

Ru(II)-thyminate complexes: New metallodrug candidates against tumor cells

Rodrigo S. Correa^{a, b, *}, Vitória Freire^a, Marília I.F. Frazão^a, Daniel P. Bezerra^c, Larissa M. Bomfim^c,

Diogo R. M. Moreira^c; Milena B. P. Soares^{c,d}, Javier Ellena^e, , Alzir A. Batista^{a,*}

^a Departamento de Química, Universidade Federal de São Carlos – UFSCar, Rodovia Washington Luís
KM 235, CP 676, 13561-901, São Carlos-SP, Brazil.

^b Departamento de Química, ICEB, Universidade Federal de Ouro Preto, CEP 35400-000, Ouro Preto-MG,
Brazil.

^c Centro de Pesquisas Gonçalo Moniz, Fundação Oswaldo Cruz (CPqGM-FIOCRUZ-BA), Salvador,
Bahia-BA Brazil.

^d Centro de Biotecnologia e Terapia Celular, Hospital São Rafael, Salvador, Bahia-BA, Brazil.

^e Departamento de Física e Informática, Instituto de Física de São Carlos, Universidade de São Paulo,
CP 369, 13560-970, São Carlos-SP, Brazil.

* To whom correspondence should be addressed:

Rodrigo S. Correa (rodricorrea@iceb.ufop.br). Alzir A. Batista (daab@ufscar.br). Tel.: +55
1633518285; Fax: +55 1633518350.

Supplementary information

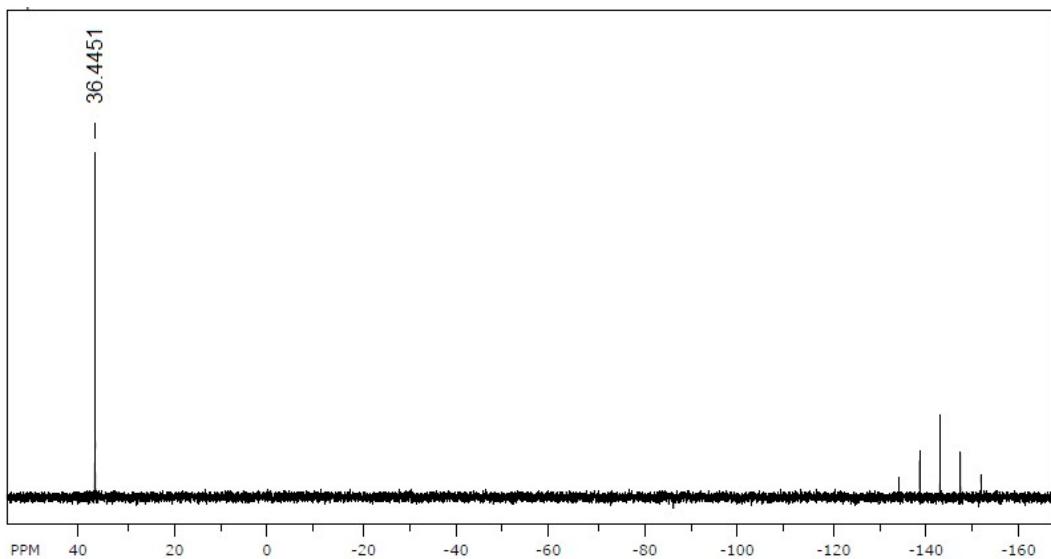


Figure 1S. $^{31}\text{P}\{\text{H}\}$ NMR spectrum for 1, in acetone- d_6 .

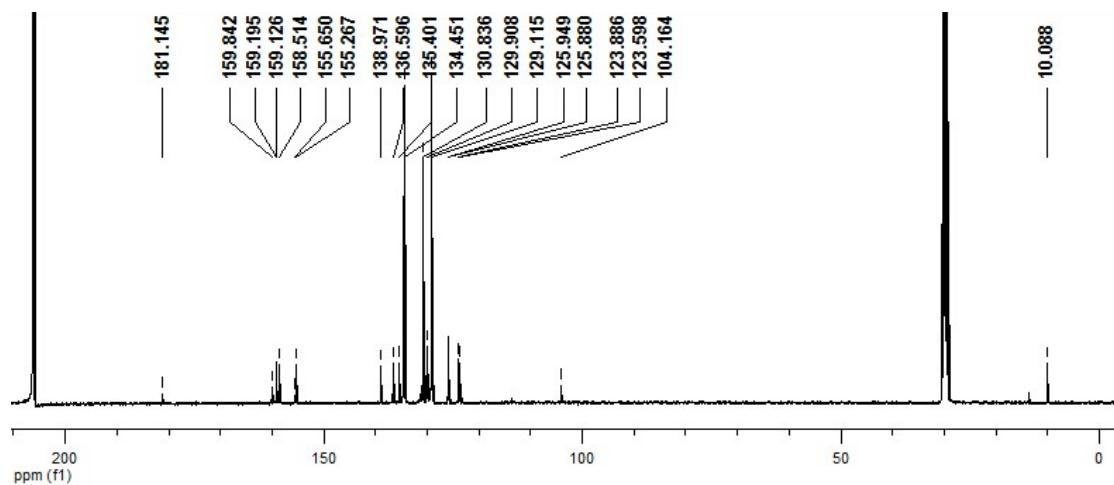


Figure 2S. $^{13}\text{C}\{\text{H}\}$ NMR spectrum for 1, in acetone- d_6 .

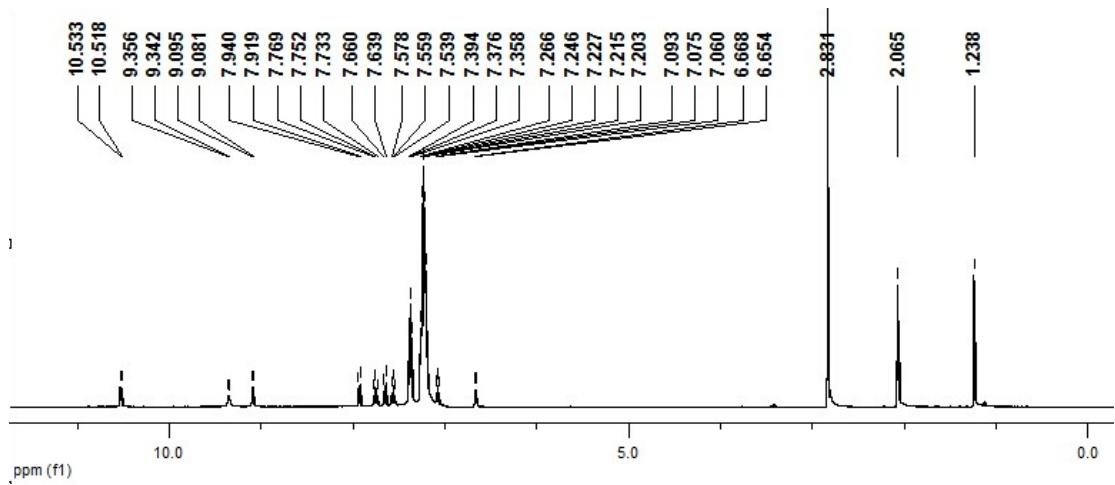


Figure 3S. ^1H NMR spectrum for 1, in acetone- d_6 .

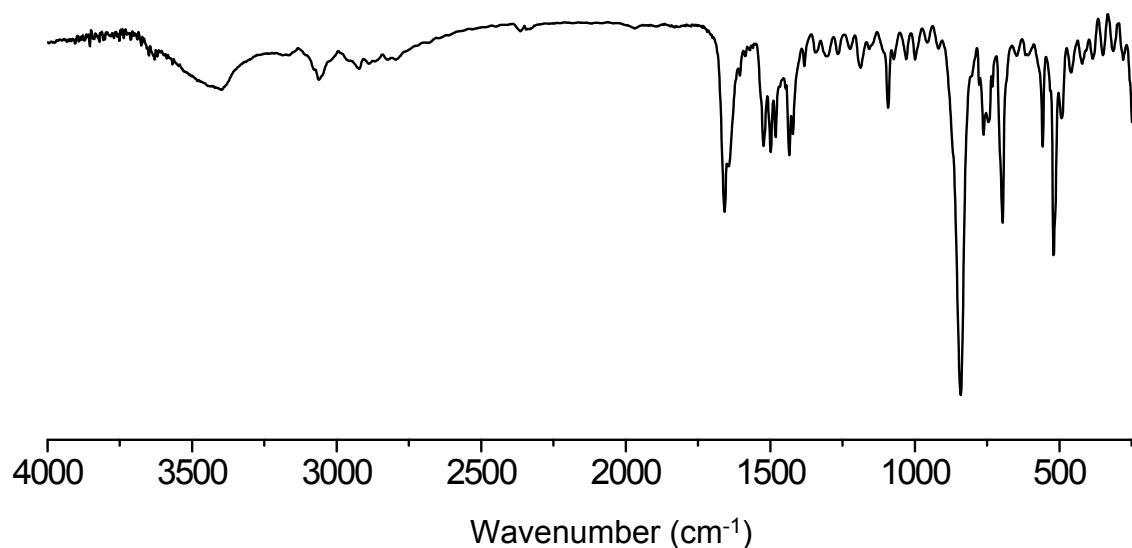


Figure 4S. Infrared spectrum for 1, in CsI pallet.

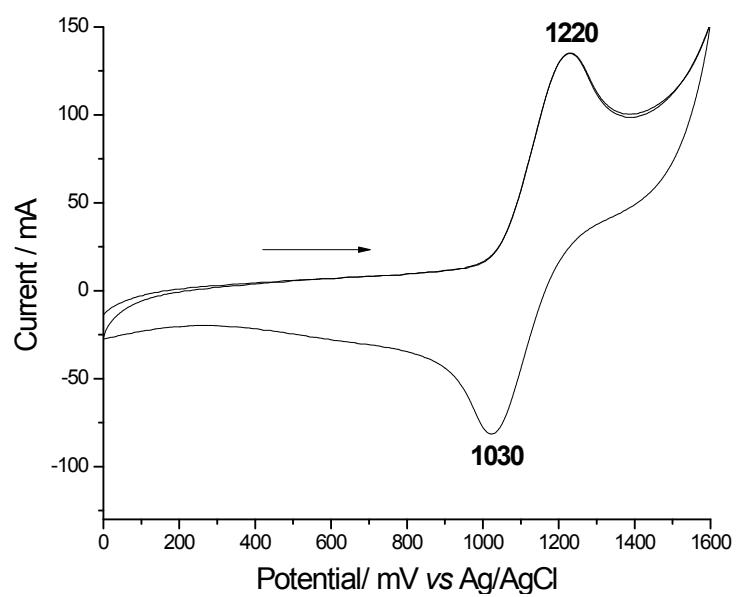


Figure 5S. Cyclic voltammetry for 1, 1.0×10^{-3} molL⁻¹ in CH₂Cl₂ with 0.1 molL⁻¹ of NBu₄ClO₄, scan rate 100 mVs⁻¹, measured at a platinum electrode.

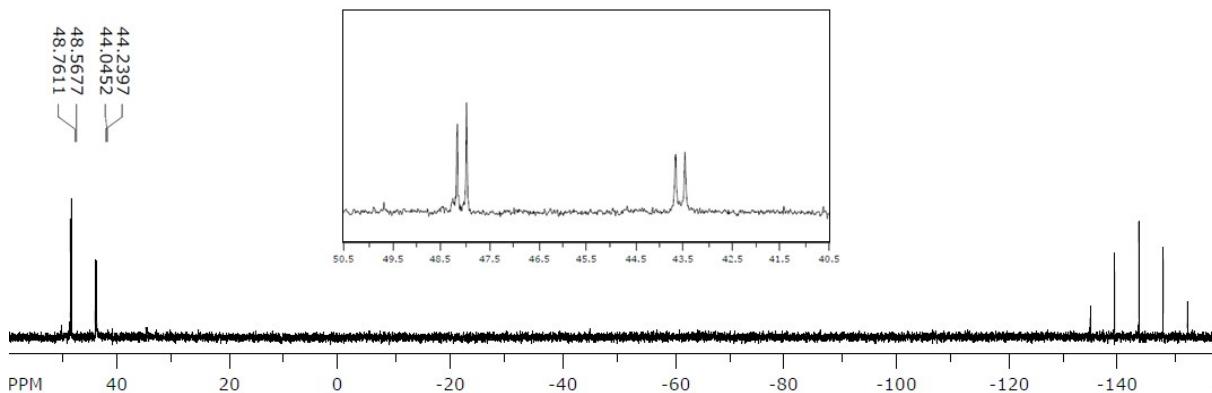


Figure 6S. ³¹P{¹H} NMR spectrum for 2, in CDCl₃.

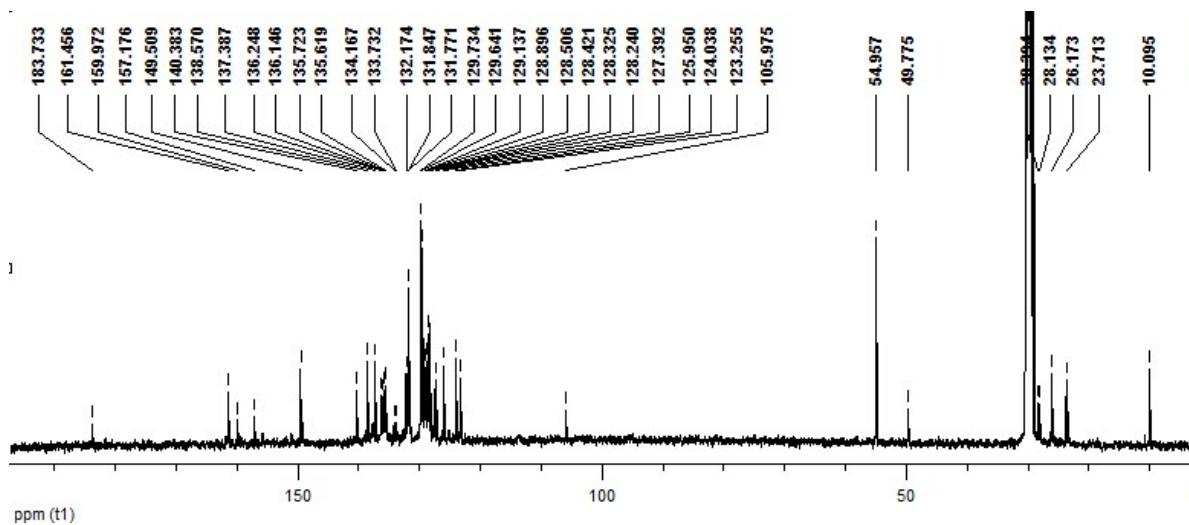


Figure 7S. ¹³C {¹H} NMR spectrum for 2, in CDCl₃.

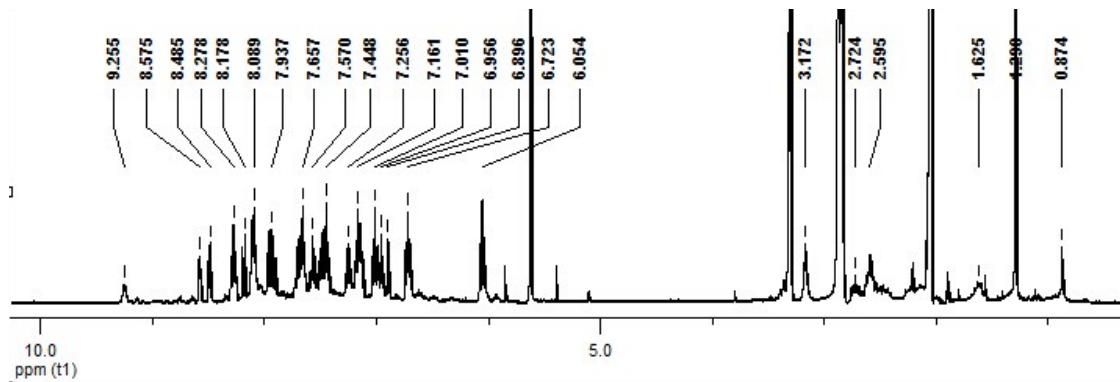


Figure 8S. ¹H NMR spectrum for 2, in CDCl₃.

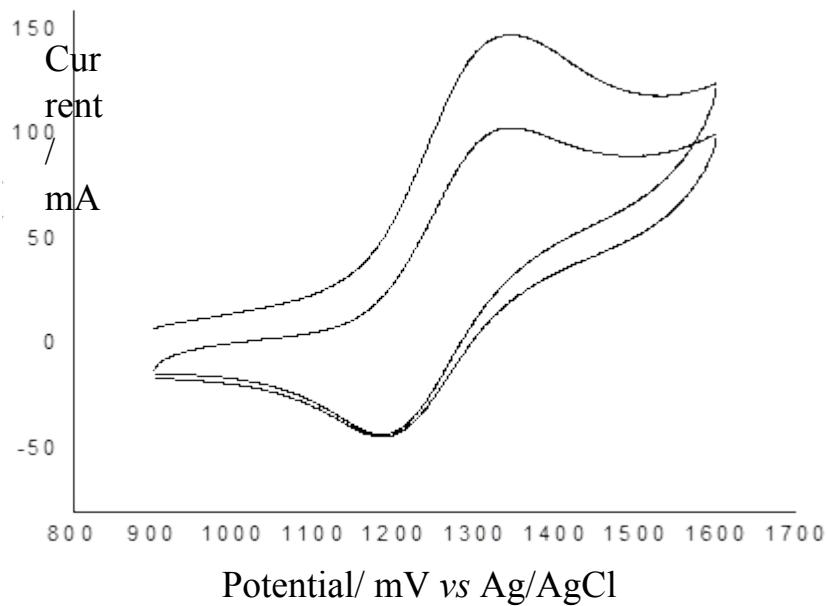


Figure 9S. Cyclic voltammetry for 2, 1.0×10^{-3} molL $^{-1}$ in CH₂Cl₂ with 0.1 molL $^{-1}$ of NBu₄ClO₄, scan rate 100 mVs $^{-1}$, measured at a platinum electrode.

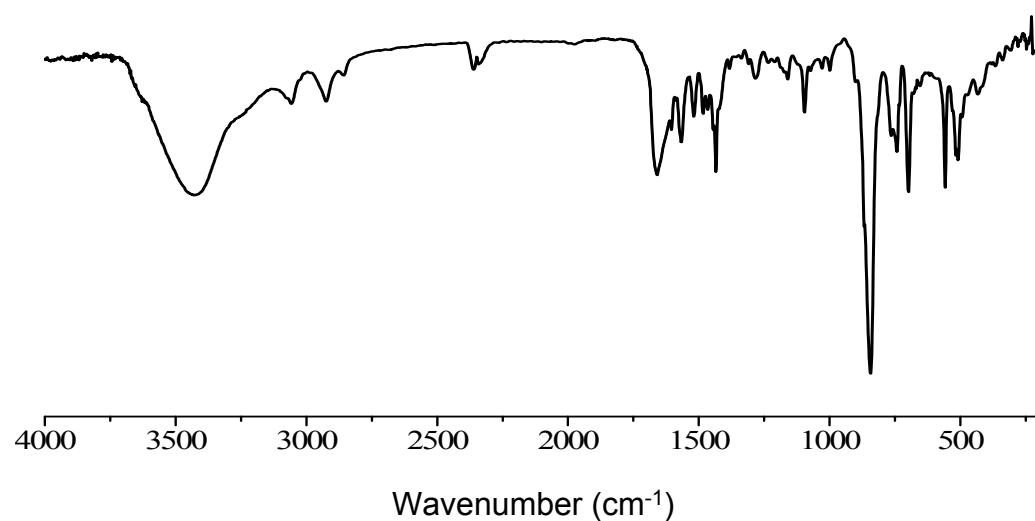


Figure 10S. Infrared spectrum for 2, in CsI pallet.

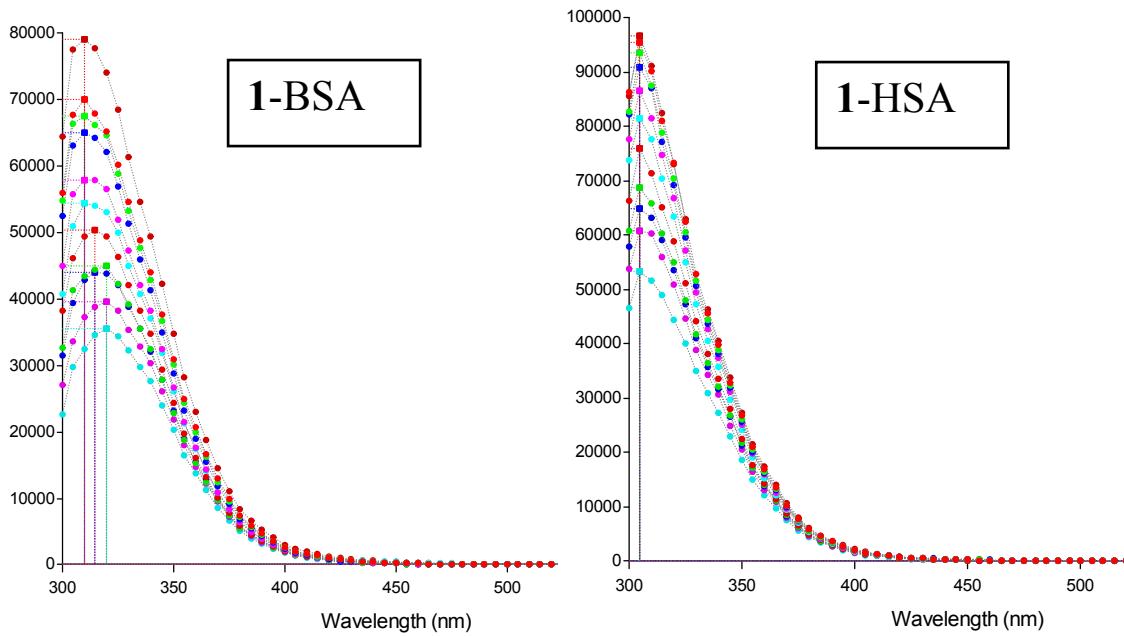


Figure 11S. Fluorescence emission spectra of the BSA (2.5 μM ; $\lambda_{\text{ex}}=270 \text{ nm}$) and HSA (5 μM ; $\lambda_{\text{ex}}=270 \text{ nm}$) at different concentrations of complex **1** at 310 K.

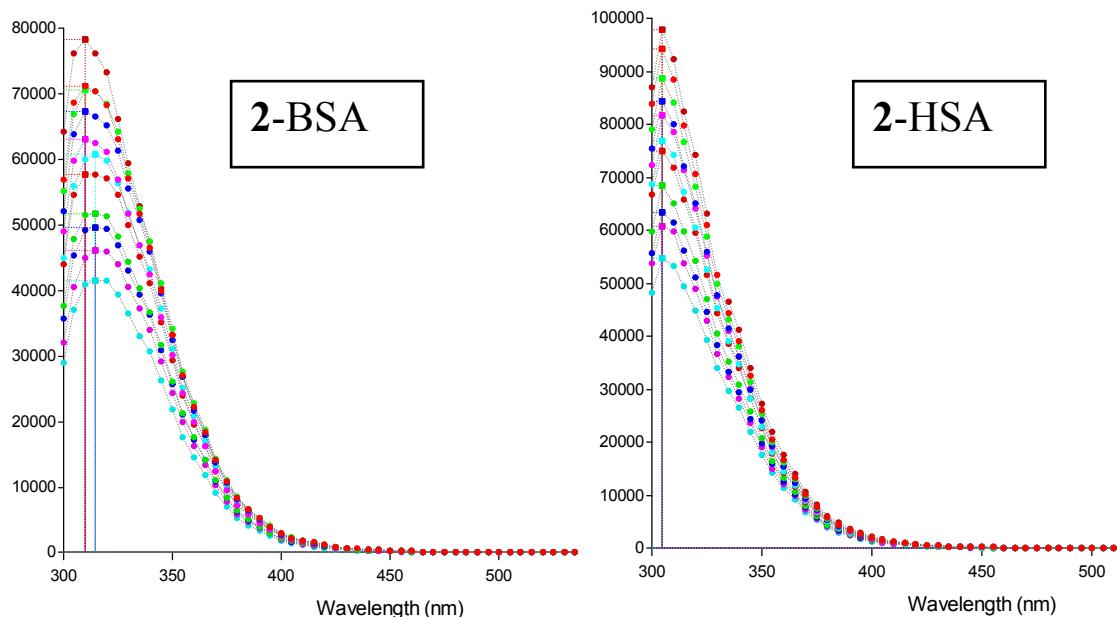


Figure 12S. Fluorescence emission spectra of the BSA (2.5 μM ; $\lambda_{\text{ex}}=270 \text{ nm}$) and HSA (5 μM ; $\lambda_{\text{ex}}=270 \text{ nm}$) at different concentrations of complex **2** at 310 K.

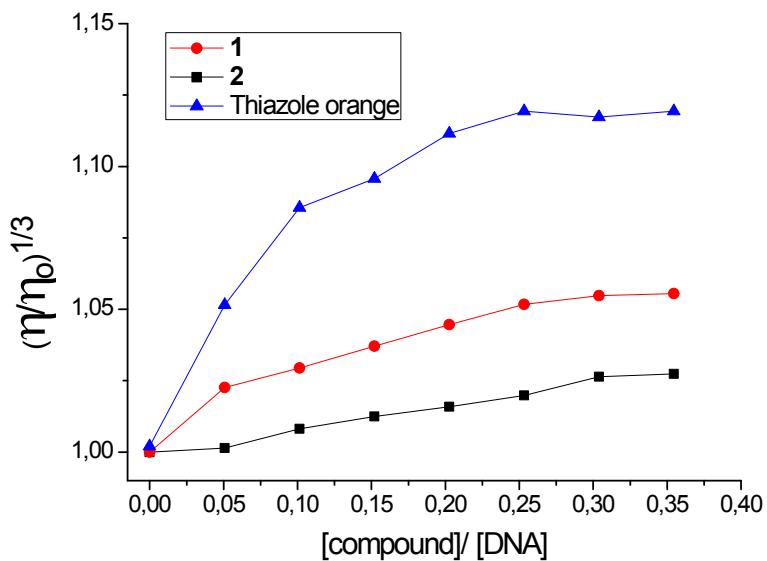


Figure 13S. Viscosity of ctDNA (η/η_0)^{1/3} in the presence of the complexes 1 and 2 at increasing amounts. For comparison, experiments with the classical intercalator thiazole orange were carried out. All experiments were performed at 310 K, in a Tris-HCl buffer, pH 7.4.

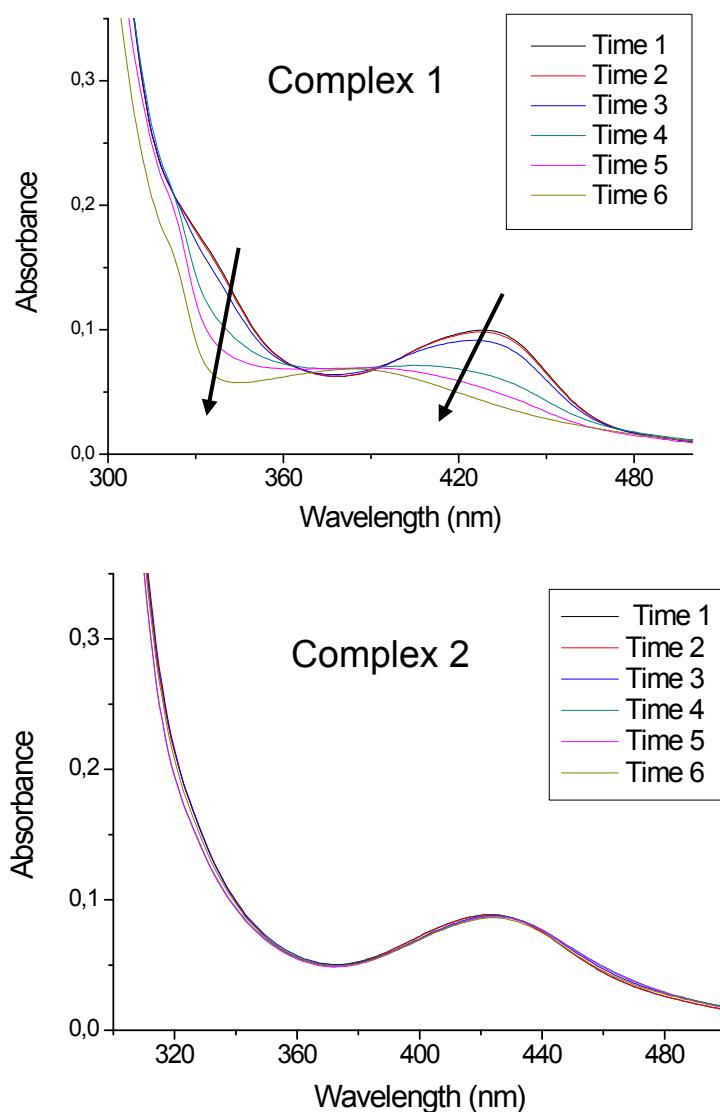


Figure 14S. UV-Visible spectra of complexes 1 and 2 in DMSO:water 9:1 *v/v*. The data were recorded in six different times: Time 1 = 0h; Time 2 = 1h; Time 3 = 6h; Time 4 = 24h; Time 4 = 36h and Time 4 = 48h.

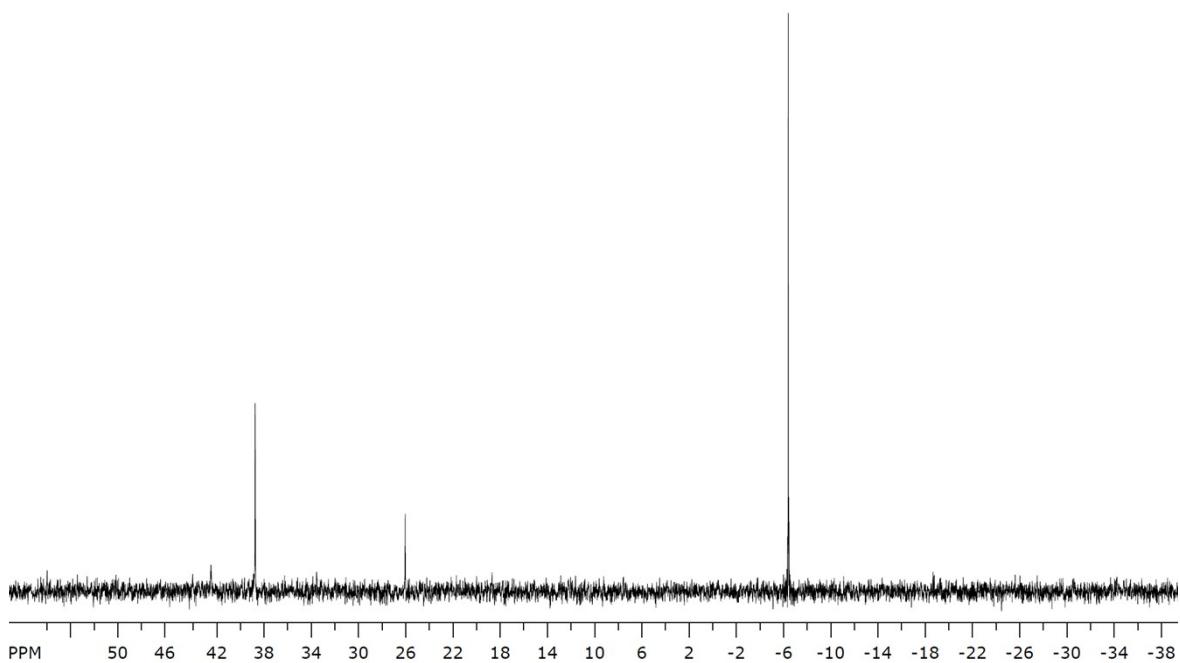
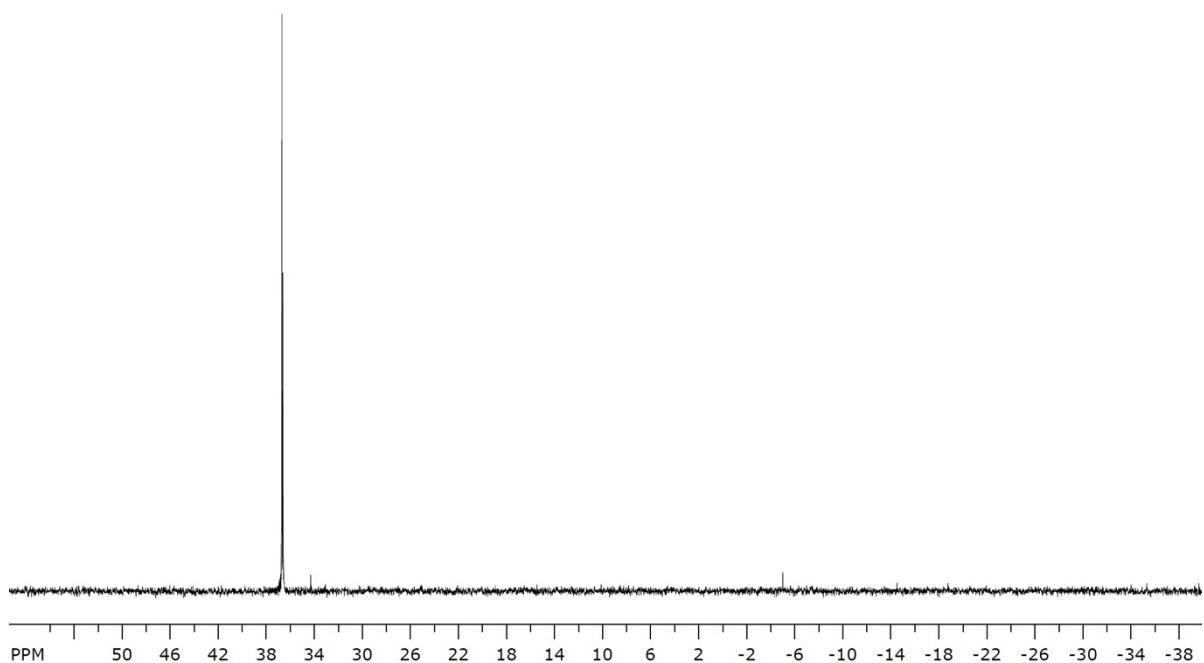


Figure 15S. $^{31}\text{P}\{\text{H}\}$ NMR spectra in DMSO:water (9:1 v/v) of complex 1 at 298 K. (Top: after 1h); (Bottom: after 24h).

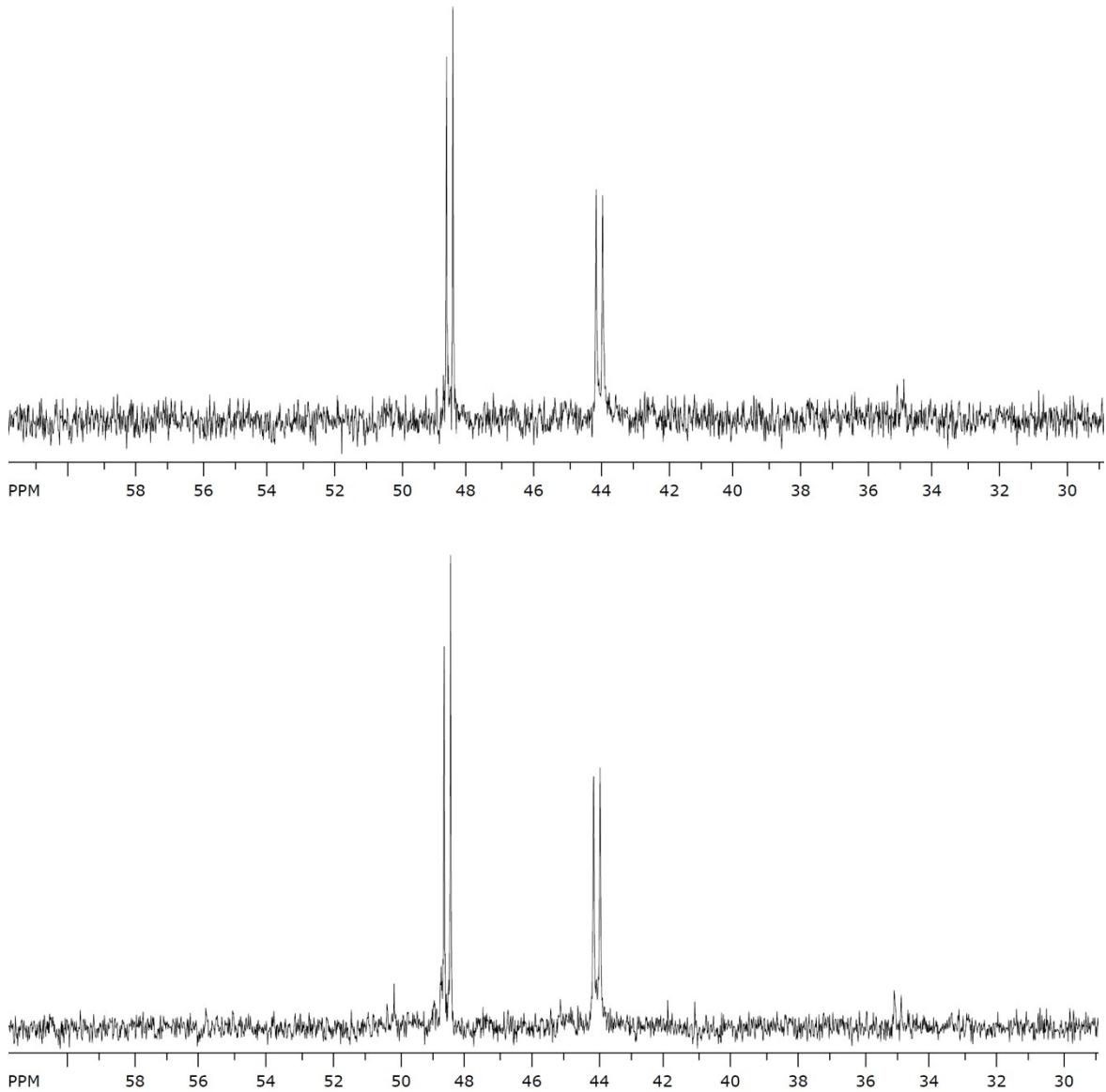


Figure 16S. $^{31}\text{P}\{\text{H}\}$ NMR spectra in DMSO:water (9:1 v/v) of complex 2 at 298 K. (Top: after 1h); (Bottom: after 24h).