Supporting Information to

Making organoruthenium complexes of 8-hydroxyquinolines more hydrophilic: Impact of a novel L-phenylalanine-derived arene ligand on the biological activity

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Table S1. Calculated log P (clog *P*) values for ligands **1**–**5** as calculated with ChemDraw 12.0. Taken from ref. 1.

ligand	**clog *P***
1	2.08
2	3.34
3	3.69
4	4.14
5	3.73

Table S2. Details of collected X-ray data for **B**.

	B
Formula	$C_{26}H_{34}Cl_4N_2O_6Ru_2$
CCDC Nr.	1585951
Molecular weight (g mol^{-1})	814.49
Temperature (K)	100(2)
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	$P2_1$
a (Å)	9.7994(4)
b (Å)	10.2685(4)
c (Å)	15.0143(5)
β (°)	94.369(2)
Volume ($Å^3$)	1506.43(10)
Z	2
Calculated density (g cm^{-3})	1.796
Absorption coefficient (mm^{-1})	1.400
F(000)	816
Crystal size (mm × mm × mm)	0.380 × 0.220 × 0.080
2θ (min, max) (°)	2.401 to 27.840
Limiting indices	-12<=h<=12 -13<=k<=13 -19<=l<=19
Reflections collected / unique	17862 / 6938
Data / restraints / parameters	6938 / 1 / 364
Goodness-of-fit on F^2	1.007
Final R indices [I>2σ(I)]	R1 = 0.0362, wR2 = 0.0711
R indices (all data)	R1 = 0.0581, wR2 = 0.0805
Largest diff. peak and hole (e $Å^{-3}$)	0.603 and -0.850

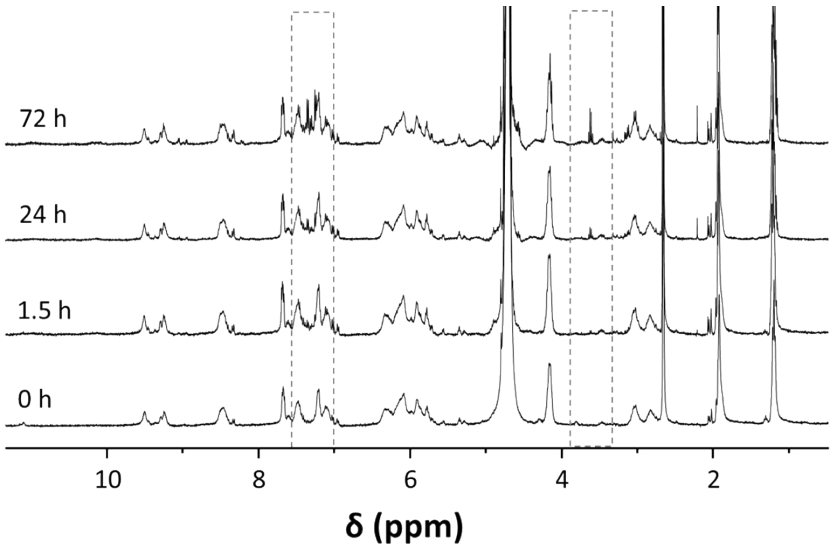

Figure S1. ^{1}H NMR spectroscopic study on the stability of **1a** in D_6-DMSO over the time course of 72 h.

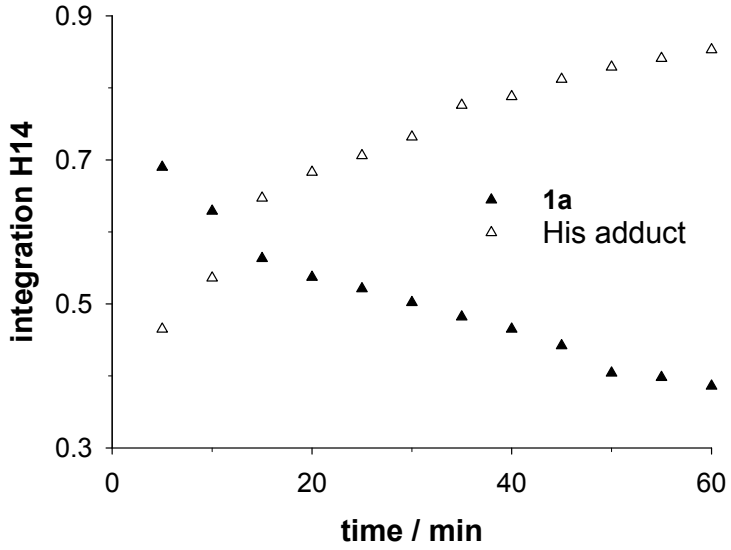

Figure S2. Time dependent decrease and increase of the ^{1}H NMR signals for H14 at 9.6 and 9.5 ppm, respectively, observed during the reaction between **1a** and His in 10% D_6-DMSO/D_2O within the first 60 min of incubation.

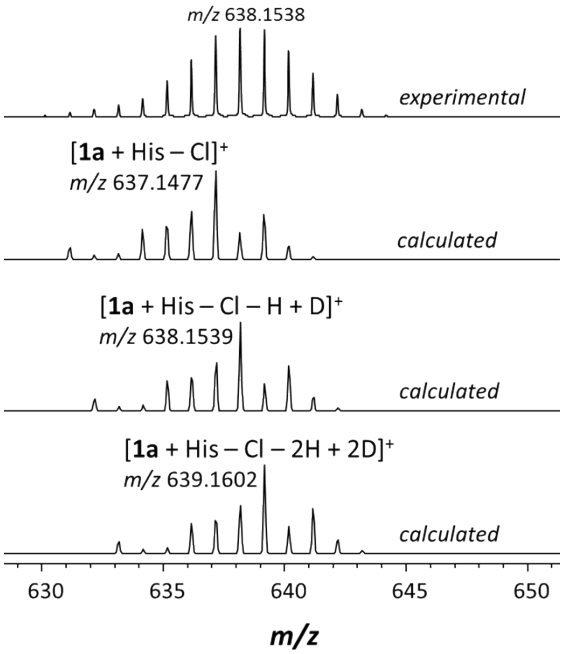

Figure S3. Section of the mass spectrum recorded for a 48-h incubation mixture of **1a** and His in D_6-DMSO (5% in 95% D_2O) and diluted with acetonitrile before analysis with ESI-MS. The peak at *m/z* 638.1538 was assigned to [**1a** + His – Cl]$^+$ and is the result of overlapping species with different degrees of H/D exchange.

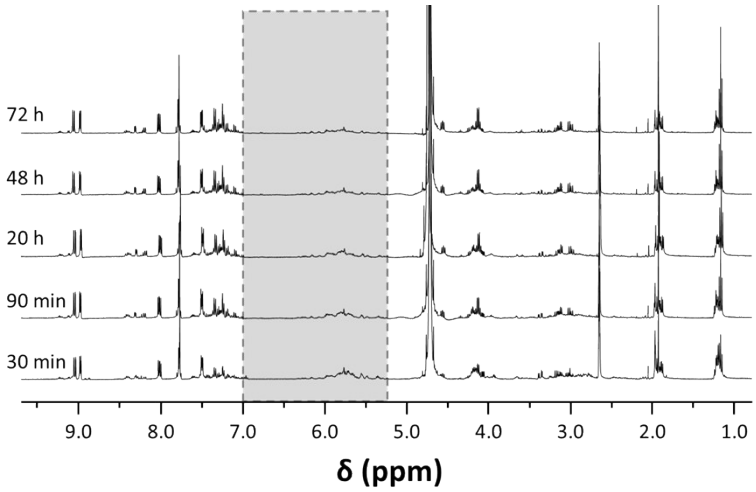

Figure S4. ^{1}H NMR spectroscopic study on the reaction of **1a** with Cys over the time course of 72 h.

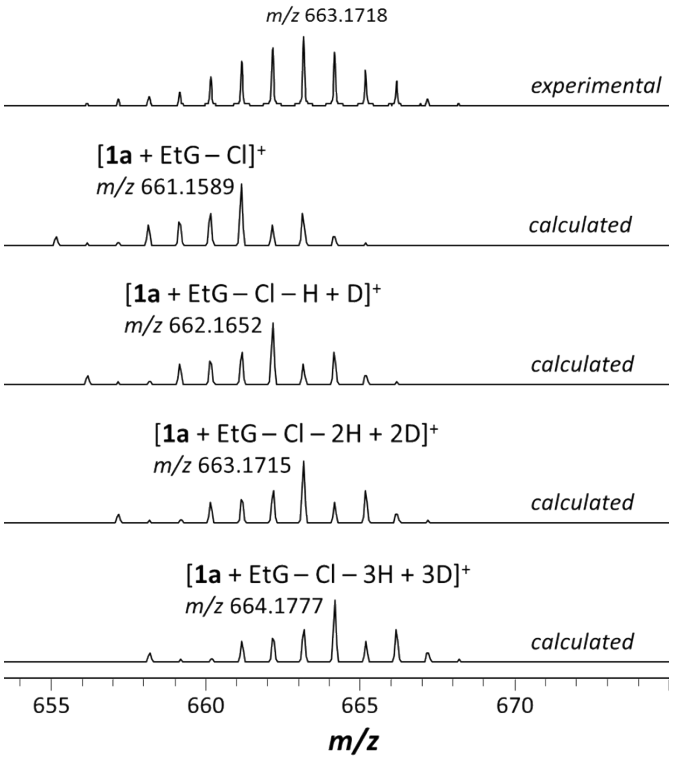

Figure S5. Section of the mass spectrum recorded for a mixture of **1a** and 9-ethylguanine (EtG) in D_6-DMSO (5% in 95% D_2O) and diluted with acetonitrile before analysis with ESI-MS. The peak at *m/z* 663.1718 was assigned to [**1a** + EtG – Cl]$^+$ and is the result of overlapping species with different degrees of H/D exchange.

References

1. M. Kubanik, H. Holtkamp, T. Söhnel, S. M. F. Jamieson and C. G. Hartinger, *Organometallics*, 2015, **34**, 5658-5668.