Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

ELECTRONIC SUPPLEMENTARY INFORMATION

Esterification of free carboxylic group from the lutidinic acid ligand as a tool to improve the cytotoxicity of Ru(II) complexes

João Honorato, Legna C. A. Vegas, Rodrigo S. Correa, Adriana P. M. Guedes, Marcelo Miyata, Fernando R. Pavan, Javier Ellena, Alzir A. Batista*

Table S1 Crystal data and structure refinement parameters obtained for the complexes 1 and 2.

	1	**2**
Empirical formula	$[RuC_{45}H_{40}N_3O_4P_2]PF_6$	$[RuC_{47}H_{44}N_3O_4P_2]PF_6$
Formula weight	994.81	1022.83
Temperature (K)	293(2)	298(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic
Space group	C2/c	P21/n
a (Å)	40.71(2)	13.5183(4)
b (Å)	15.001(9)	12.8666(3)
c (Å)	14.658(9)	28.1285(7)
α (°)	90	90
β (°)	95.496(7)	100.746(10)
γ (°)	90	90
Volume ($Å^3$)	8910(9)	4806.7(2)
Z	8	4
Density (calculated) (Mg/m^3)	1.415	1.413
Absorption coeficiente (mm^{-1})	0.523	0.494
F(000)	3864	2088.0
Crystal size (mm^3)	0.26 x 0.26 x 0.20	0.21 x 0.10 x 0.09
Theta range for data collection (°)	1.977 to 27.485	2.719 to 30.508
Index ranges	$-52 \le h \le 52$, $-19 \le k \le 19$, $-18 \le l \le 18$	$-19 \le h \le 19$, $-18 \le k \le 18$, $-40 \le l \le 40$
Reflections collected	39930	73392
Independent reflections	10192 [R(int) = 0.0614]	14670 [R(int) = 0.0394]
Completeness to theta (%)	100.0	100.0
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	10192 / 0 / 563	14670 / 0 / 574
Goodness-of-fit on F^2	1.140	1.098
Final R indices [I>2sigma(I)]	R1 = 0.0563, wR2 = 0.1403	R1 = 0.0548, wR2 = 0.1384
R indices (all data)	R1 = 0.0744, wR2 = 0.1610	R1 = 0.0782, wR2 = 0.1616
Extinction coeficiente	0.00268(15)	0.00068(13)
Largest diff. peak and hole ($e.Å^{-3}$)	0.848 and -0.938	1.36 and -0.95

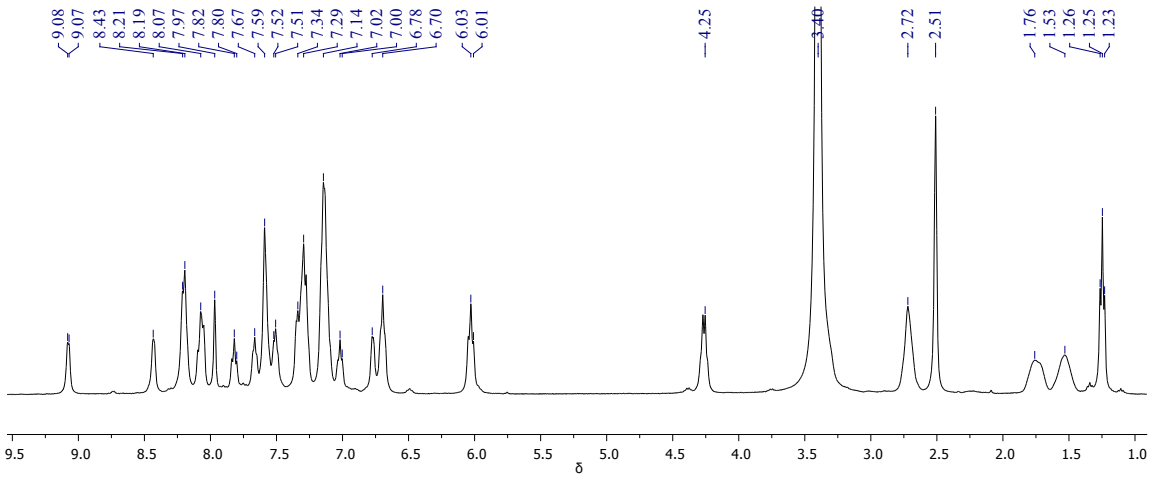

Figure S1 ^{1}H NMR spectra of the complex 2 with peak assignation (DMSO-d_6)

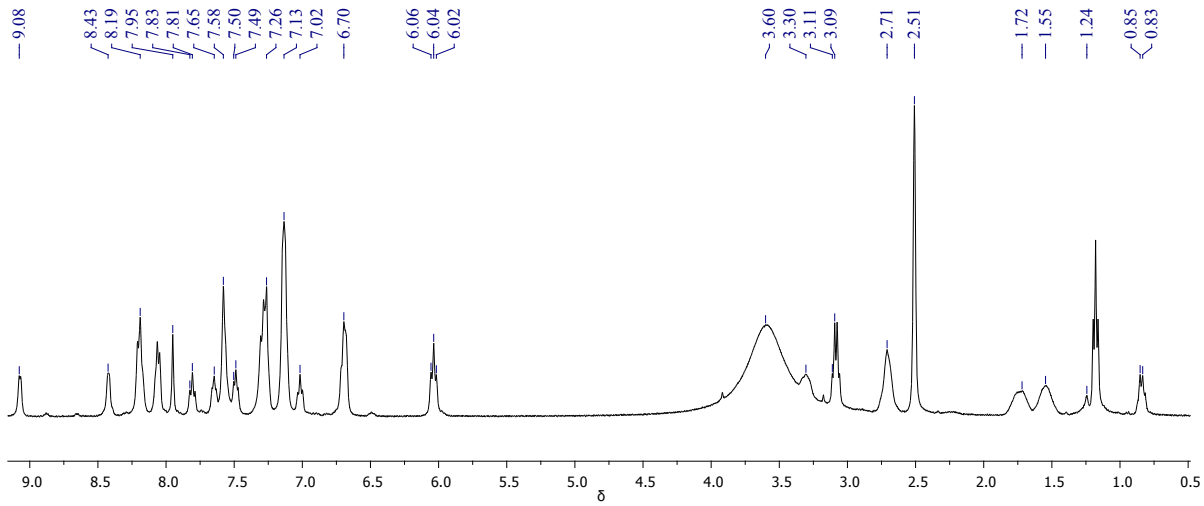

Figure S2 ^{1}H NMR spectra of the complex 1 with peak assignation (DMSO-d_6)

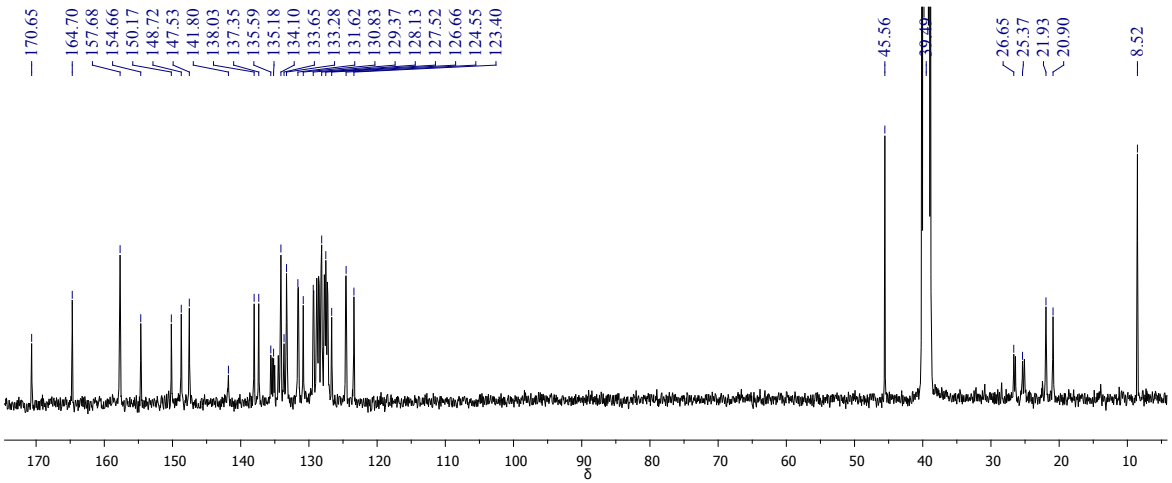

Figure S3 $^{13}C\{^{1}H\}$ NMR spectra of the complex 1 with peak assignation (DMSO-d_6)

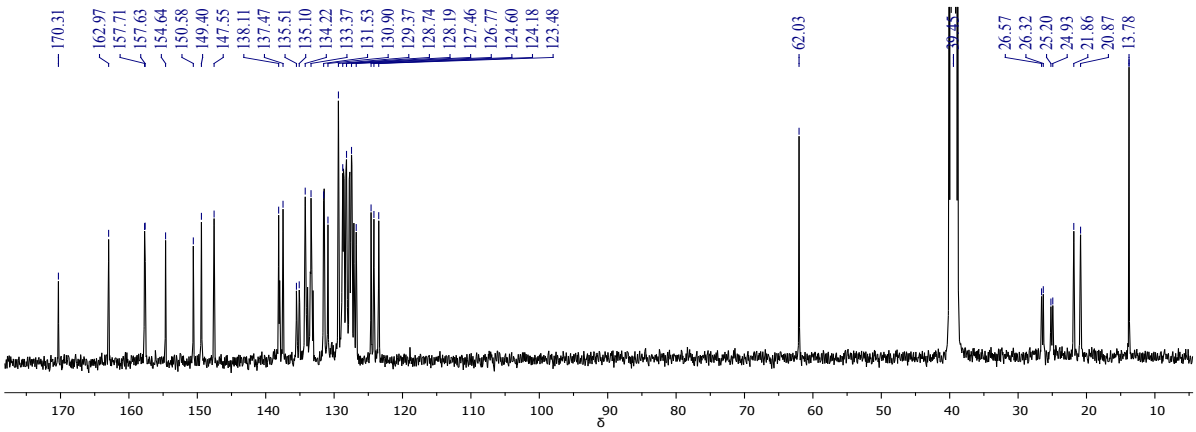

Figure S4 $^{13}C\{^{1}H\}$ NMR spectra of the complex 2 with peak assignation (DMSO-d_6)

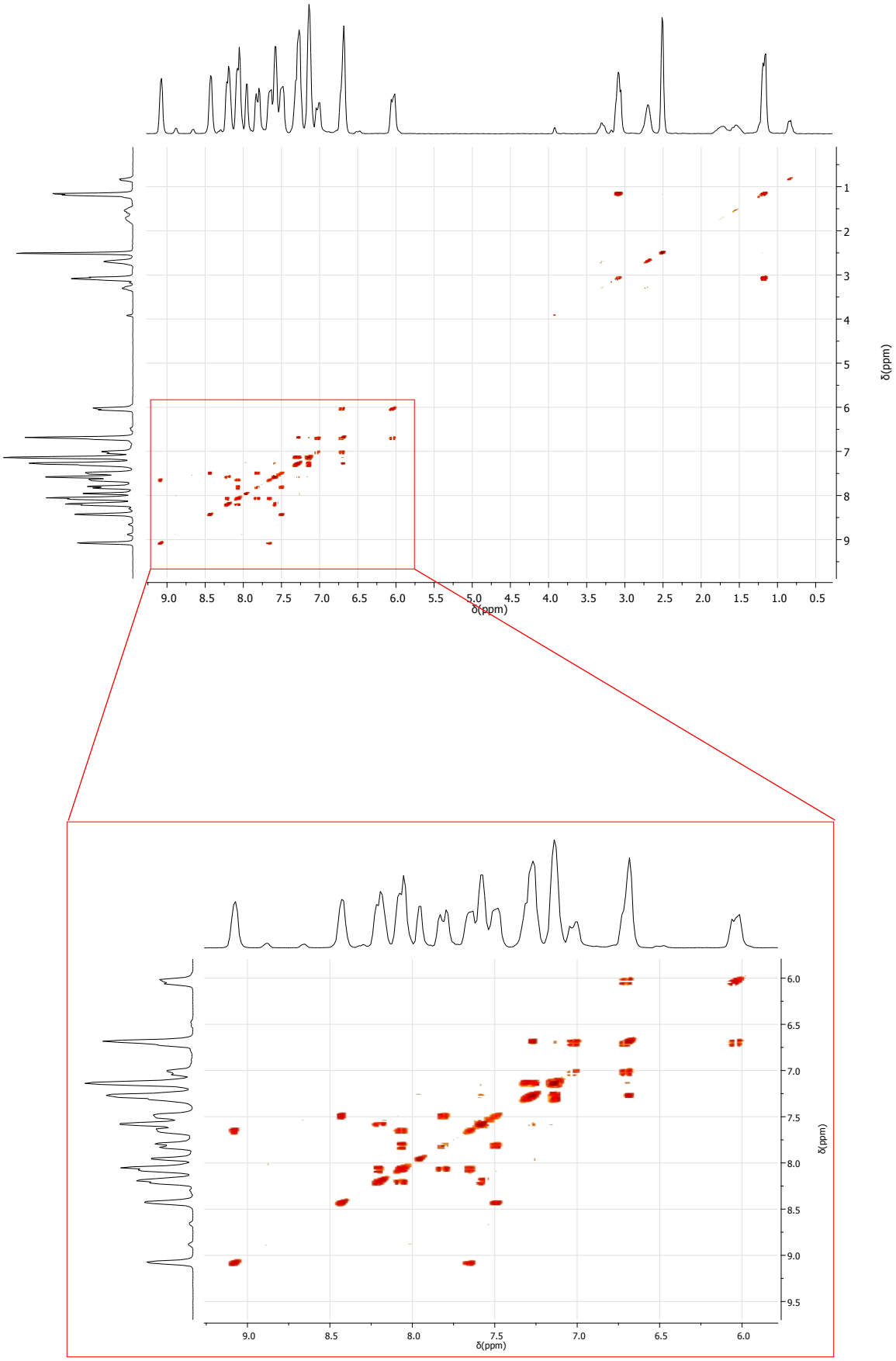

Figure S5 ^{1}H-^{1}H COSY NMR spectra of the complex 1 (DMSO-d_6)

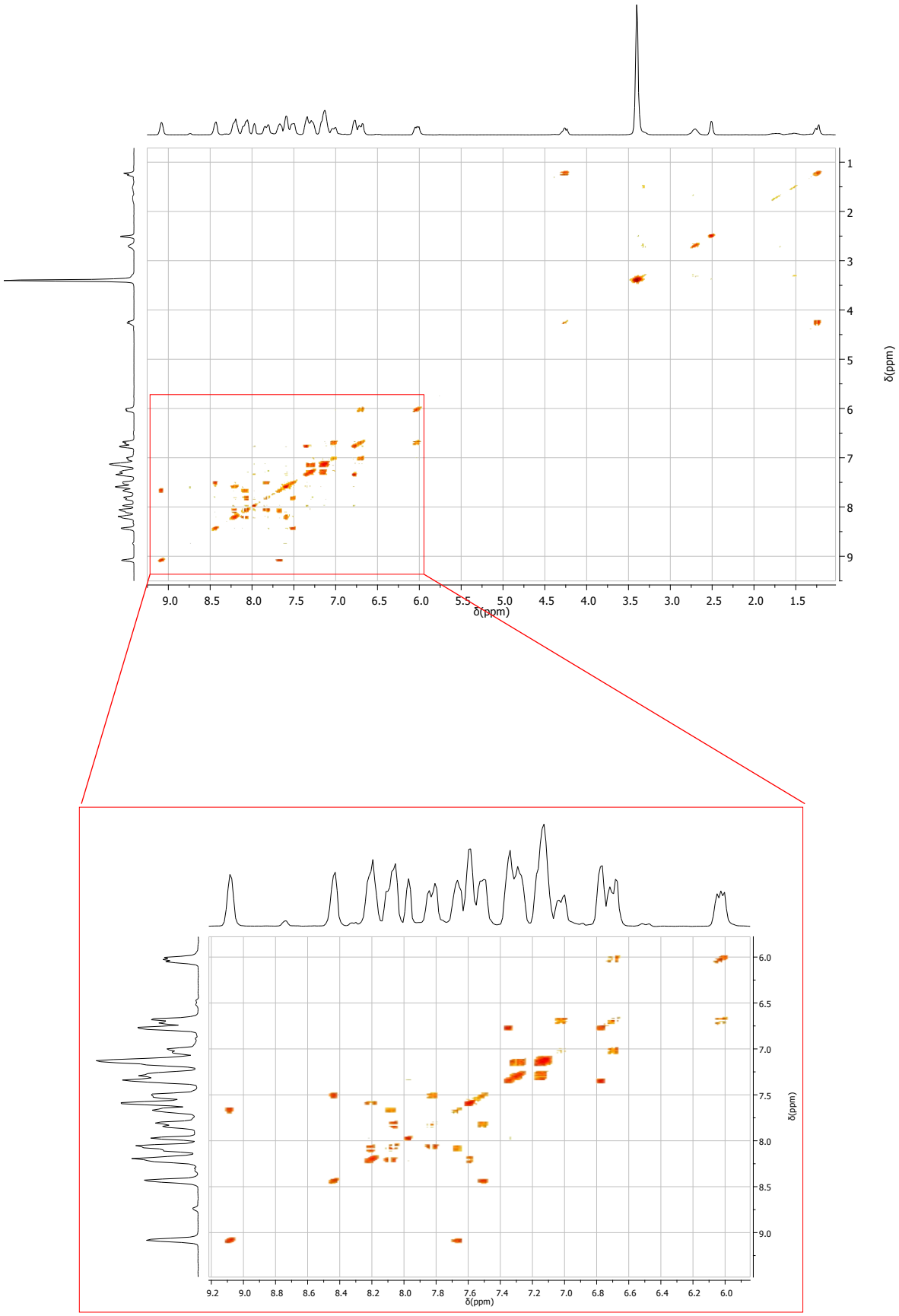

Figure S6 ^{1}H-^{1}H COSY NMR spectra of the complex 2 (DMSO-d_6)

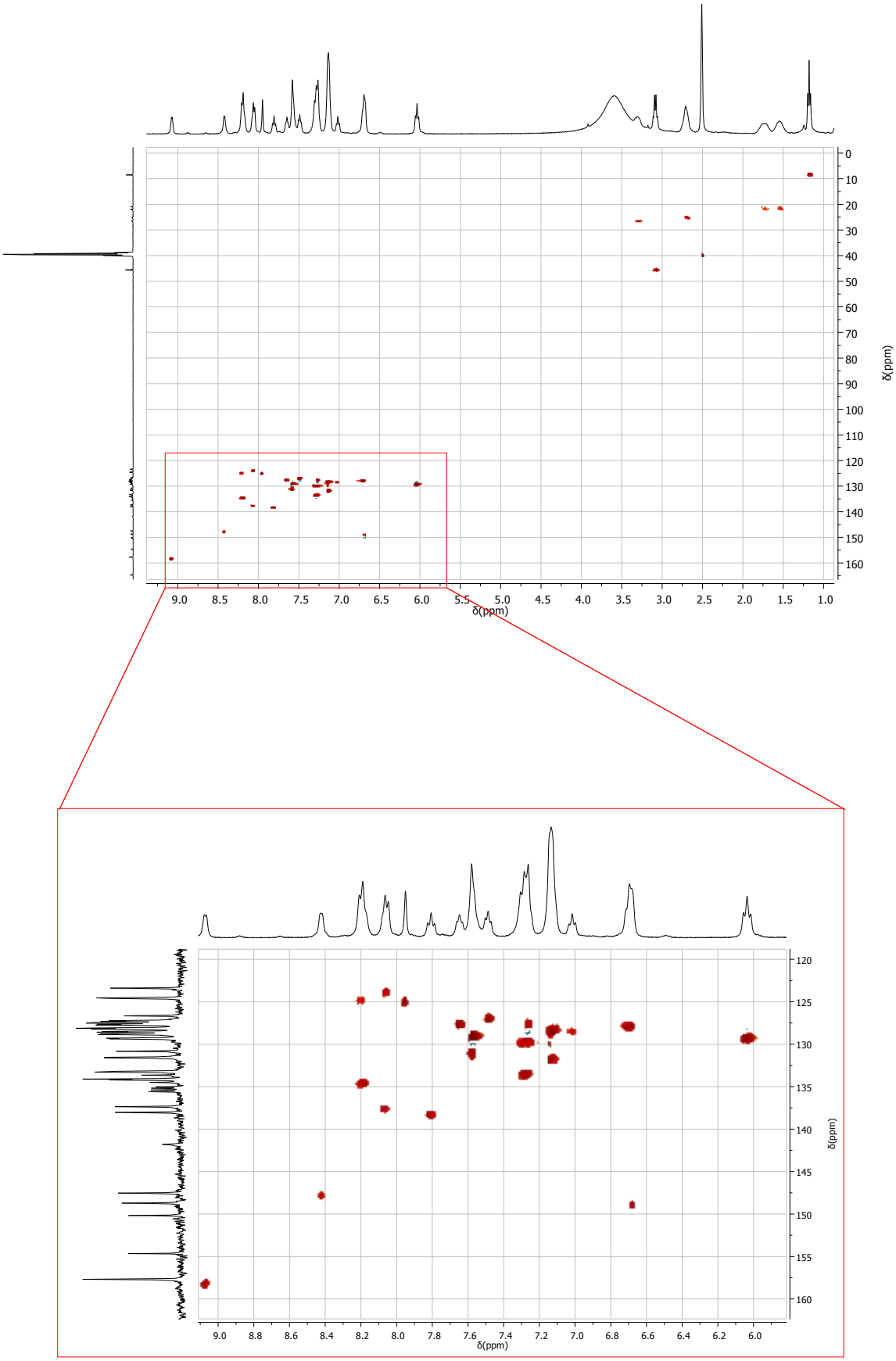

Figure S7 ^{1}H-^{13}C HSQC NMR spectra of the complex 1 (DMSO-d_6)

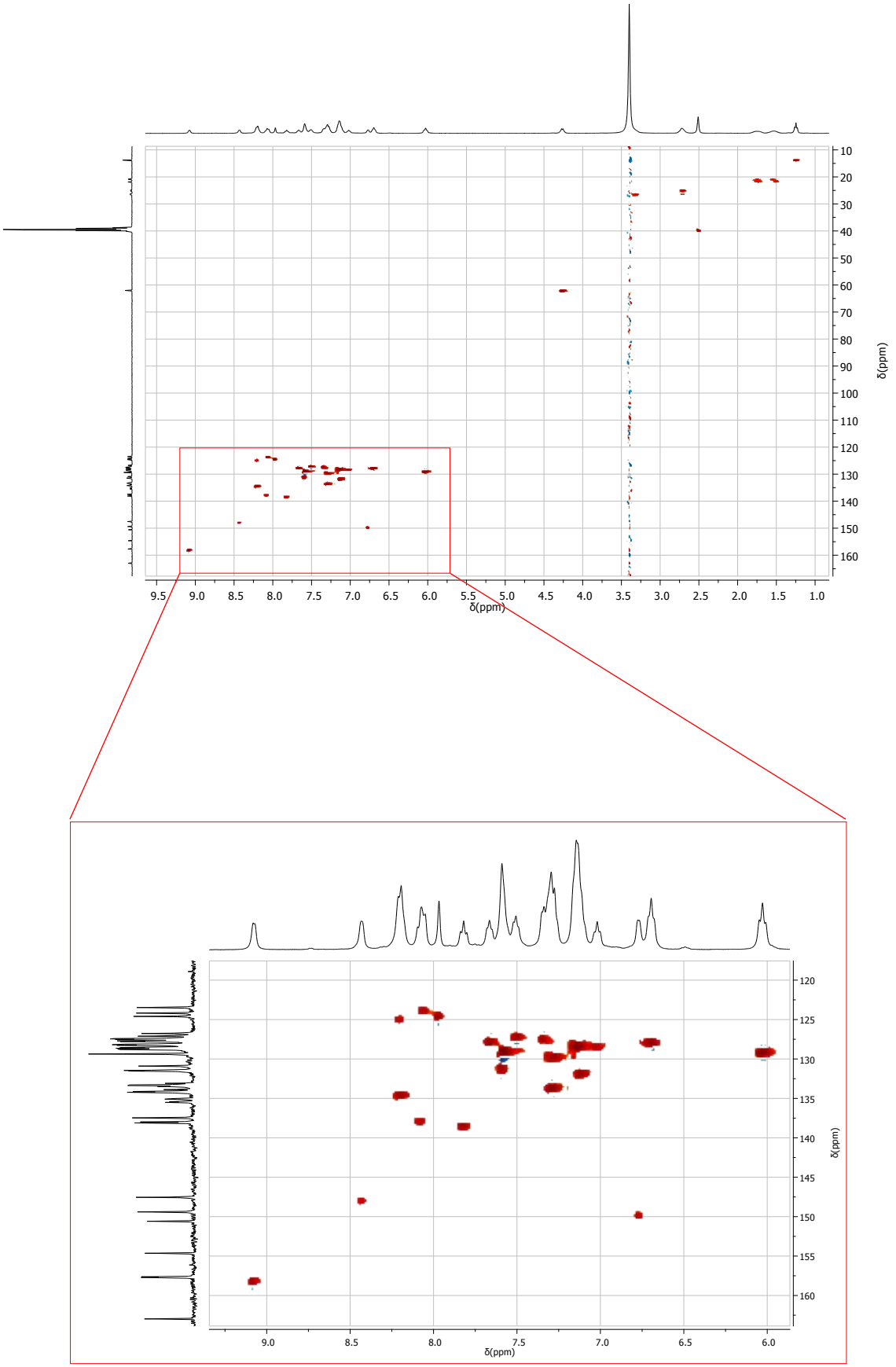

Figure S8 ^{1}H-^{13}C HSQC NMR spectra of the complex 2 (DMSO-d_6)

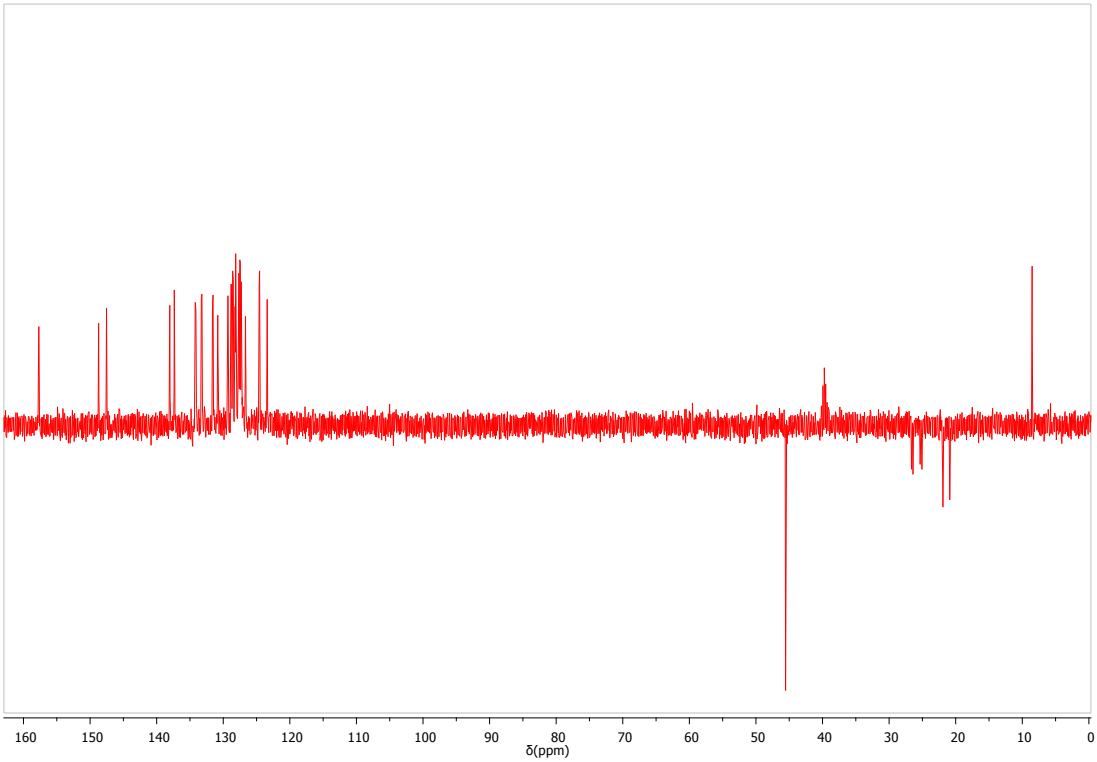

Figure S9 ^{13}C DEPT NMR spectra of the complex 1 (DMSO-d_6)

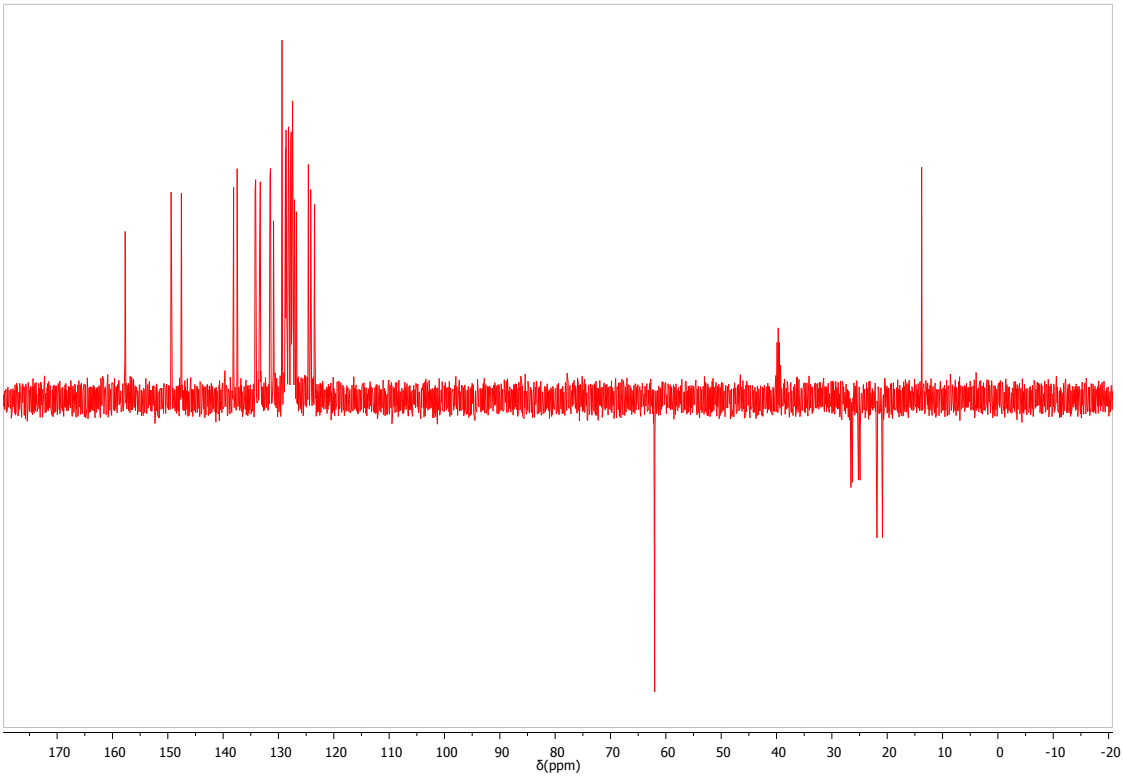

Figure S10 ^{13}C DEPT NMR spectra of the complex 2 (DMSO-d_6)

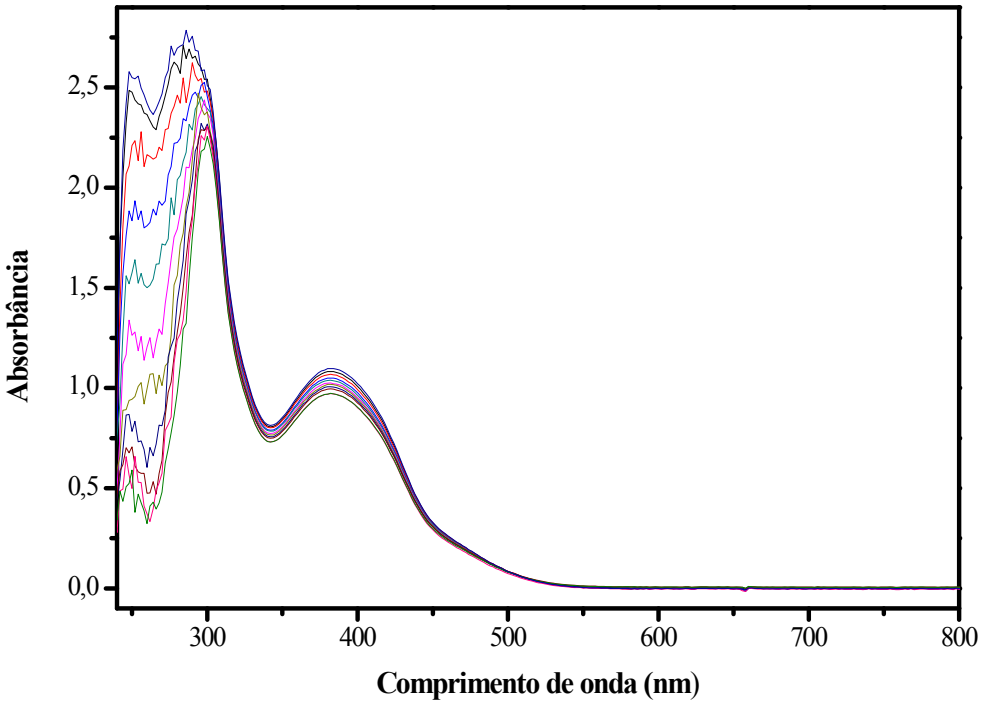

Figure S11 Spectrophotometric titration spectra of 1 with calf thymus (ct-DNA).

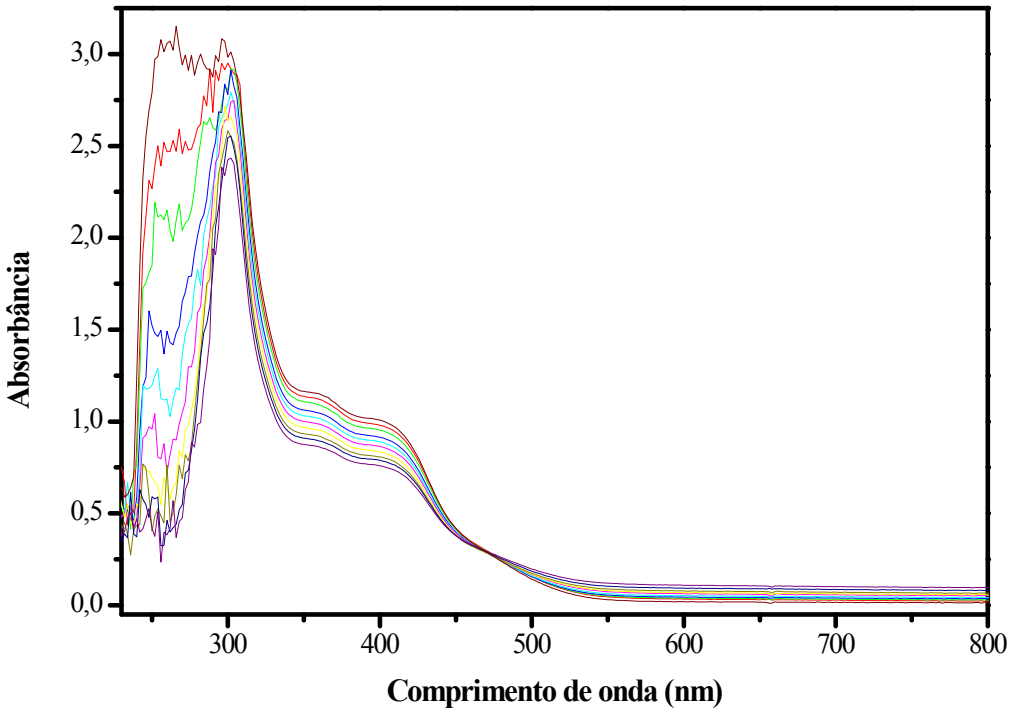

Figure S12 Spectrophotometric titration spectra of 3 with calf thymus (ct-DNA).

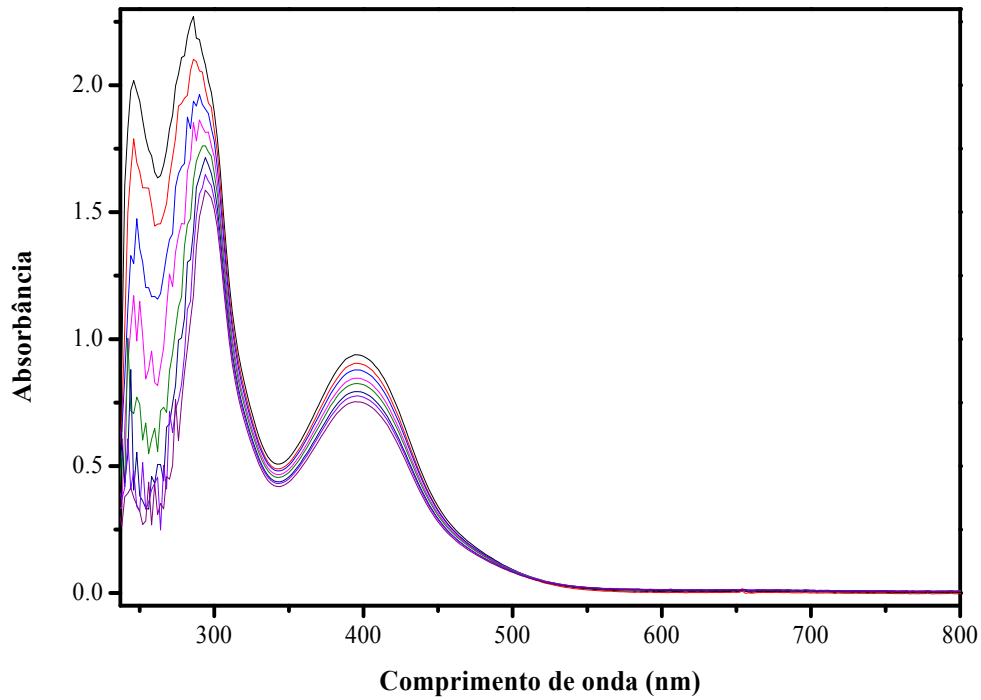

Figure S13 Spectrophotometric titration spectra of 2 with calf thymus (ct-DNA).

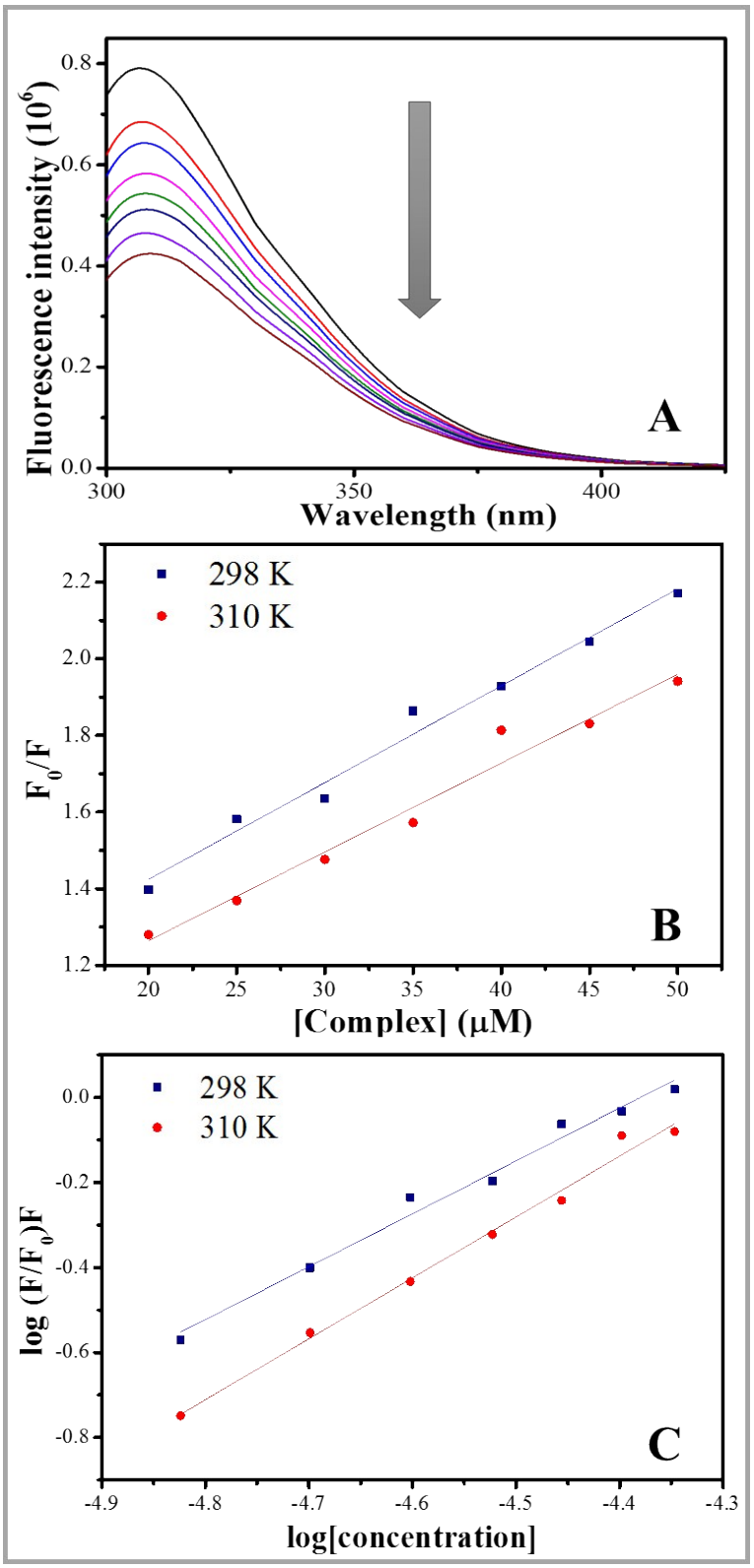

Figure S14 (A) Fluorescence quenching spectra of HSA with different concentrations of complex 2 in a Trizma-HCl buffer, pH 7.4; (B and C) Stern–Volmer plots for complex 2 showing tryptophan quenching at 310 and 289 K.

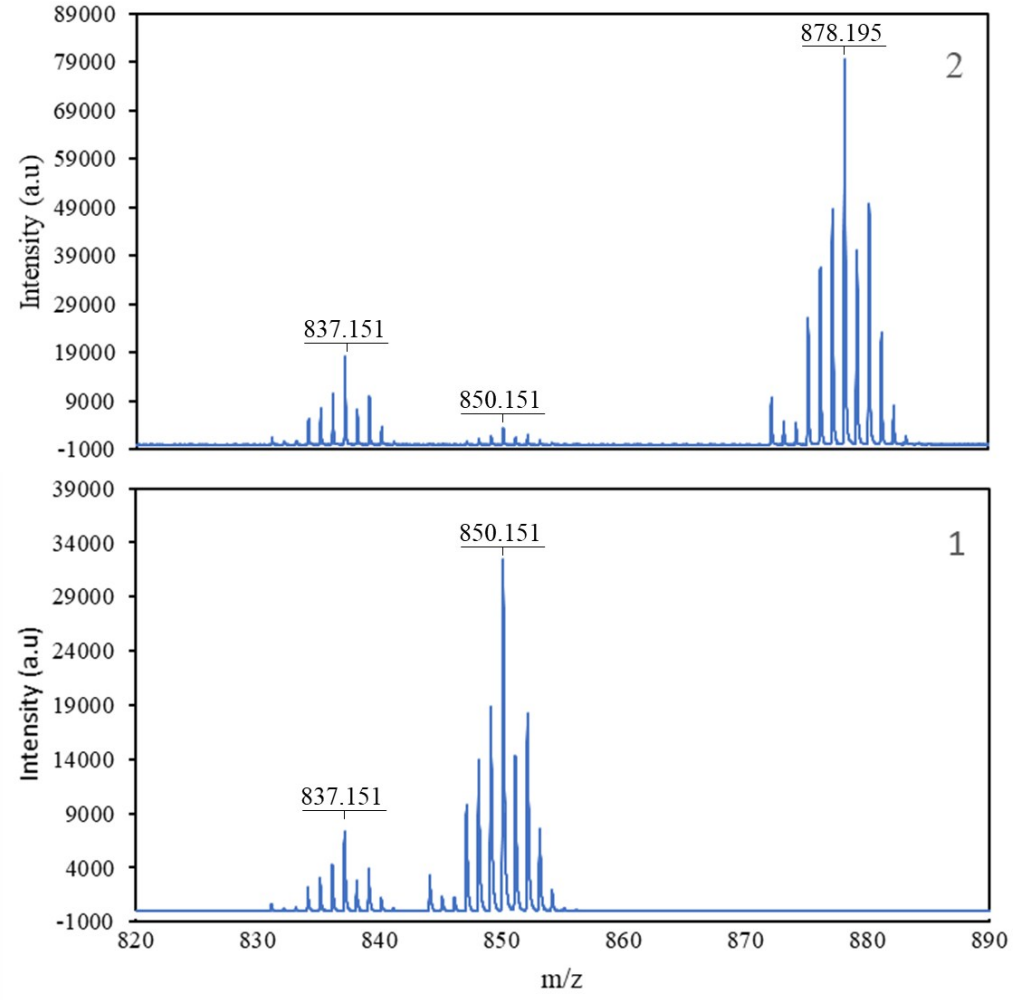

Figure S15 Maldi-TOF/MS spectra of complexes 1 and 2, using the dihidroxibenzoic acid as calibrant