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SUPPLEMENTARY MATERIAL TO

DNA/BSA interactions and cytotoxic studies of tetradentate *N*,*N*,*O*,*O*-Schiff base copper(II) complexes

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THE INTRINSIC EQUILIBRIUM BINDING CONSTANT FOR DNA STUDIES

$$\frac{[DNA]}{\varepsilon_A - \varepsilon_f} = \frac{[DNA]}{\varepsilon_b - \varepsilon_f} \pm \frac{1}{K_b / (\varepsilon_b - \varepsilon_f)} \qquad \text{(Equation S-1)}$$

To determine the intrinsic binding constant K_b, the ratio of the intercept of the curve [DNA]/(ε_A - ε_f) versus [DNA], where [DNA] is the DNA concentration in base pairs and the slope was used. The apparent extinction coefficient ε_A is consistent with A_{obsd}/[complex]. The extinction coefficients ε_f and ε_b refer to the unbound and fully bound complex, respectively.

STERN-VOLMER EQUATION FOR DNA AND BSA STUDIES

Stern-Volmer quenching constant, K_{sv}, for DNA and BSA as well as the quenching rate constant, k_q, for BSA were calculated using the Stern-Volmer equation:

$$\frac{I_0}{I} = 1 + K_{sv}[Q] \qquad \text{(Equation S-2)}$$

In Equation S-2, the total concentration of the quencher is given by [Q], while I_0 describes the emission intensity in the absence of the quencher and the emission intensity in the presence of the quencher is described by I.

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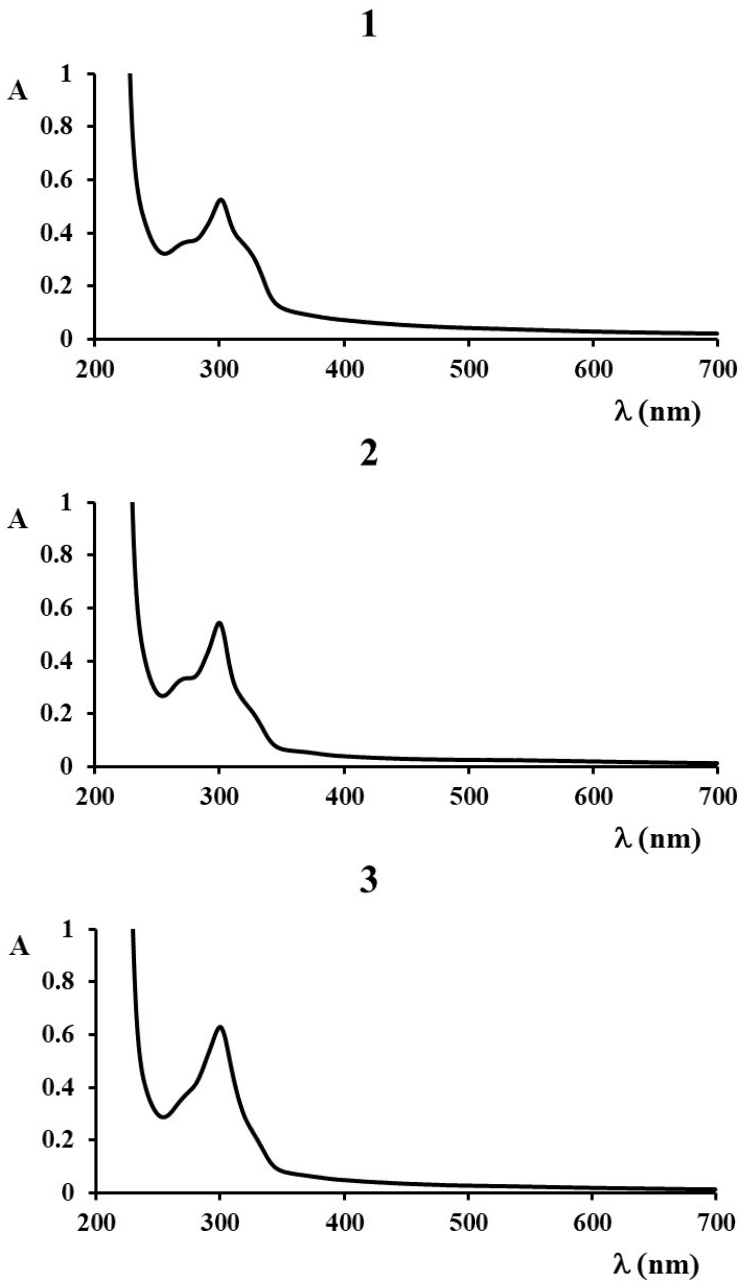


Fig. S-1. UV-Vis spectra of studied complexes [Cu(acac2pn)] (1), [Cu(phacac2pn)] (2), [Cu(tfacac2pn)] (3)

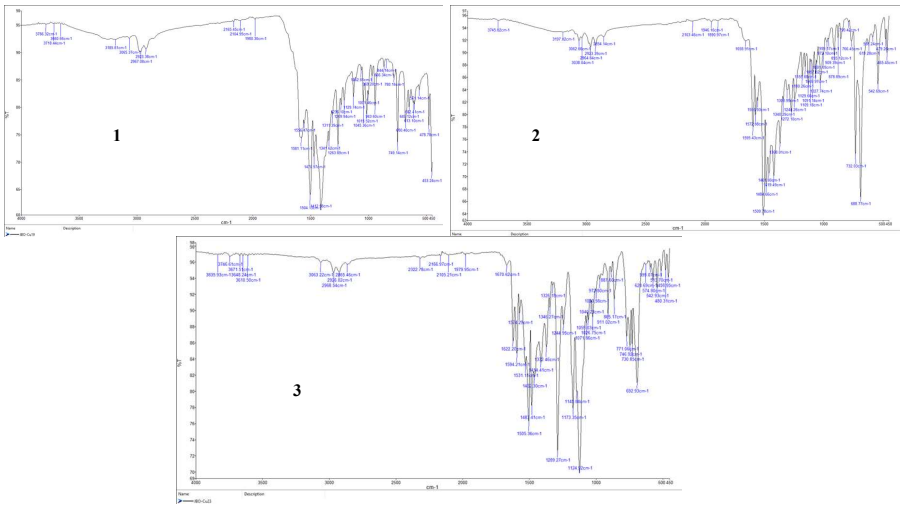
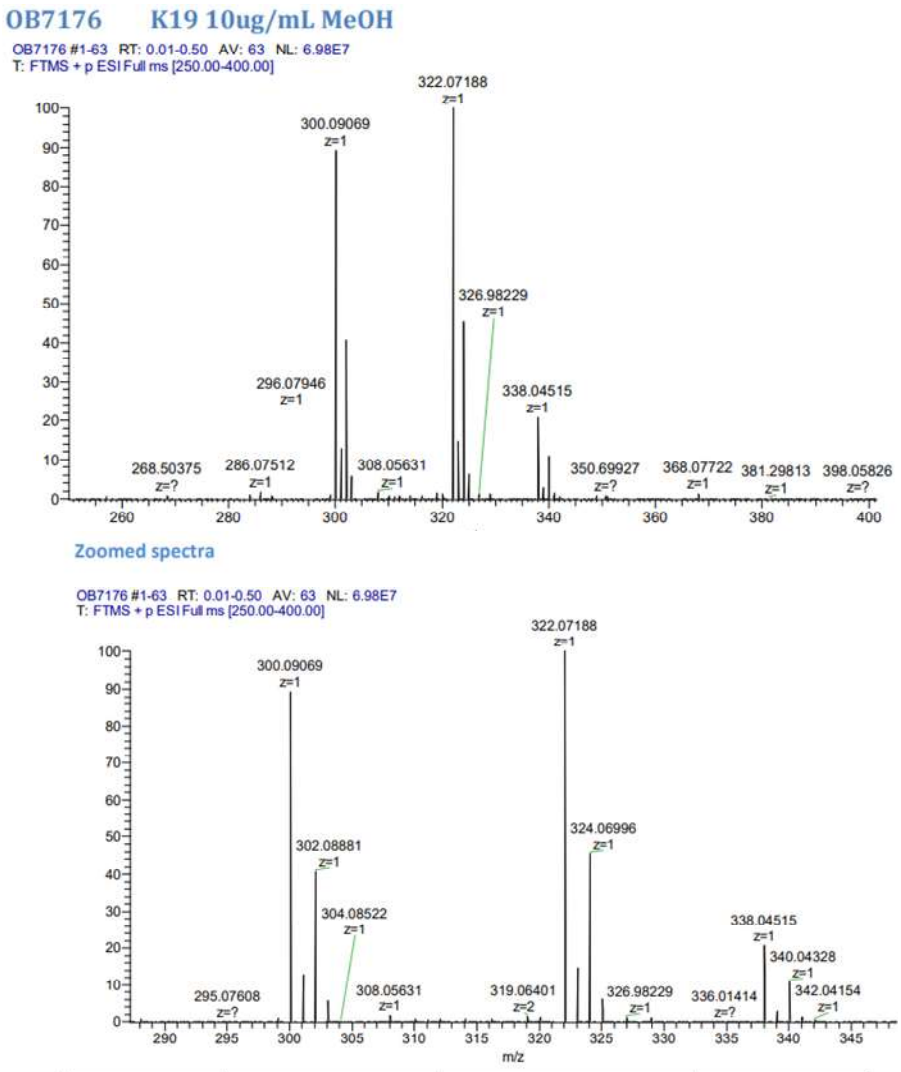
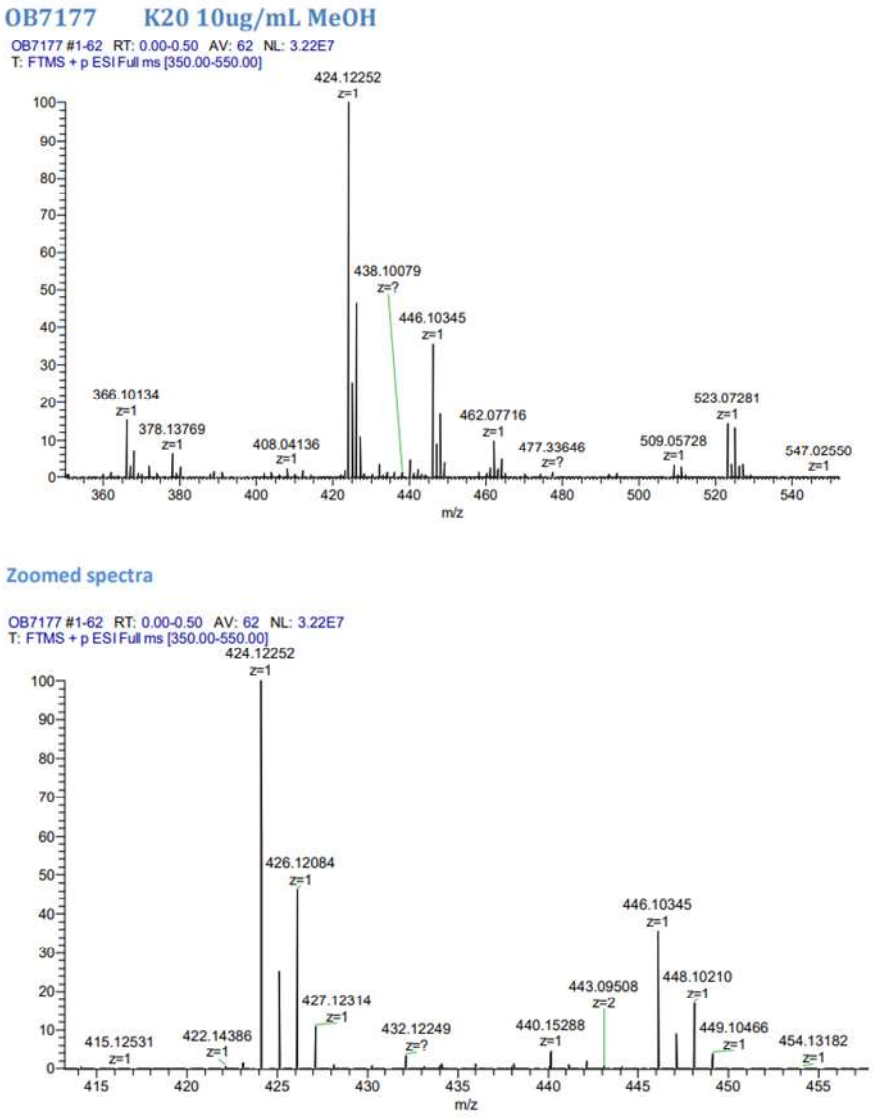


Fig. S-2. IR spectra of studied complexes [Cu(acac2pn)] (1), [Cu(phacac2pn)] (2), [Cu(tfacac2pn)] (3)



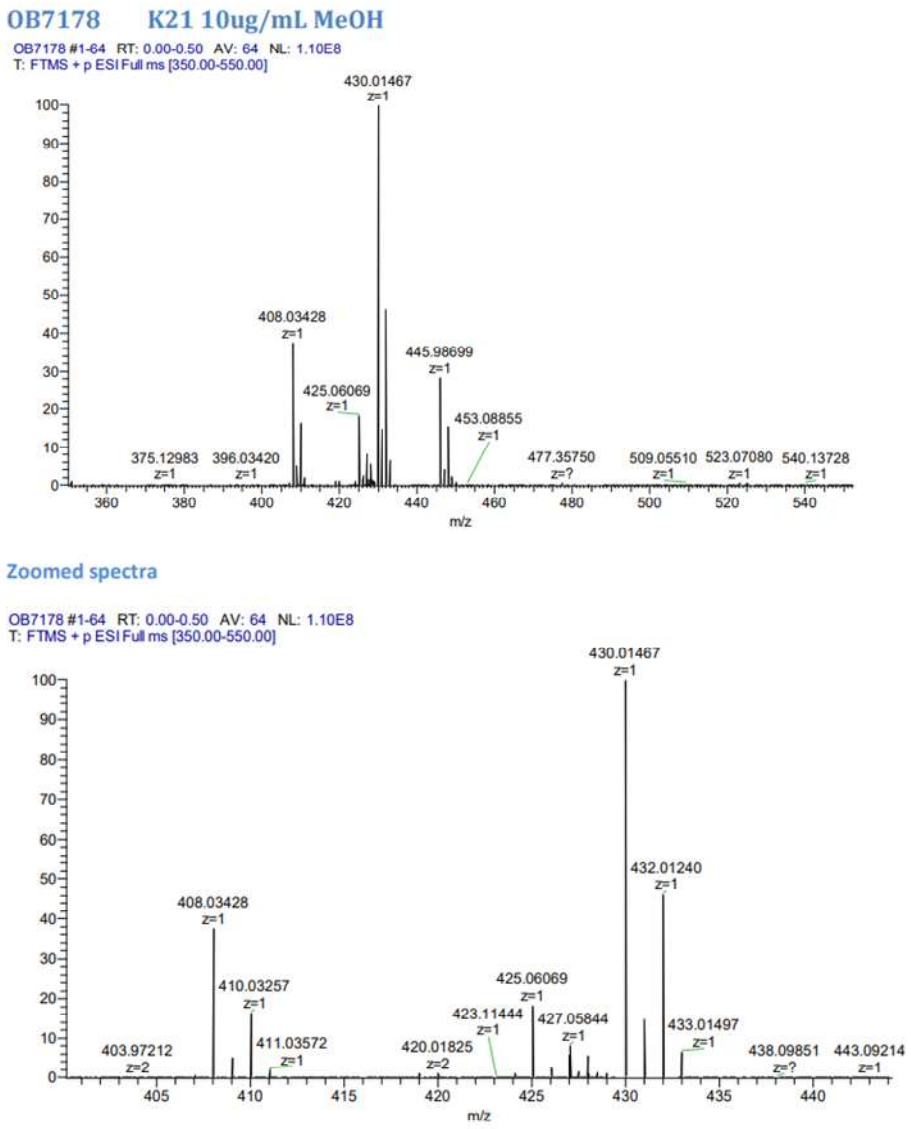
Exact mass	Observed mass	Observed ion type	Error (ppm)
300.08935	300.09069	$[M+H]^+$	4.47
322.0713	322.07188	$[M+Na]^+$	1.80

Fig. S-3. Mass spectra for complex [Cu(acac2pn)] (1) (10 ng/mL MeOH).



Exact mass	Observed mass	Observed ion type	Error (ppm)
424.12065	424.12252	$[M+H]^+$	4.41
446.1026	446.10345	$[M+Na]^+$	1.91

Fig. S-4. Mass spectra for complex [Cu(phacac2pn)] (2) (10 ng/mL MeOH).



Exact mass	Observed mass	Observed ion type	Error (ppm)
408.03282	408.03428	$[M+H]^+$	3.52
430.01477	430.01467	$[M+Na]^+$	0.23

Fig. S-5. Mass spectra for complex [Cu(tfacac2pn)] (3) (10 ng/mL MeOH).

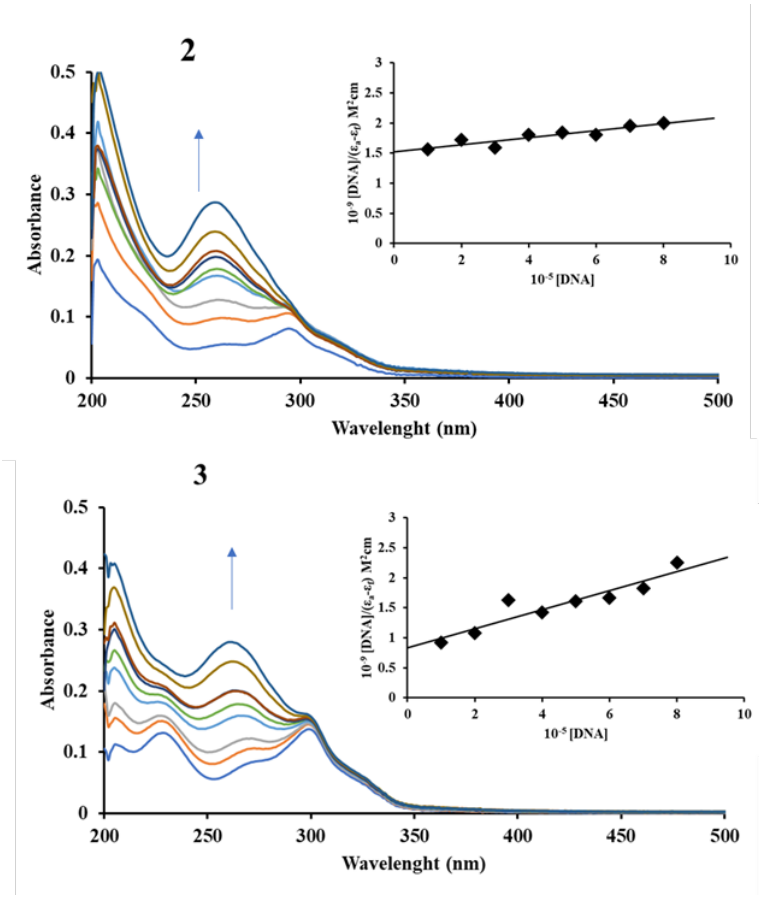


Fig. S-6. UV-Vis titration spectra for 8 μM solution of complexes **2** and **3** in 0,01 M PBS with increasing ct-DNA concentration (0 - 40 μM). Arrow shows hyperchromism in the spectral band. Insepts: Plots of [DNA]/($\varepsilon_a - \varepsilon_f$) versus [DNA] for the titration of the complexes with ct-DNA; with (■) are shown the experimentl data points and the full line represents the exponential fitting of the data.

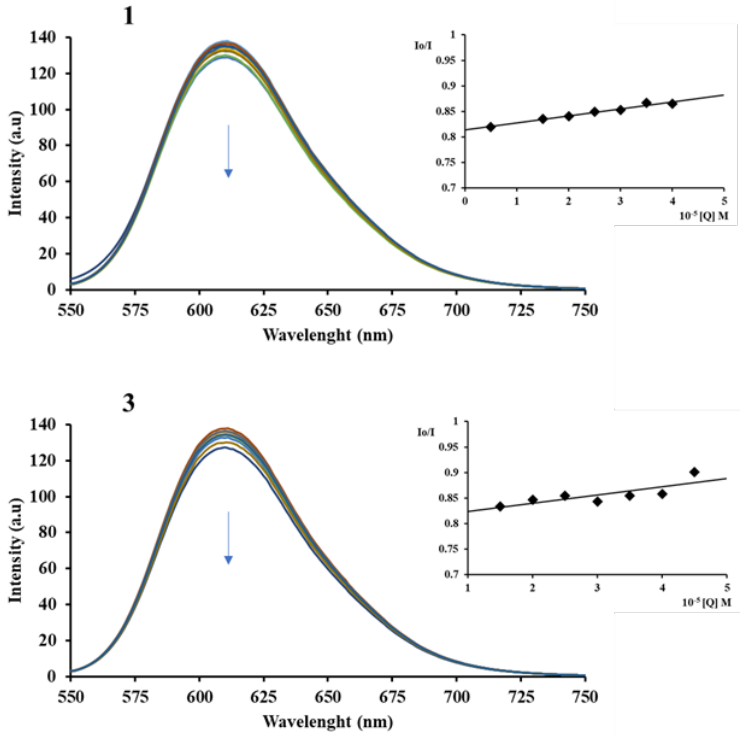


Fig. S-7. Fluorescence titration spectra of EtBr-DNA and of EtBr (25 μM) bound to DNA (25 μM) in the presence of varying amounts of complexes **1** and **3** (phosphate buffer solution = 0,01 M, pH = 7.4). Arrow shows changes in fluorescence intensity upon increasing concentration of complexes (0-50 μM). Insert: plots of I_o/I versus [Q]; with (■) are shown the experimental data points and the full line represents the exponential fitting of the data.

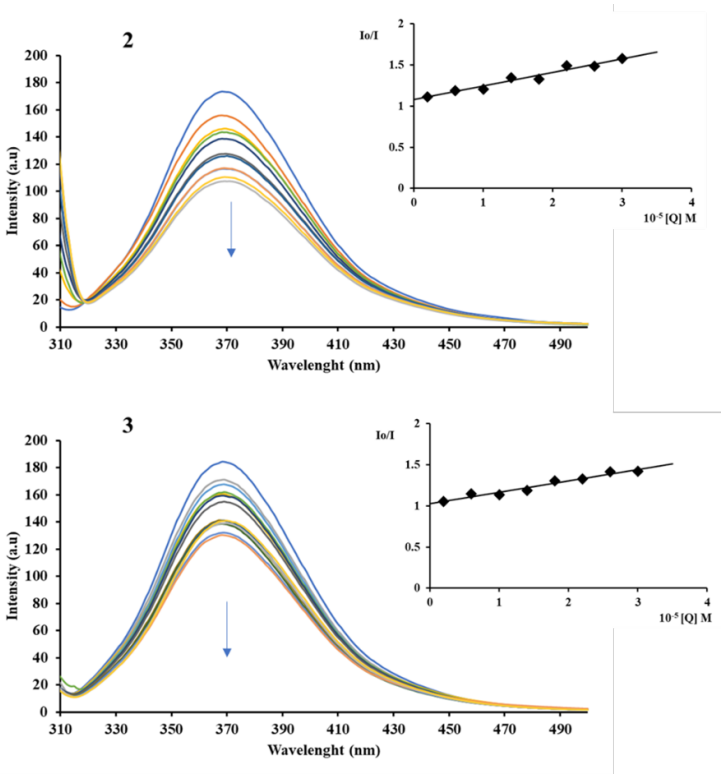


Fig. S-8. Fluorescence titration spectra of BSA (2 μM) at different concentrations of complexes **2** and **3** (phosphate buffer solution = 0,01 M, pH = 7.4). Arrow shows changes in fluorescence intensity upon increasing concentration of complexes (0-30 μM). Insets: Stern-Volmer plots of the interaction with BSA.

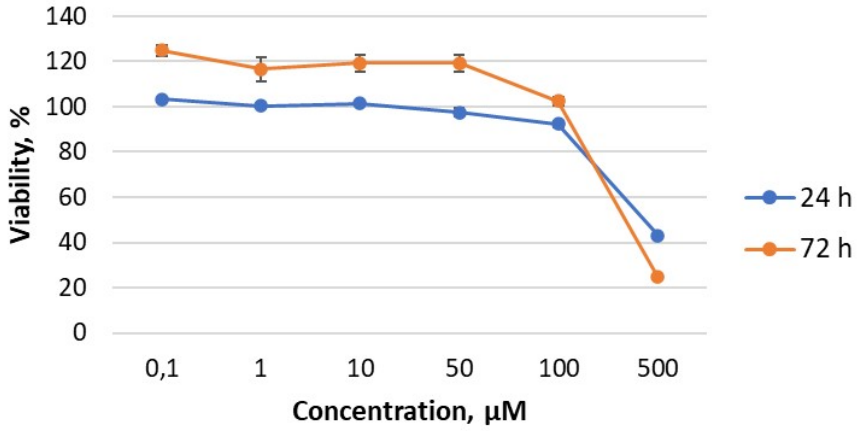


Fig. S-9. Effects of **1** on HCT-116 cells, expressed as the complex concentations related to the number of viable cells after 24 and 72 h of exposure.

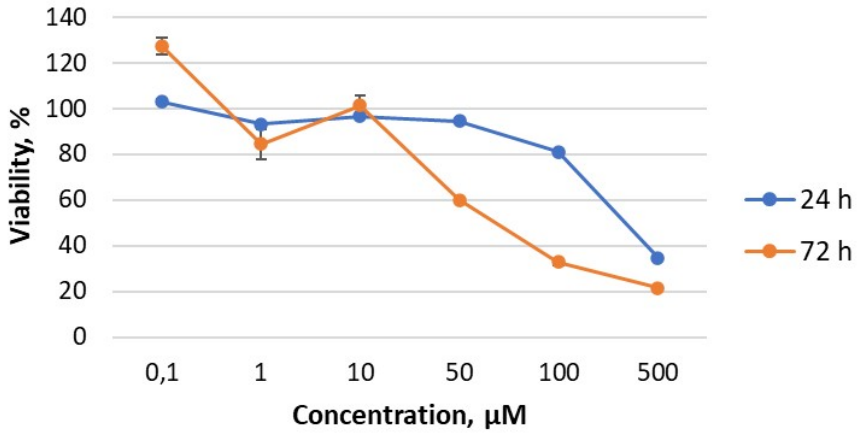


Fig. S-10. Effects of **2** on HCT-116 cells, expressed as the complex concentrations related to the number of viable cells after 24 and 72 h of exposure.

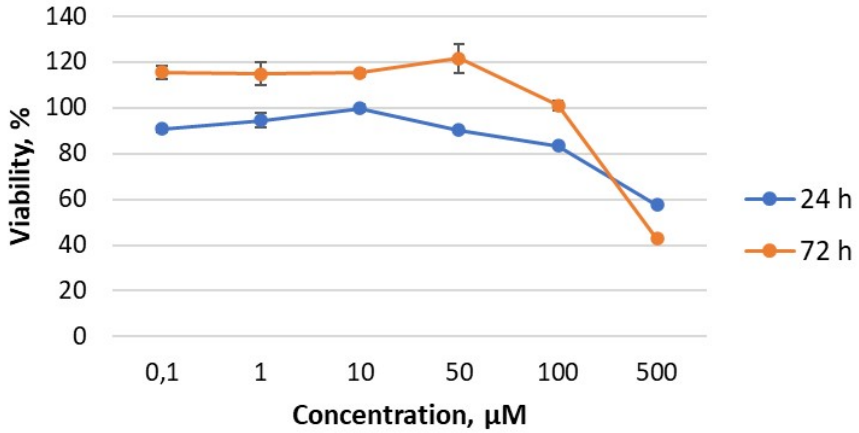


Fig. S-11. Effects of **3** on HCT-116 cells, expressed as the complex concentrations related to the number of viable cells after 24 and 72 h of exposure.

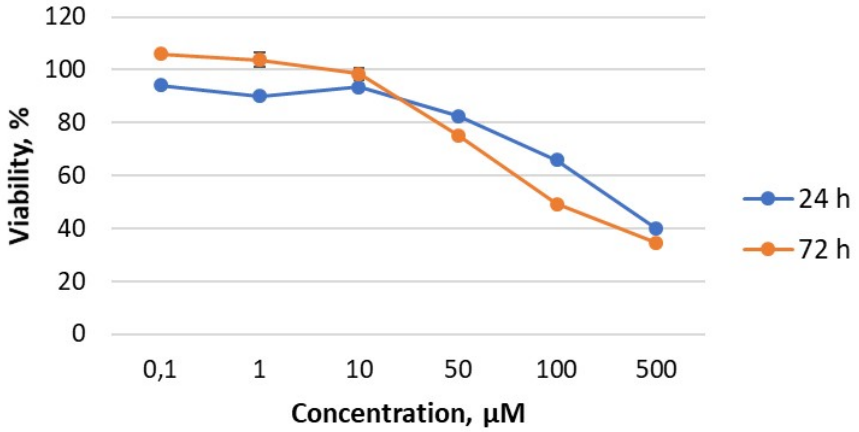


Fig. S-12. Effects of complex **1** on to MRC-5 cells, expressed as the complex concentrations related to the number of viable cells after 24 and 72 h of exposure.

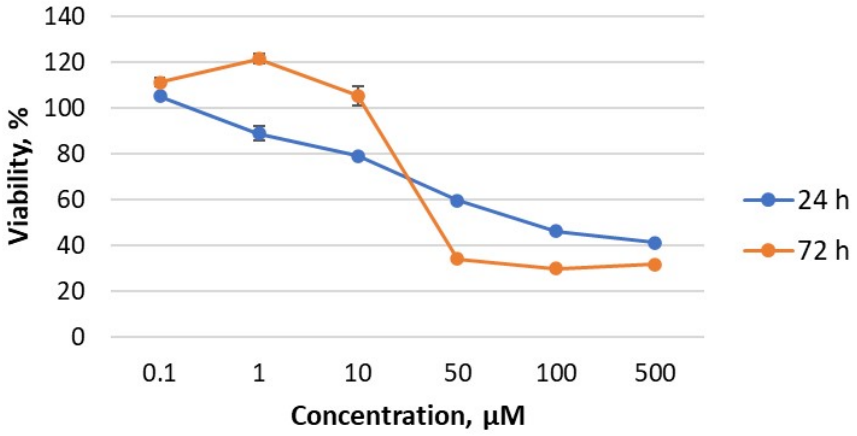


Fig. S-13. Effects of complex **2** on to MRC-5 cells, expressed as the complex concentrations related to the number of viable cells after 24 and 72 h of exposure.

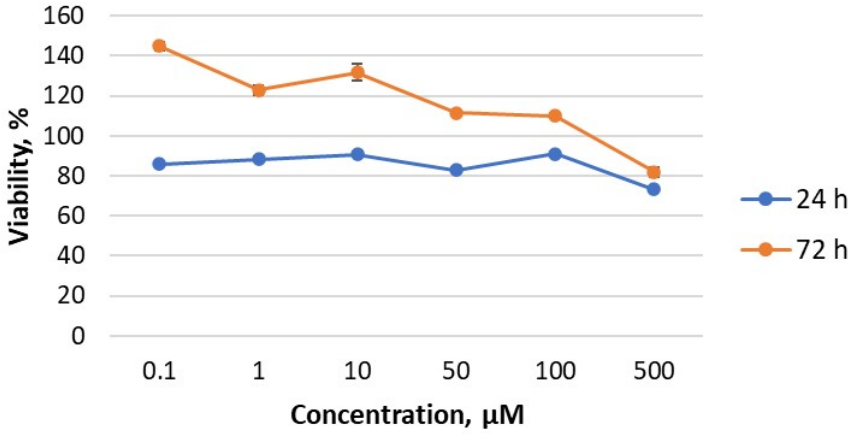


Fig. S-14. Effects of complex **3** on to MRC-5 cells, expressed as the complex concentrations related to the number of viable cells after 24 and 72 h of exposure.