Copper(II) Complexes with Mixed Heterocycle Ligands as Promising Antibacterial and Antitumor Species

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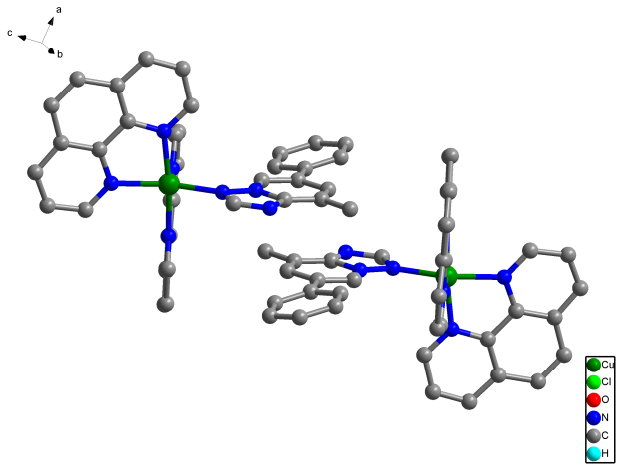

Figure S1. Supramolecular dimers of $[Cu(phen)_2(pmtp)](ClO_4)_2$ (**2**) generated through intermolecular π-π stacking interactions.

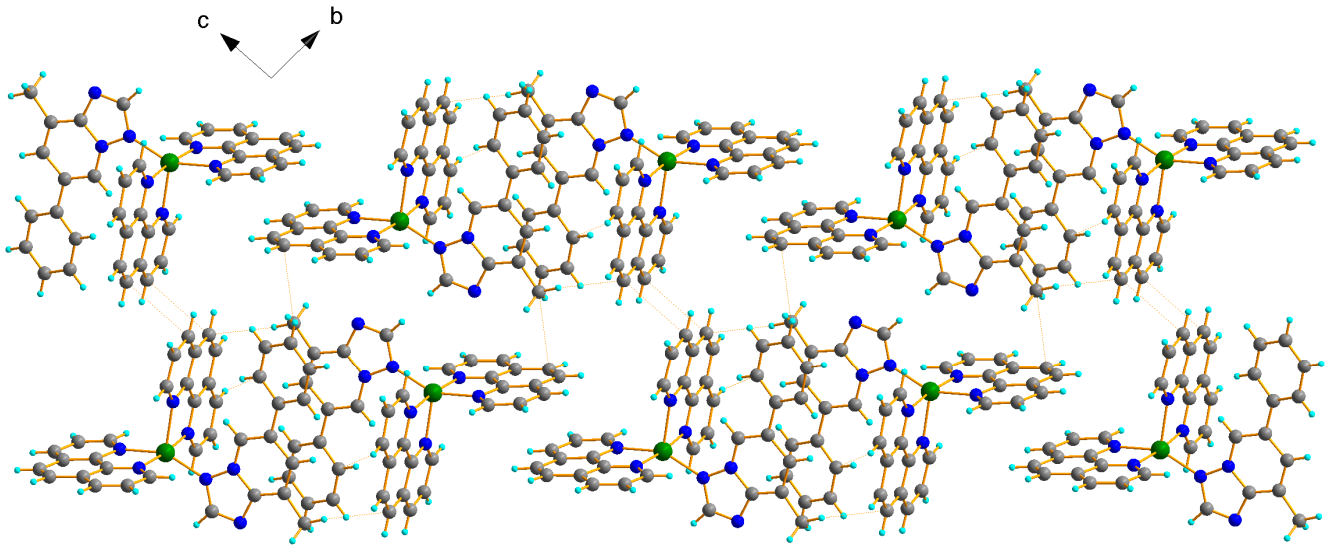

Figure S2. Packing diagram of $[Cu(phen)_2(pmtp)](ClO_4)_2$ (**2**) showing the supramolecular chains along a axes.

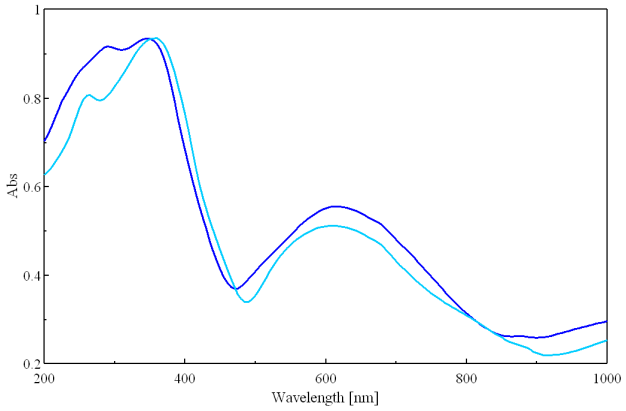

Figure S3. UV-Vis spectra of complex (**1**) (dark blue) and complex (**2**) (light blue).

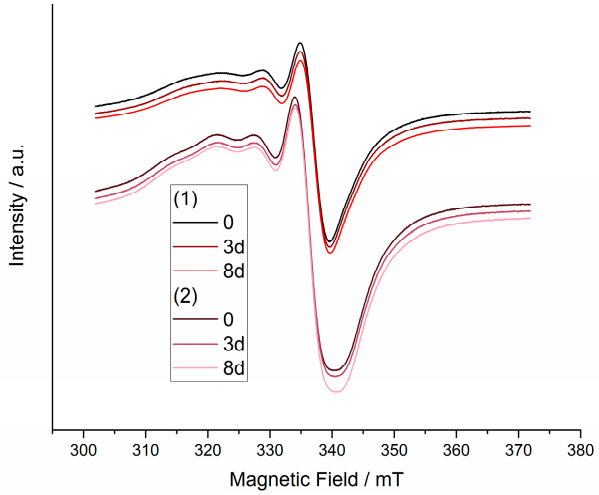

Figure S4. EPR spectra of complex (**1**) and (**2**) in DMSO.

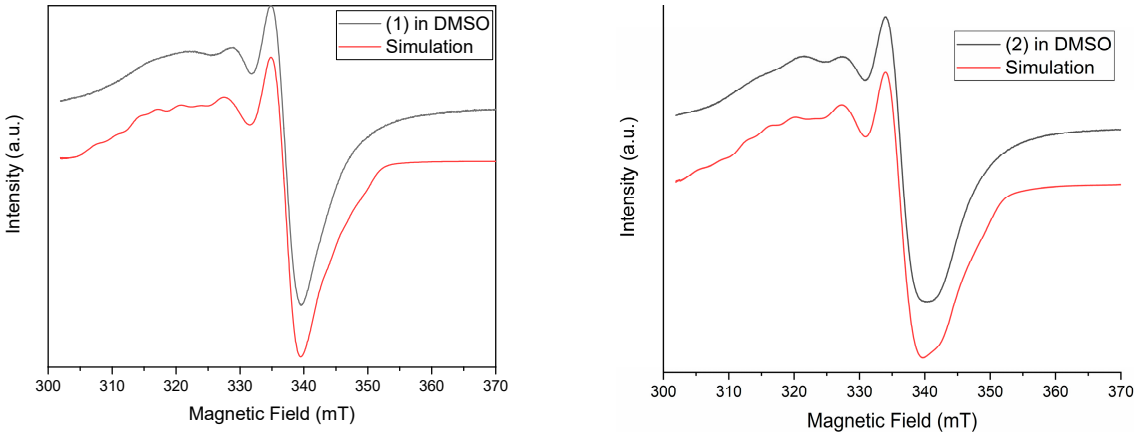

Figure S5. EPR spectra (registered and simulated) of complex (**1**) and (**2**) in DMSO.

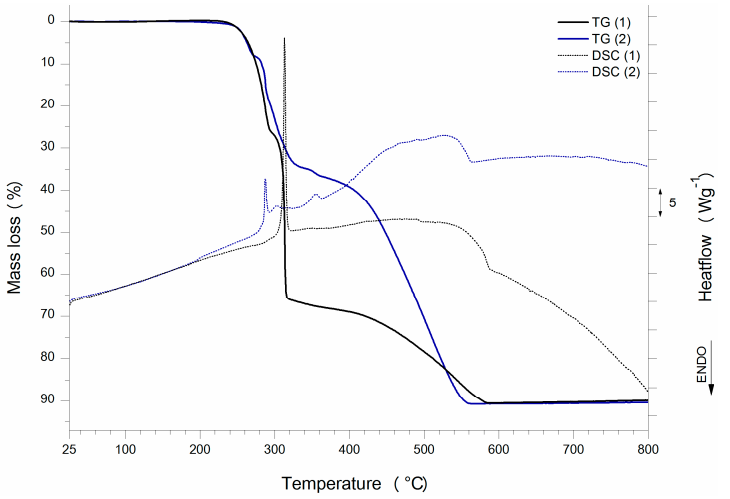

Figure S6. TG and DSC curves for complexes.

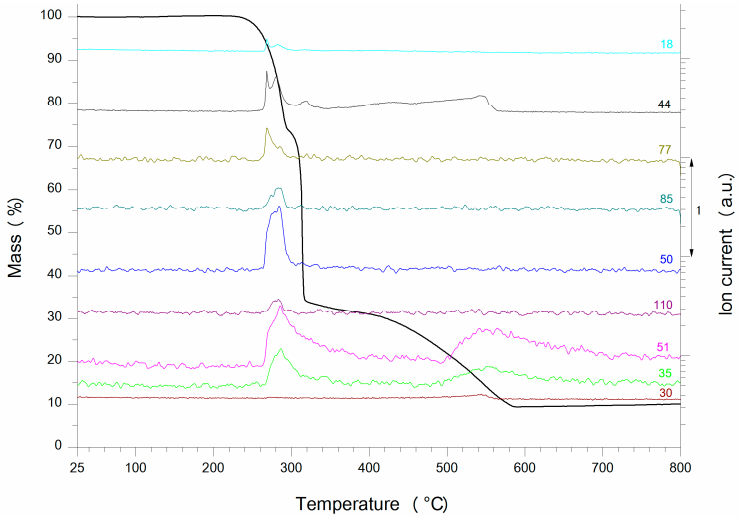

Figure S7. TG curve together with evolved gases for complex (**1**).

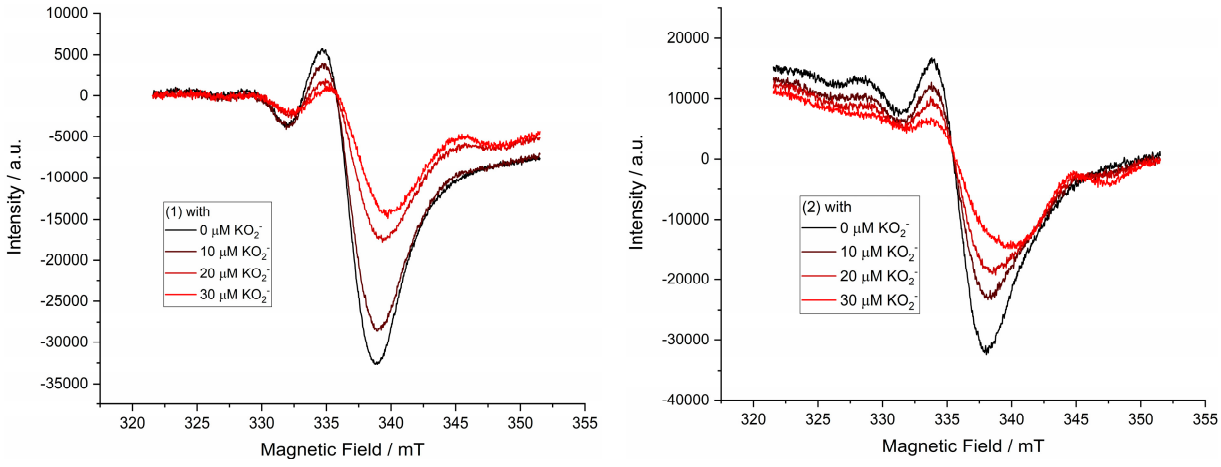

Figure S8. EPR spectra of complex (**1**) and (**2**) modification in interaction with superoxide.

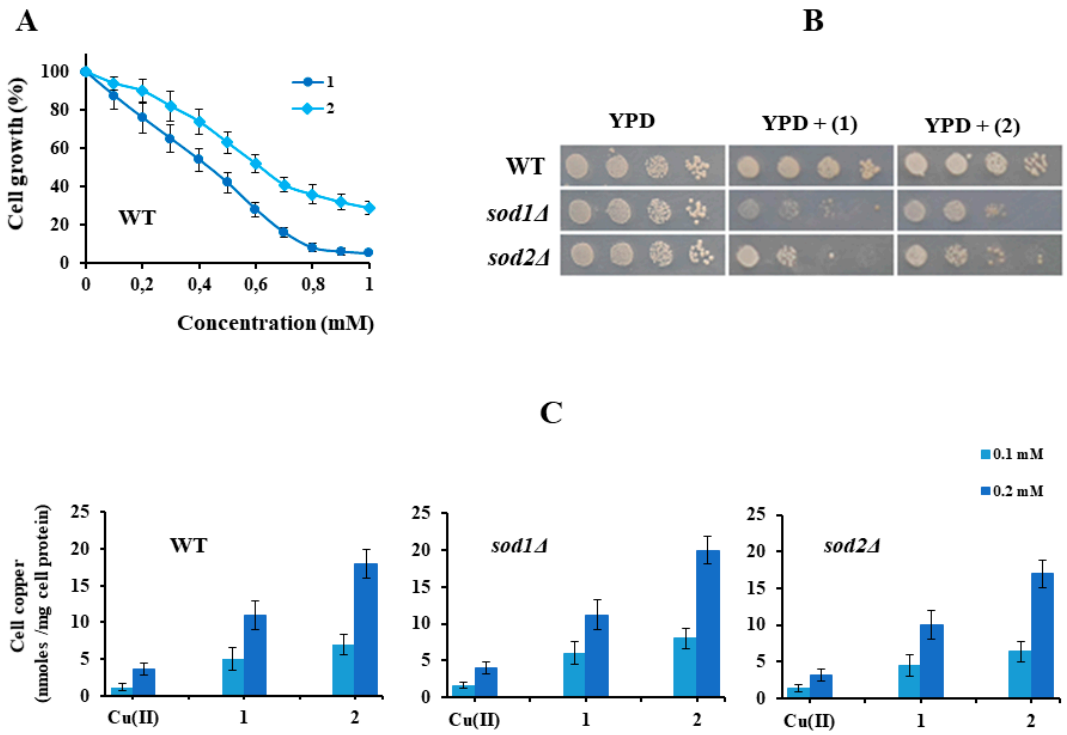

Figure S9. Effect of compounds (**1**) and (**2**) on *Saccharomyces cerevisiae* (effect on growth yeast cell proliferation determined after 16 hours of exposure to various concentrations of complexes expressed relatively to cell growth in the absence of compounds (**A**), effect of compounds on growth of superoxide dismutase-deficient mutants *sod1Δ* and *sod2Δ* (**B**) and compound's uptake expressed as copper accumulation (**C**)).

Table S1. Continuous shape measure for the coordination polyhedron around the Cu(II) atom.

Geometry	Cu1 (compound 1)	Cu2 (compound 1)	Cu1 (compound 2)
PP-5	29.381	28.943	29.021
vOC-5	5.897	6.019	2.779
TBPY-5	0.891	0.957	2.277
SPY-5	4.307	4.487	2.381
JTBPY-5	4.513	4.331	5.488

Table S2. Thermal data for complexes in air atmosphere.

Compound	Step	Thermal effect	Temperature range / °C	Δm_{exp} /%	Identified product by EGA with corresponding *m*/*z* values
(**1**)	1.	Exothermic	198-294	27.00	moieties from pmtp (15 (CH_3), 60, 61 ($C_2H_9N_2$), 77, 78 (C_6H_5), 85 ($C_2H_5N_4$), 109, 110 ($C_5H_8N_3$)), moieties from dipy (80 (C_5H_6N), 112, 113 ($C_6H_{13}N_2$)), moieties from perchlorate (Cl (35), CHCl (49), ClO (50, 51), Cl_2 (70)), H_2O (18), CO_2 (44)
	2.	Exothermic	294-356	41.15	moieties from perchlorate (Cl (35), CHCl (49), ClO (50, 51), ClO_2 (69), Cl_2 (70), HCl_2 (72)), 44(CO_2)
	3.	Exothermic	356-660	22.68	moieties from perchlorate (Cl (35), ClO (51), ClO_2 (69), Cl_2 (70), HCl_2 (72)), 30 (NO), 44(CO_2)
(**2**)	1.	Exothermic	195-266	8.18	moieties from pmtp (15 (CH_3), 77, 78 (C_6H_5), 85 ($C_2H_5N_4$), 110 ($C_5H_8N_3$)), moieties from dipy (112, 113 ($C_6H_{13}N_2$)), moieties from perchlorate (Cl (35), CHCl (49), ClO (50, 51), Cl_2 (70))
	2.	Exothermic	266-287	12.17	moieties from pmtp (15 (CH_3), 77, 78 (C_6H_5), 85 ($C_2H_5N_4$), 110 ($C_5H_8N_3$)), moieties from dipy (112, 113 ($C_6H_{13}N_2$)), moieties from perchlorate (Cl (35), CHCl (49), ClO (50, 51), Cl_2 (70)), H_2O (18), 44(CO_2)
	3.	Exothermic	287-358	16.43	ClO (50, 51), 30 (NO), 44(CO_2)
	4.	Exothermic	358-570	53.96	ClO (50, 51), 30 (NO), 44(CO_2)