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Electronic Supplementary Information

Tailoring copper(II) complexes with pyridine-4,5-dicarboxylate esters for anti-*Candida* activity

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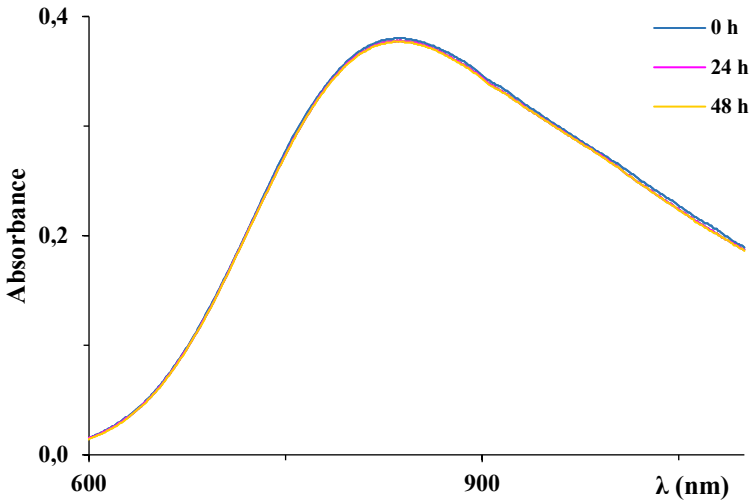

Fig. S1 Time stability of complex **1** followed by UV-Vis spectrophotometry at room temperature in DMSO.

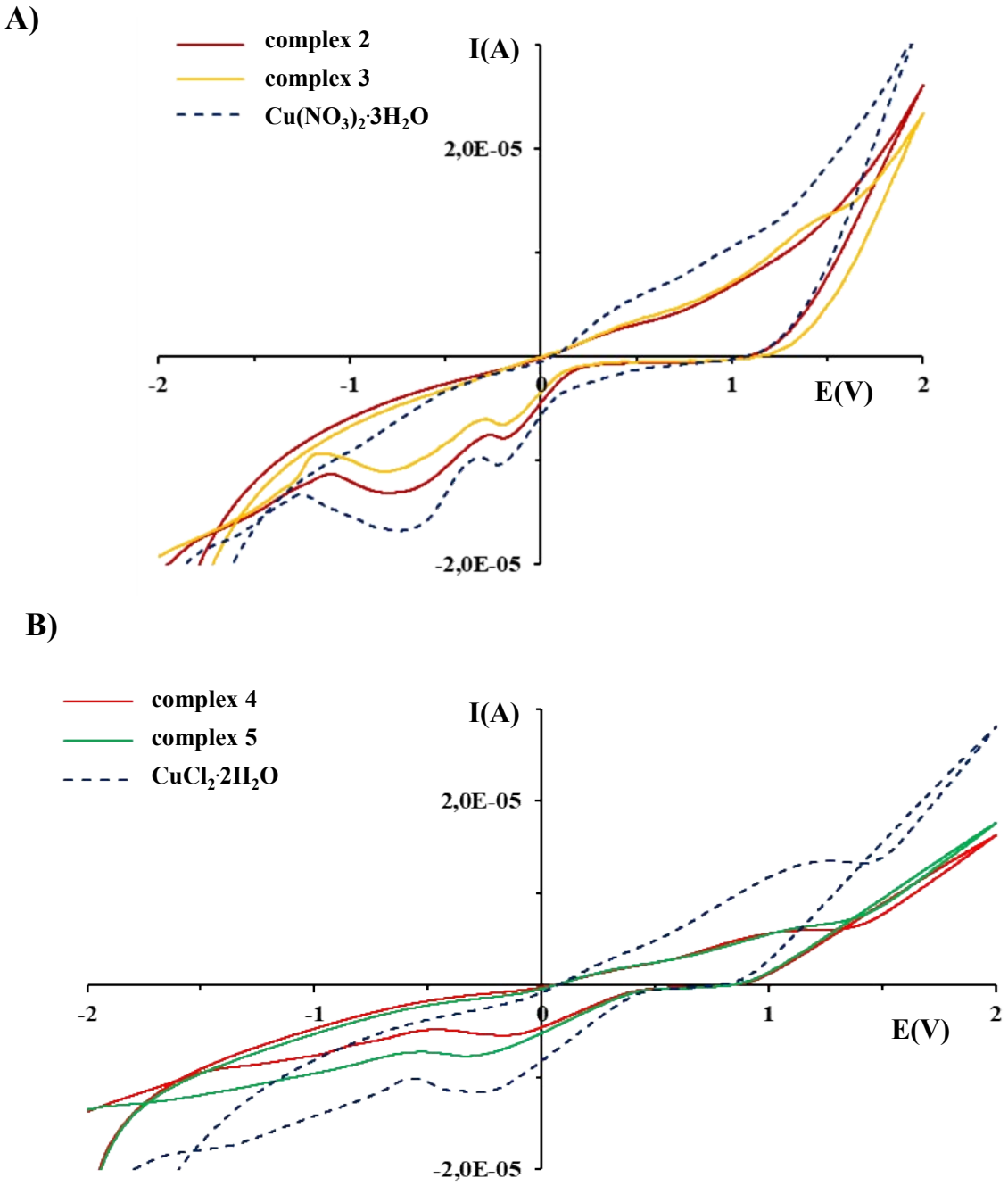

Fig. S2 Cyclic voltammograms of the copper(II) complexes **2** and **3** (**A**) and **4** and **5** (**B**), alongside the corresponding CuX_2 salt (X = NO_3^- and Cl^-) at GC electrode in DMSO and 0.1 M TBAHP as a supporting electrolyte with a scan rate of 50 mV s^{-1}. The conditions were the following: E_{begin} = -2.0 V, E_{end} = 2.0 V and E_{step} = 0.002 V.

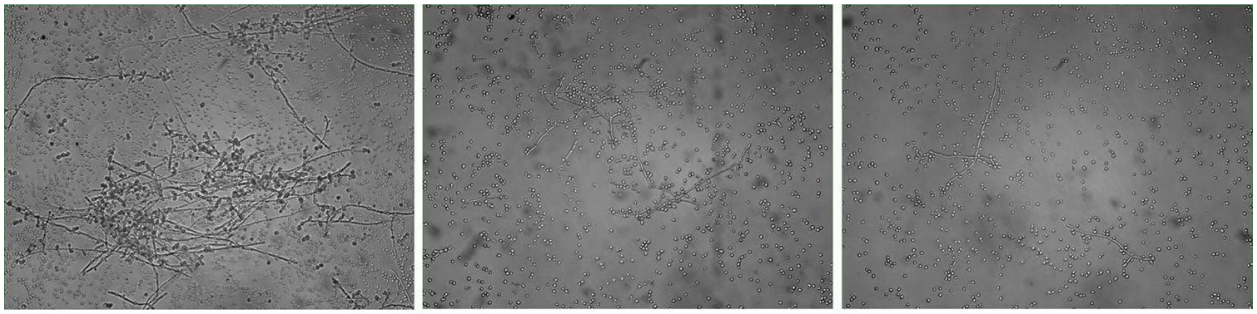

Fig. S3 Filamentation of *C. albicans* ATCC 10231 in presence of subinhibitory concentrations (0.5 × MIC) of complexes **1** and **4** in liquid RPMI medium (Olympus BX51, Applied Imaging Corp., San Jose, CA, United States, under 20 × magnification).

Table S1 Values of the binding constants of copper(II) complexes **1 – 5** with ct-DNA.

Complex	K_{sv} (M^{-1})	Hypochromism (%)	K_q ($M^{-1}s^{-1}$)	K_A (M^{-1})	n
1	$(1.06\pm0.01)\cdot10^3$	15.6	$1.06\cdot10^{11}$	$8.75\cdot10^2$	0.97
2	$(8.15\pm0.40)\cdot10^2$	12.0	$8.15\cdot10^{10}$	$8.51\cdot10^2$	0.99
3	$(9.66\pm0.15)\cdot10^2$	15.4	$9.66\cdot10^{10}$	$1.12\cdot10^2$	0.75
4	$(1.22\pm0.03)\cdot10^3$	17.1	$1.22\cdot10^{11}$	$7.09\cdot10^2$	0.93
5	$(1.01\pm0.04)\cdot10^3$	15.5	$1.01\cdot10^{11}$	$3.55\cdot10^2$	0.86

Table S2 Details of the crystal structure determination for copper(II) complexes **1 – 5**.

Complex	**1**	**2**	**3**	**4**	**5**
CCDC No.	2041822	2041823	2041819	2041821	2041820
Empirical formula	$C_{12}H_{16}CuN_4O_{13}S$	$C_{13}H_{14}Cu_1N_4O_{11}S$	$C_{14}H_{16}Cu_1N_4O_{12}$	$C_{24}H_{20}Cl_4Cu_2N_4O_8S_2$	$C_{26}H_{24}Cl_4Cu_2N_4O_8S_2$
Formula weight	519.89	497.88	495.85	825.44	853.49
Temperature/K	150(2)	150(2)	150(2)	150(2)	150(2)
Crystal system	triclinic	monoclinic	monoclinic	triclinic	monoclinic
Space group	$P\bar{1}$	$P2_1/c$	Cc	$P\bar{1}$	$P2_1/c$
a/Å	7.8810(3)	9.1313(6)	10.3255(6)	7.7848(5)	12.0032(7)
b/Å	12.4005(4)	24.6456(11)	22.7235(11)	9.0261(6)	17.3134(8)
c/Å	20.9376(6)	8.5875(5)	8.0546(5)	11.9040(5)	7.6901(4)
α/°	79.593(3)	90	90	101.778(4)	90
β/°	88.991(2)	106.946(7)	101.849(6)	100.435(4)	99.719(5)
γ/°	88.486(3)	90	90	109.621(6)	90
Volume/Å^3	2011.66(12)	1848.67(19)	1849.59(19)	742.48(8)	1575.19(14)
Z	4	4	4	1	2
ρ_{calc}/g cm^{-3}	1.717	1.789	1.781	1.846	1.799
μ/mm^{-1}	1.265	1.364	1.259	6.887	1.878
F(000)	1060	1012	1012	414	860
Crystal size/mm^3	0.5 × 0.3 × 0.05	0.35 × 0.10 × 0.10	0.30 × 0.05 × 0.05	0.15 × 0.10 × 0.02	0.1 × 0.1 × 0.05
Radiation	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)	Cu Kα (λ = 1.54184)	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.696 to 60.912	5.228 to 60.76	6.134 to 60.586	7.882 to 150.492	4.706 to 54.962
Index ranges	-11 ≤ h ≤ 11, -17 ≤ k ≤ 17, -29 ≤ l ≤ 29	-6 ≤ h ≤12, -34 ≤ k ≤ 21, -12 ≤ l ≤ 9	-14 ≤ h ≤9, -32 ≤ k ≤ 21, -11 ≤ l ≤ 11	-9 ≤ h ≤ 9, -11 ≤ k ≤ 10, -14 ≤ l ≤ 12	-15 ≤ h ≤ 11, -22 ≤ k ≤ 22, -9 ≤ l ≤ 9
Reflections collected	25294	10122	5050	7240	8104
Independent reflections	10742 [R_{int} = 0.0300, R_{sigma} = 0.0389]	4849 [R_{int} = 0.0299, R_{sigma} = 0.0521]	3279 [R_{int} = 0.0284, R_{sigma} = 0.0494]	3047 [R_{int} = 0.0347, R_{sigma} = 0.0420]	3608 [R_{int} = 0.0277, R_{sigma} = 0.0374]
Data/restraints/ parameters	10742/6/594	4849/2/282	3279/6/298	3047/0/201	3608/0/211
Goodness-of-fit on F^2	1.057	1.031	1.053	1.074	1.048
Final R indexes [I ≥ 2σ (I)]	R_1 = 0.0378, wR_2 = 0.0961	R_1 = 0.0382, wR_2 = 0.0769	R_1 = 0.0336, wR_2 = 0.0714	R_1 = 0.0400, wR_2 = 0.1044	R_1 = 0.0315, wR_2 = 0.0732
Final R indexes [all data]	R_1 = 0.0473, wR_2 = 0.1029	R_1 = 0.0556, wR_2 = 0.0846	R_1 = 0.0391, wR_2 = 0.0745	R_1 = 0.0465, wR_2 = 0.1108	R_1 = 0.0400, wR_2 = 0.0787
Largest diff. peak/hole /e Å^{-3}	+1.135/-0.872	+0.484/-0.463	+0.501/-0.369	+0.772/-0.835	+0.55/-0.46