

Supplementary information
Anti-proliferative and anti-migration activity of arene-ruthenium(II)
complexes with azole therapeutic agents

Legna Colina-Vegas, Katia M. de Oliveira, Beatriz N. Cunha, Marcia Cominetti, Maribel Navarro^{*}, Alzir Azevedo Batista^{*}

Table of contents

Fig S1. Spectrofluorometric titration spectra of HSA with the ruthenium compounds **2-4**.

Fig S2. ^1H NMR spectrum of guanosine and complex **3** at different times (only resonances of H_8 , NH and NH_2 are assignments).

Fig S3. Hoechst 33258 (H33258) displacement assay for metal complexes **2-4**.

Fig S4. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum in the mixture 70:30 DMSO: Culture medium (DMEM) of complex **3** at different times.

Equation description:

Classical Stern–Volmer equation (1) was used to determine the Stern–Volmer quenching constant (K_{sv}):

$$F_0/F = 1 + K_q\tau_0[Q] = 1 + K_{sv}[Q] \quad (1)$$

where F_0 and F are the fluorescence intensities in the absence and presence of quencher, respectively, $[Q]$ is the quencher concentration.

Binding constant (K_b) and number of binding sites (n) were determined by plotting the double log graph of the fluorescence data using the equation (2):

$$\log [(F_0-F)/F] = \log K_b + n\log[Q] \quad (2)$$

The thermodynamic parameters were calculated from equations (3) and (4):

$$\ln (K_2/K_1) = [(1/T_1)-(1/T_2)]\Delta H/R \quad (3)$$

where K_1 and K_2 are the binding constants at temperatures T_1 and T_2 , respectively, and enthalpy (ΔH) and R is the gas constant.

Additionally, the change in free energy (ΔG) and entropy (ΔS) were calculated from the following equation:

$$\Delta G = -RT \ln K = \Delta H - T\Delta S \quad (4)$$

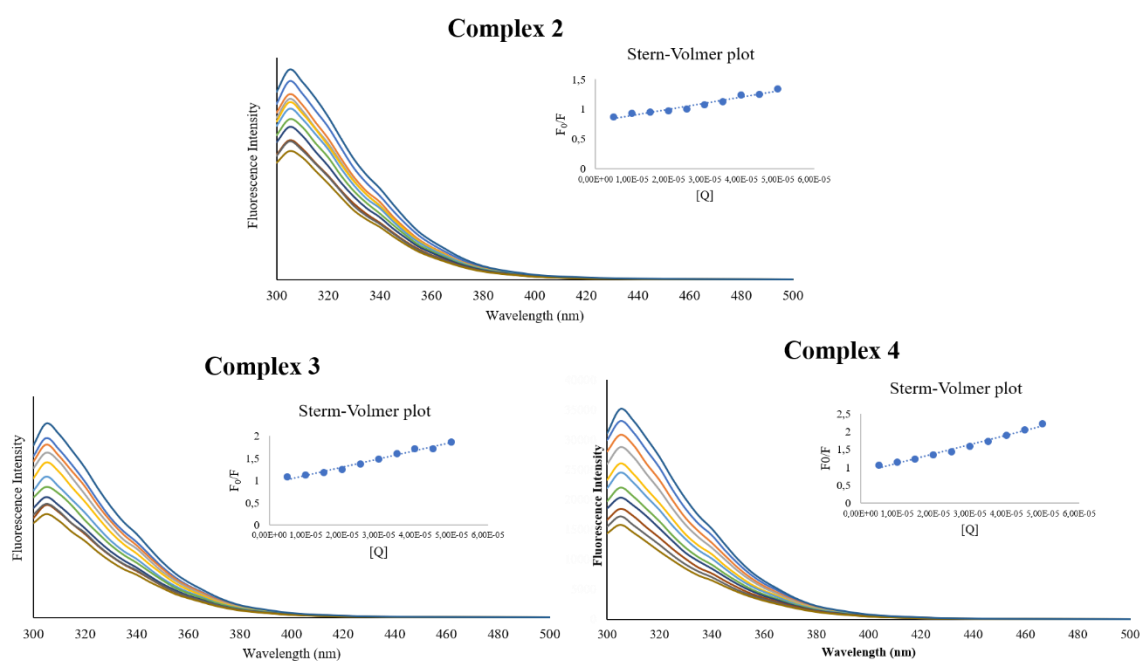


Fig S1. Spectrofluorometric titration spectra of HSA with the ruthenium compounds **2-4**

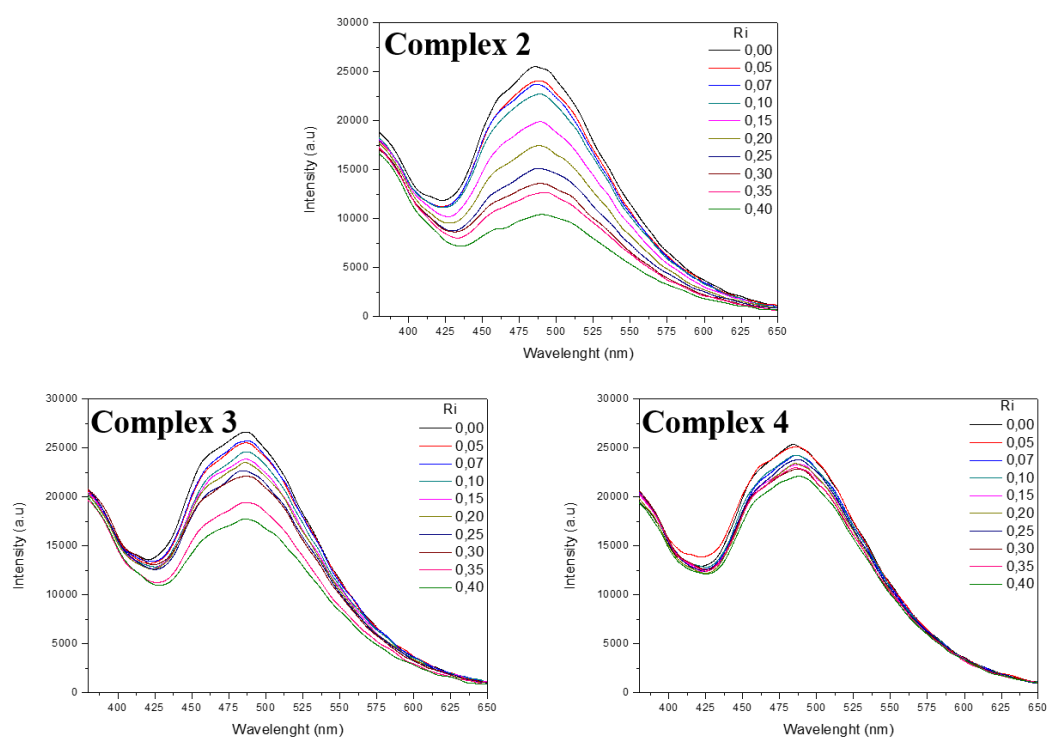


Fig S2. Hoechst 33258 (H33258) displacement assay for metal complexes **2-4**

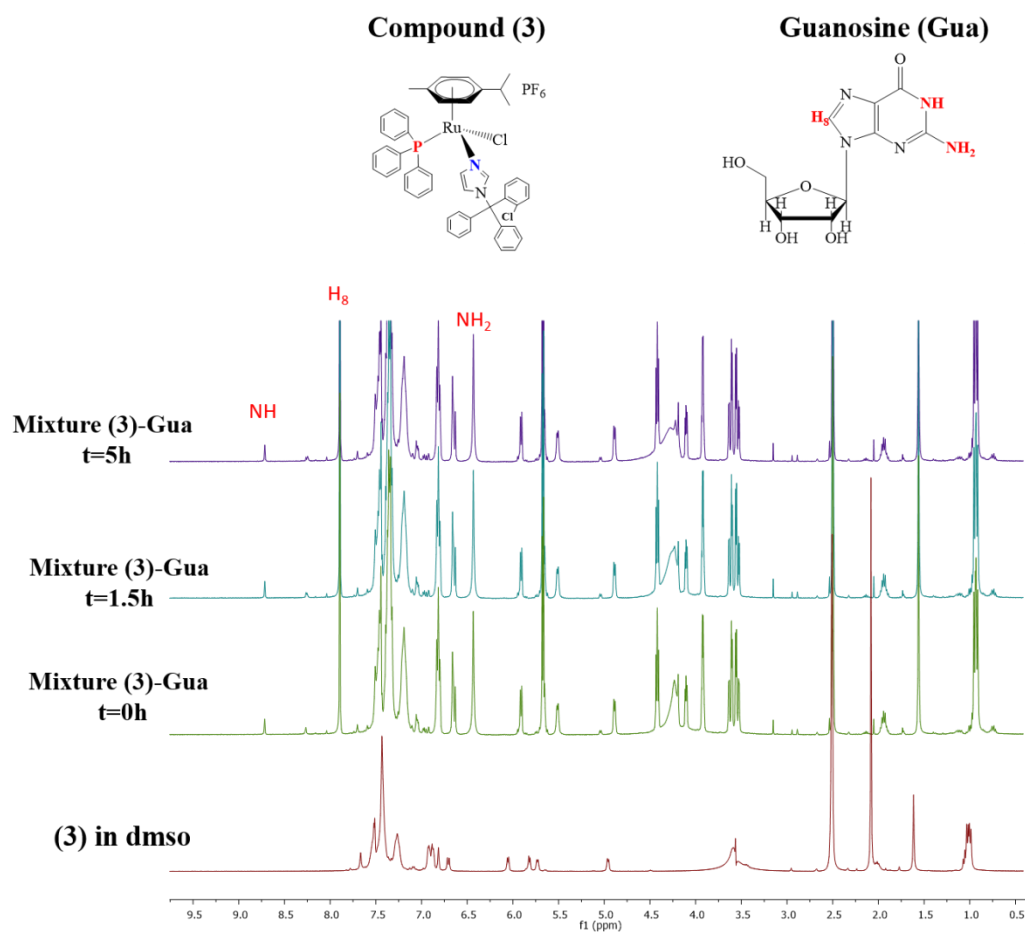


Fig S3. ^1H NMR spectrum of guanosine and complex **3** at different times (only resonances of H_8 , NH and NH_2 are assignments)

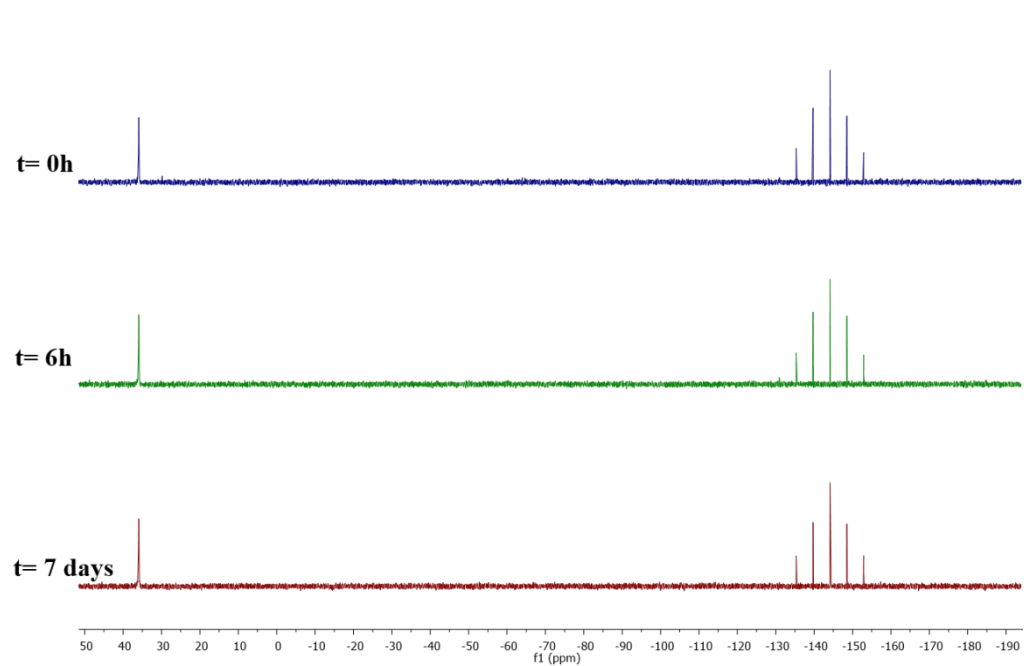


Fig S4. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum in the mixture 70:30 DMSO:Culture medium (DMEM) of complex **3** at different times