Electronic supplementary information

Antiparasitic activity and ultrastructural alterations provoked by organoruthenium complexes against *Leishmania amazonensis*

Legna Colina-Vegas, Joseane Lima Prado Godinho, Thallita Coutinho, Rodrigo S. Correa, Wanderley de Souza, Juliany Cola Fernandes Rodrigues, Maribel Navarro, Alzir Azevedo Batista

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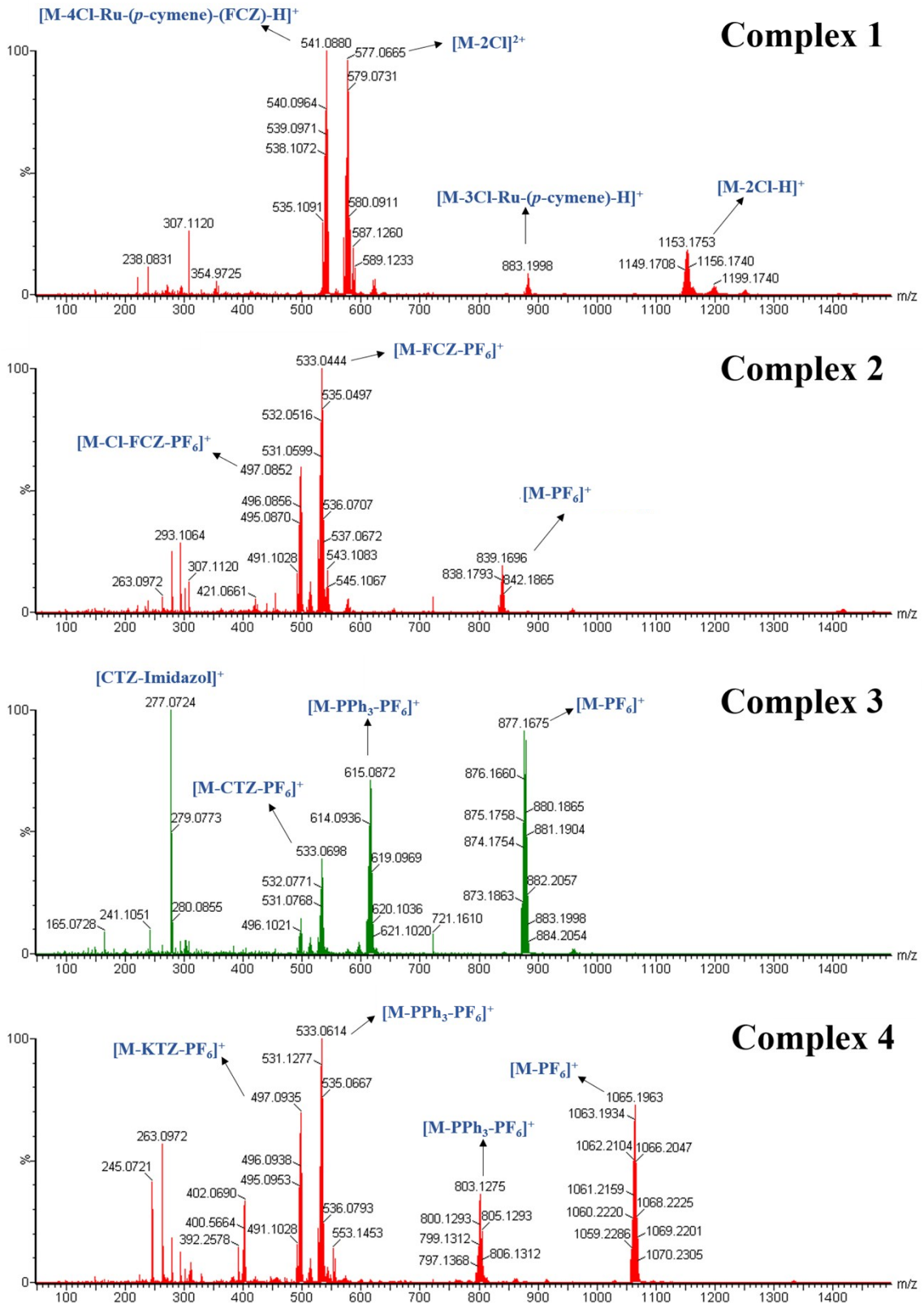

Fig 1S. TOF-MS-ES+ spectrum of complex **1-4** in acetone

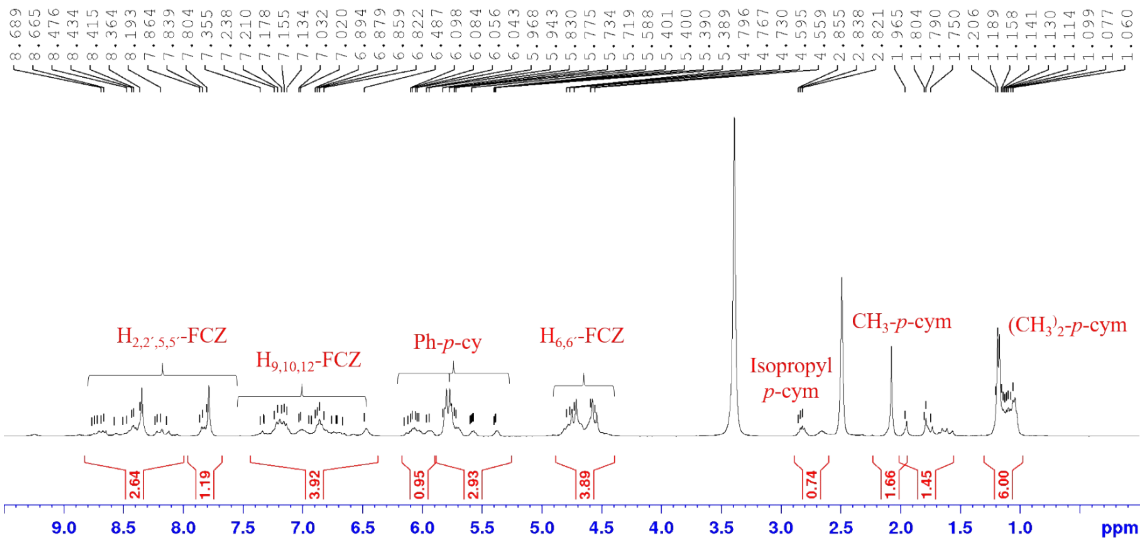

Fig 2S. ^{1}H NMR spectra of **1** in dmso-d_6 at 298 NMR

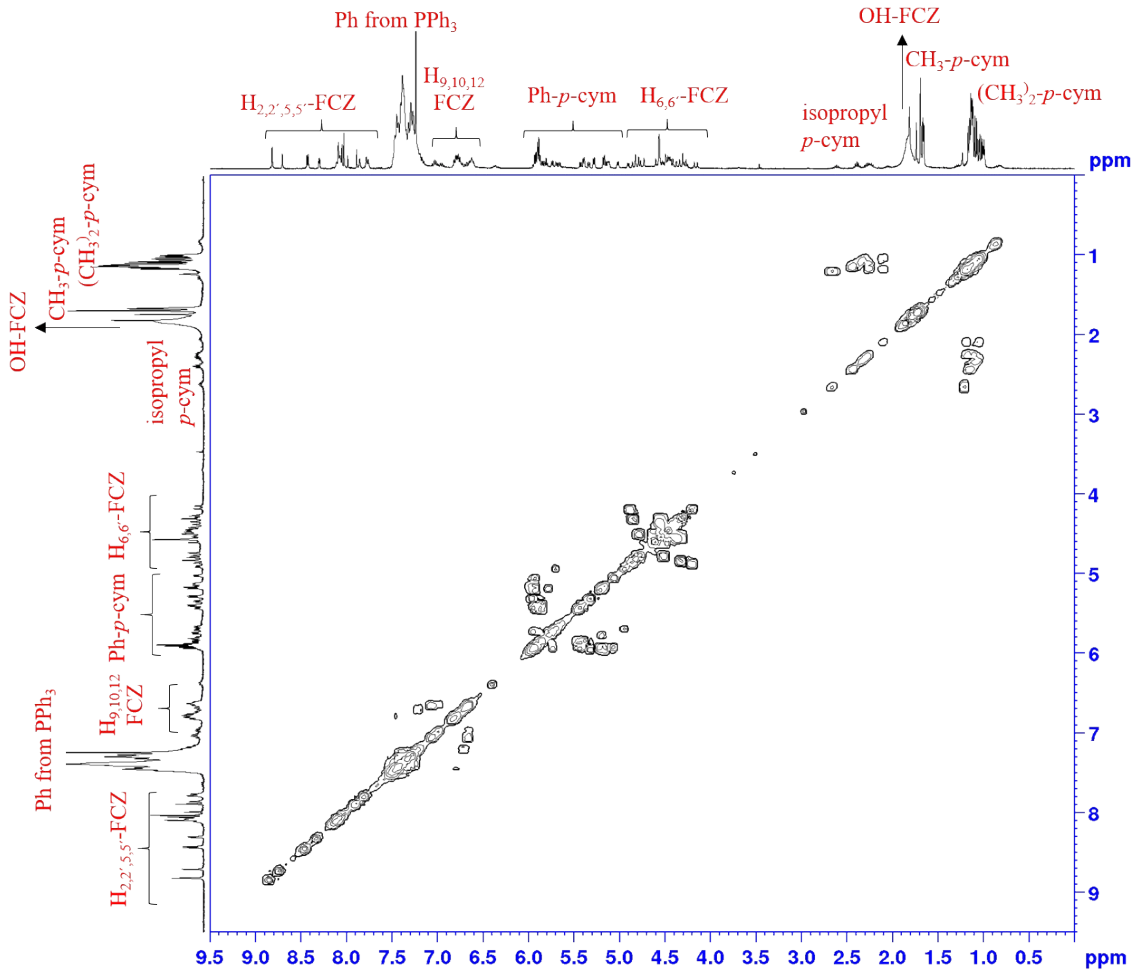

Fig 3S. ^{1}H-^{1}H COSY NMR spectra of **2** in $CDCl_3$ at 298 K

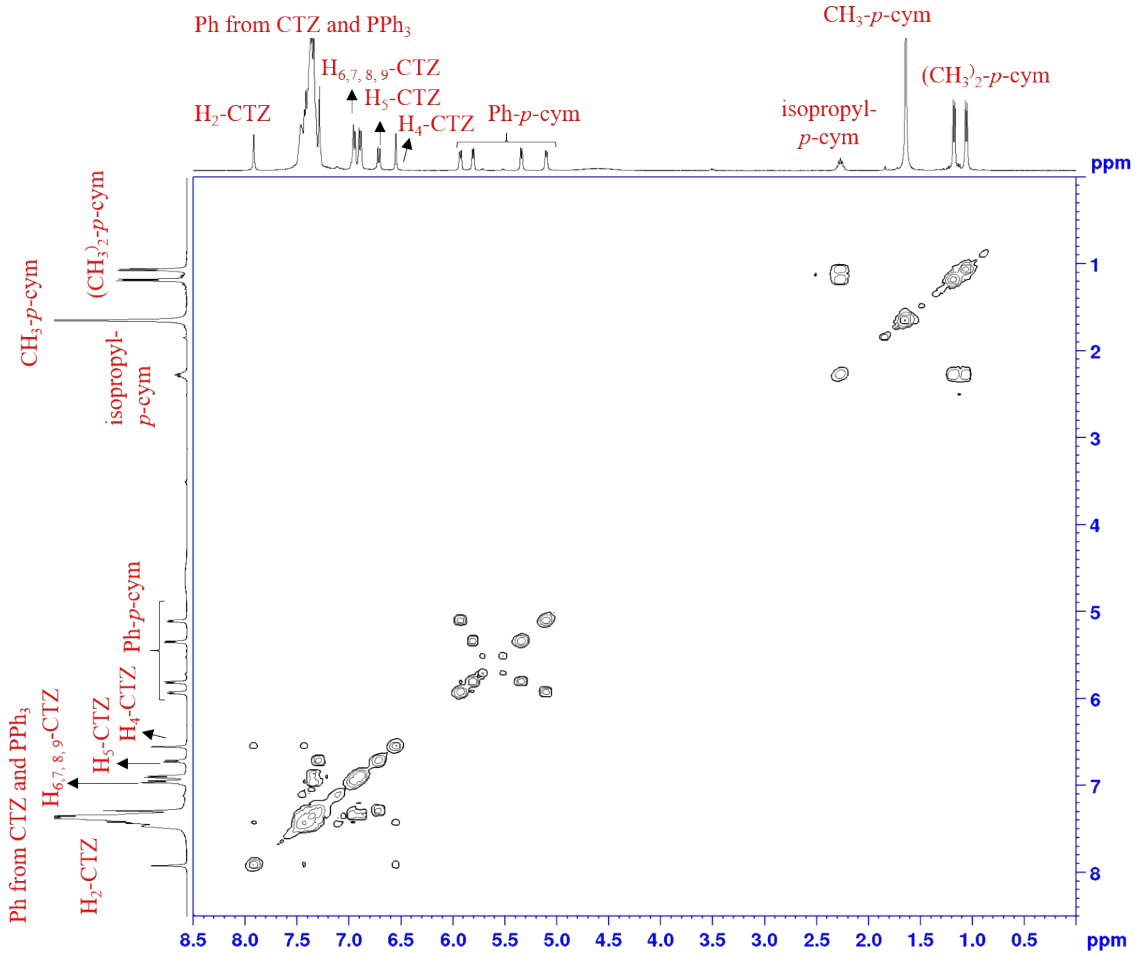

Fig 4S. ^{1}H-^{1}H COSY NMR spectra of **3** in $CDCl_3$ at 298 K

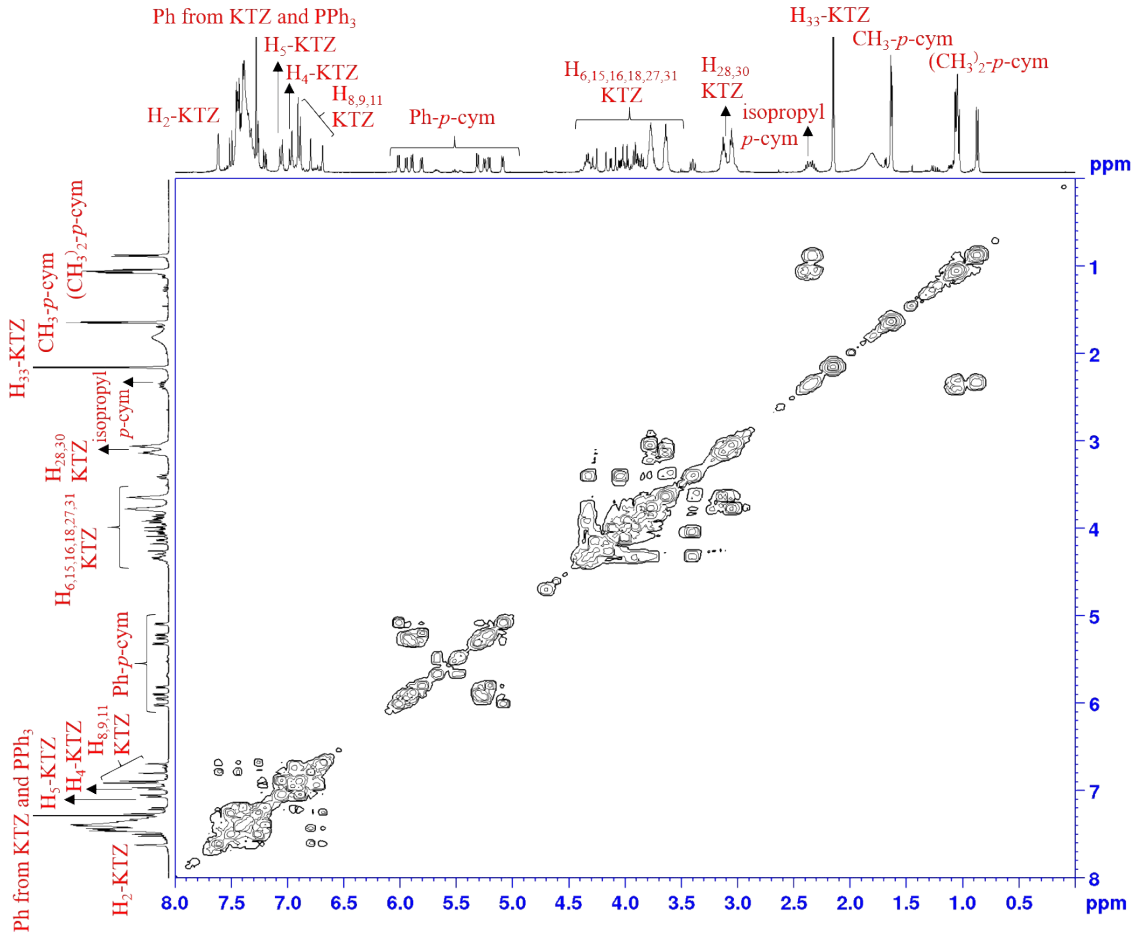

Fig 5S. ^{1}H-^{1}H COSY NMR spectra of **4** in $CDCl_3$ at 298 K

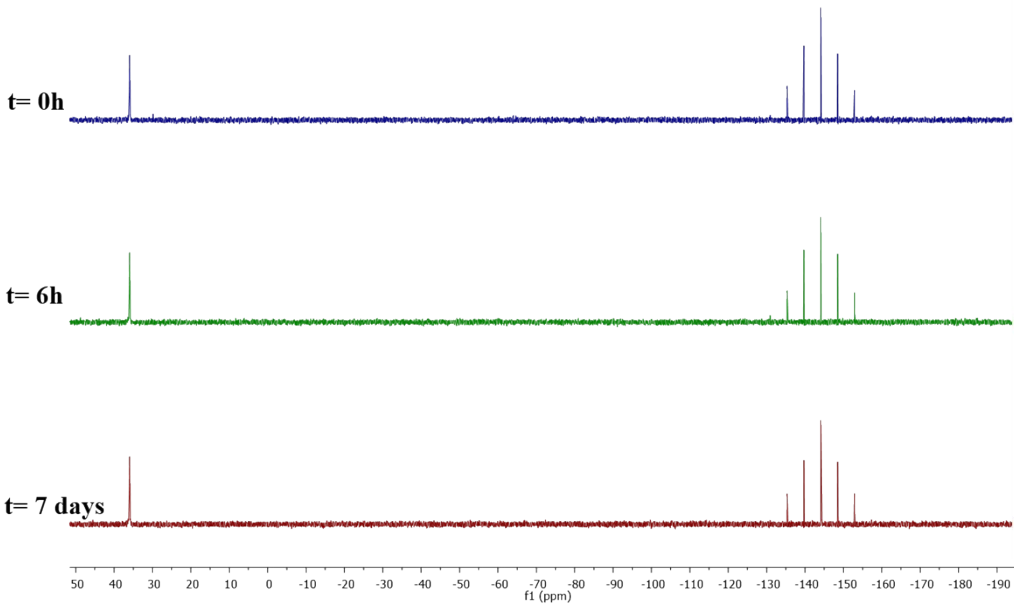

Fig 6S. $^{31}P\{^{1}H\}$ NMR spectrum in the mixture 70:30 DMSO:Culture medium (DMEM) of complex **3** at different times

Table 1S. Crystal data and structure refinement for complexes **1** and **5**.

Empirical formula	$[Ru_2C_{46}H_{52}F_4N_{12}O_2]Cl_2.2CH_3OH.H_2O$	$[RuC_{28}H_{31}OClP]PF_6$
Formula weight	1307.04	695.99
Temperature (K)	293(2)	293(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	Triclinic	Orthorhombic
Space group	P-1	Iba2
Unit cell dimensions (Å, °)	a = 8.9997(9); α= 82.615(3) b = 11.4597(6); β= 81.957(4) c = 13.9001(9); γ = 81.799(4)	a = 20.732(3) b = 16.101(1) c = 17.977(3)
Volume ($Å^3$)	1396.30(18)	6000.9(1)
Z	2	8
Density (Mg/m^3)	1.554	1.541
Absorption coefficient (mm^{-1})	0.801	0.776
F(000)	666	2816
Crystal size (mm^3)	0.40 x 0.17 x 0.16	0.35 x 0.30 x 0.21
θ range for data collection (°)	3.31 to 25.50	2.94 to 25.68.
Index ranges	-10≤h≤10, -13≤k≤13, -16≤l≤16	25≤h≤-25, 19 ≤k≤-19, 21 ≤l≤-21
Reflections collected	19541	10295
Independent reflections	5102 [Rint = 0.0390]	5650 [R_{int} = 0.0546, R_{sigma} = 0.0606]
Completeness to theta (%)	98.3	99.4
Data / restraints / parameters	5102/0/318	5650/1/356
Goodness-of-fit on F^2	1.080	1.040
Final R indices [I>2sigma(I)]	R_1 = 0.0523, wR_2 = 0.1376	R_1 = 0.0510, wR_2 = 0.1307
R indices (all data)	R_1 = 0.0592, wR_2 = 0.1439	R_1 = 0.0704, wR_2 = 0.1433
Absolute structure parameter	-	-0.08(4)
Extinction coefficient	0.065(6)	0.0047(5)
Largest diff. peak and hole ($e.Å^{-3}$)	1.23 and -1.03	0.96 and -1.01

R: refinement, wR: weighted R

Table 2S. Selected bond distances (Å) and angles (°) for the complex **5**

Bond lengths	Bond angles
Molecule 1	

Ru1-O1w	2.145(10)	O1w-Ru1-Cl1	81.0(3)
Ru1-P1	2.373(3)	O1w-Ru1-P1	86.2(3)
Ru1-Cl1	2.413(3)	P1-Ru1-Cl1	86.78(10)
Ru1-*Ct*1*	1.735(9)	O1w-Ru1-*Ct*1	128.6(4)
		Molecule 2	
Ru2-O2w	2.142(10)	O2w-Ru2-Cl2	81.2(3)
Ru2-P2	2.375(3)	O2w-Ru2-P2	86.6(3)
Ru2-Cl2	2.412(3)	P2-Ru2-Cl2	86.67(11)
Ru2-*Ct*2*	1.745(9)	O2w-Ru2-*Ct*2	127.8(4)

* *Ct* is defined as the centroid of the *p*-cymene ring.