1.998(2)
Cu2–N210	2.0069(19)	-	2.0073(19)

Table S3. The geometry of selected hydrogen bonds for compounds **1a·6H$_2$O**, **1b** and **1b·H$_2$O**.

	D−H···A	D−H / Å	H···A / Å	D···A / Å	D−H···A /°
1a·6H$_2$O	N2−H2A···O14S	0.92(3)	2.07(4)	2.930(3)	155(3)
	N2−H2B···O13S[a]	0.85(3)	2.14(3)	2.925(3)	154(3)
	O1W−H1W2···O14S[b]	0.85(4)	2.40(5)	3.077(3)	138(4)
	O13−H13A···O13S	0.85(3)	1.92(3)	2.736(3)	164(3)
	O6W−H6W1···O11S[a]	0.85(3)	2.04(3)	2.876(3)	167(3)
1b	N1−H1A···O12S	0.84(3)	2.17(3)	3.002(4)	175(3)
	N1−H1A···O12S[c]	0.84(3)	1.97(3)	2.752(4)	154(3)
	N1−H1B···O11S[d]	0.88(3)	2.14(3)	2.956(4)	154(3)
	N1−H1B···O13S[d]	0.88(3)	2.00(3)	2.868(4)	168(3)
	O13−H13A···O11[e]	0.83(3)	2.05(3)	2.856(3)	163(3)
	O13−H13B···O11S	0.829(18)	2.09(3)	2.807(4)	145(3)
	O13−H13B···O14S[f]	0.829(18)	1.967(16)	2.737(4)	154(3)
1b·H$_2$O	N1−H1A···O12S[g]	0.87(3)	2.10(3)	2.958(3)	170(3)
	N1−H1A···O12S[g]	0.89(3)	2.01(3)	2.890(3)	170(2)
	N1−H1A···O12S[h]	0.84(3)	2.14(3)	2.947(3)	159(3)
	N1−H1A···O12S[i]	0.87(3)	2.03(3)	2.899(3)	173(2)
	O1W−H1W1···O14S[g]	0.84(2)	2.05(2)	2.868(3)	164(3)

[a]-1+*x*,*y*,*z*; [b]1+*x*,*y*,*z*; [c]-*x*,*y*,1/2-*z*; [d]*x*,1+*y*,*z*; [e]-*x*,-*y*,1-*z*; [f]-*x*,*y*,1/2-*z*; [g]*x*,-1+*y*,-1+*z*; [h]*x*,1/2-*y*,-1/2+*z* ;[i]*x*,3/2-*y*,-1/2+*z*