Supplementary Material

Binding Kinetics of Ruthenium Pyrithione Chemotherapeutic Candidates to Human Serum Proteins Studied by HPLC-ICP-MS

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Table 1S. ICP-MS operating parameters.

Parameter	Type/Value	Type/Value
	Ru speciation analysis	Analysis of total Ru content
Sample introduction		
Nebuliser	Miramist	Miramist
Spray chamber	Scott	Scott
Skimmer and sampler	Ni	Ni
Plasma conditions		
Forward power	1550 W	1550 W
Plasma gas flow (Ar)	15.0 L min ⁻¹	15.0 L min ⁻¹
Carrier gas flow (Ar)	0.45 L min ⁻¹	1.05 L min ⁻¹
Dilution gas flow (Ar)	0.75 L min ⁻¹	/
Make up gas flow (Ar)	/	0.10 L min ⁻¹
Total carrier gas flow	1.20 L min ⁻¹	1.15 L min ⁻¹
He gas flow	4.3 mL min ⁻¹	4.5 mL min ⁻¹
Omega bias	-110 V	-120 V
Cell entrance	-40 V	-40 V
Cell exit	-60 V	-60 V
Deflect	3.8 V	3.0 V
Plate bias	-60 V	-60 V
Sample uptake rate	1.0 mL min ⁻¹	0.3 mL min ⁻¹
Data acquisition parameters		
m/z of isotopes monitored	⁹⁹ Ru, ¹⁰¹ Ru	¹⁰¹ Ru
m/z of internal standards*	¹⁰³ Rh	¹⁰³ Rh
Total acquisition time	1080 s	/

*In speciation analysis, internal standards were not used when the ID-ICP-MS procedure was applied



8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3 6.2 6.1 6.0 5.9 5.8 5.7 5.6 f1 (ppm)

Figure 1. ¹H-NMR stability spectra of the chlorido complex (1) in 0.3% MeOD-d₄/D₂O solution containing 154 mM NaCl recorded a) immediately, b) after 24 hours and c) after 48 hours. The release of *p*-cymene is labelled with an asterisk (*).



Figure S2: ¹H-NMR stability spectra of the pta complex (**2**) in D₂O solution containing 154 mM NaCl recorded a) immediately, b) after 24 hours and c) after 48 hours. The release of *p*-cymene is labelled with an asterisk (*) and ptao with squares.



Figure S3: ³¹P-NMR stability spectra of the pta complex (**2**) in D₂O solution containing 154 mM NaCl recorded a) immediately, b) after 24 hours and c) after 48 hours.