

Supporting Information

Transferring the Concept of Multinuclearity to Ruthenium Complexes for Improvement of Anticancer Activity

Maria G. Mendoza-Ferri,^a Christian G. Hartinger,^{a,b,} Marco A. Mendoza,^{c,∞} Michael Groessel,^a
Alexander Egger,^a Rene E. Eichinger,^a John B. Mangrum,^d Nicholas P. Farrell,^d Magdalena
Maruszak,^e Patrick J. Bednarski,^e Franz Klein,^c Michael A. Jakupec,^a Alexey A. Nazarov,^{a,*} Kay
Severin,^b Bernhard K. Keppler^a*

^a University of Vienna, Institute of Inorganic Chemistry, Austria

^b Institut des Sciences et Ingénierie Chimiques, Ecole Polytechnique Fédérale de Lausanne,
Switzerland

^c Department of Chromosome Biology, Max F. Perutz Laboratories, University of Vienna, Austria

^d Department of Chemistry, Virginia Commonwealth University, United States

^e Department of Pharmaceutical and Medicinal Chemistry, University of Greifswald, Germany

Table of contents:

- 1.1 Elemental Analysis Data
- 1.2 Hydrolysis of **4c** by $^1\text{H-NMR}$
- 1.3 $\text{p}K_{\text{a}}$ determination
- 1.4 Structures of **7** and **8**

1.1. Elemental Analysis Data

Table S1. Elemental Analyses Data for compounds **1a**, **3a** and **5a**

	1a		3a		5a	
	$C_{28}H_{28}N_2O_4 \cdot 2/3H_2O$		$C_{30}H_{32}N_2O_4 \cdot 1/3H_2O$		$C_{34}H_{40}N_2O_4 \cdot 2H_2O$	
	theoret.	found	theoret.	found	theoret.	found
C	71.78	71.73	73.45	73.39	70.81	70.92
H	6.31	6.35	6.71	7.03	7.69	7.78
N	5.98	5.87	5.71	5.67	4.86	4.79

Table S2. Elemental Analyses Data for compounds **1b**, **3b** and **5b**

	1b		3b		5b	
	$C_{14}H_{16}N_2O_4 \cdot$		$C_{16}H_{20}N_2O_4$		$C_{20}H_{28}N_2O_4$	
	theoret.	found	theoret.	found	theoret.	found
C	60.86	61.11	63.14	62.87	66.64	66.52
H	5.84	6.09	6.62	6.70	7.83	7.63
N	10.14	10.43	9.20	9.06	7.77	7.40

Table S3. Elemental Analyses Data for compounds **1c**, **3c** and **5c**

	1c		3c		5c	
	$C_{34}H_{42}N_2O_4Ru_2Cl_2$		$C_{36}H_{46}N_2O_4Ru_2Cl_2$		$C_{40}H_{54}N_2O_4Ru_2Cl_2$	
	theoret.	found	theoret.	found	theoret.	found
C	50.06	49.87	51.24	50.96	53.39	53.09
H	5.19	5.21	5.49	5.59	6.05	6.23
N	3.43	3.14	3.32	3.24	3.11	3.12

1.2. Hydrolysis of **4c**

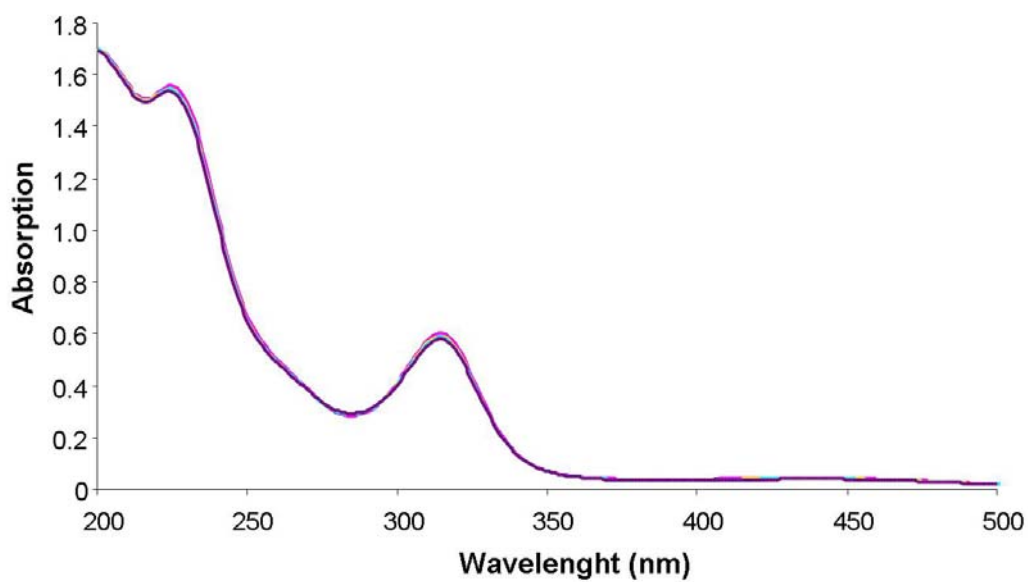


Figure S1. UV-vis spectra of **4c** in water measured over 2 d.

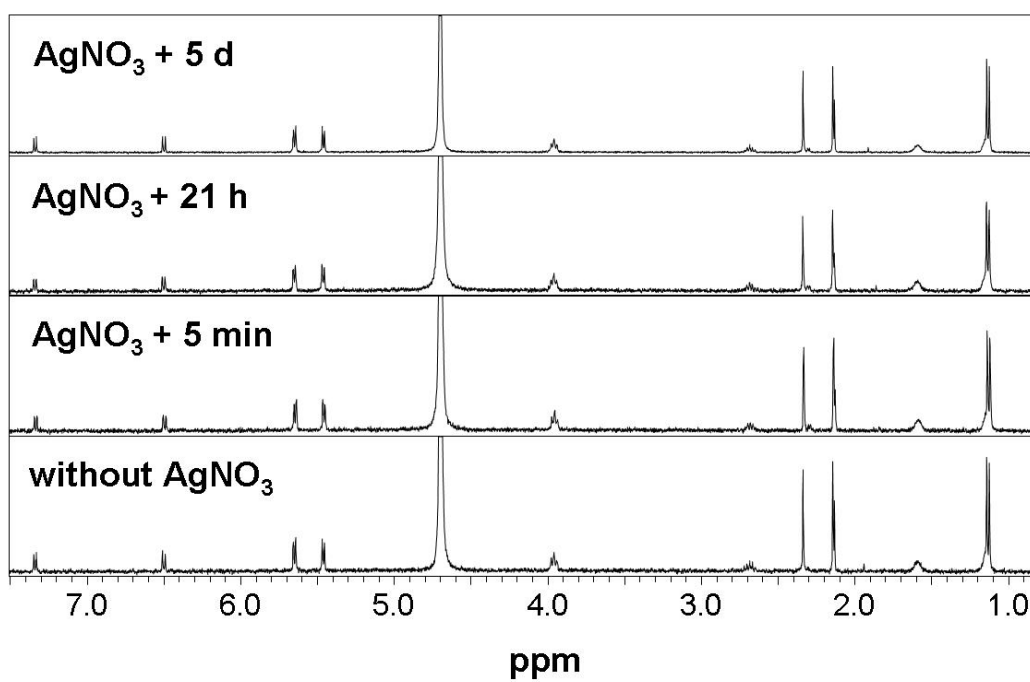


Figure S2. Time-resolved ¹H-NMR spectra of **4c** in D₂O before and after addition of AgNO₃.

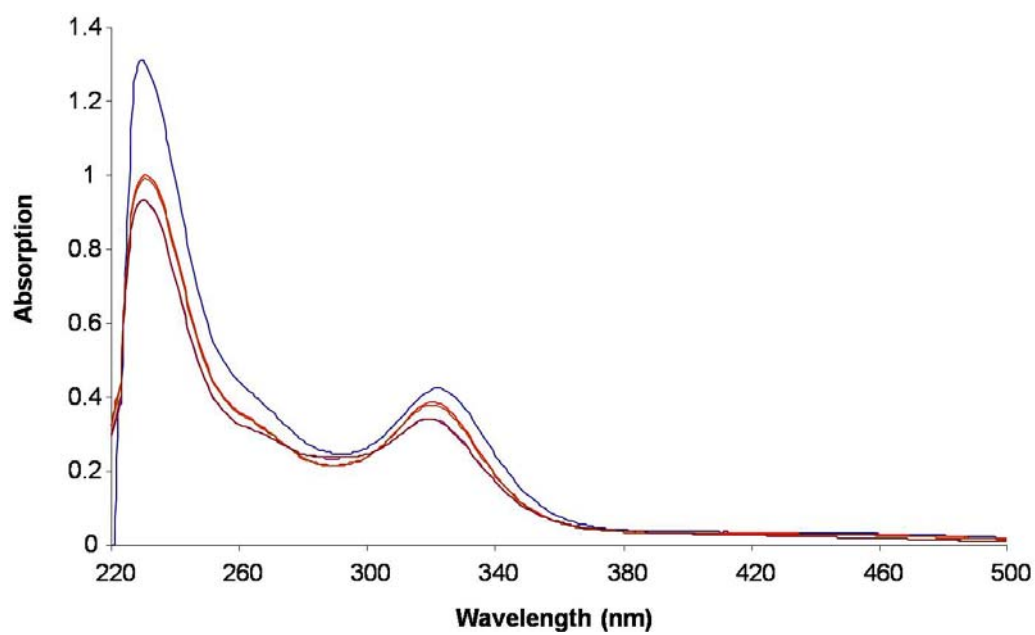


Figure S3. Time course of UV-vis spectra of **4c** prepared in dry methanol and after addition of 10% water to the sample.

1.3. pK_a determination

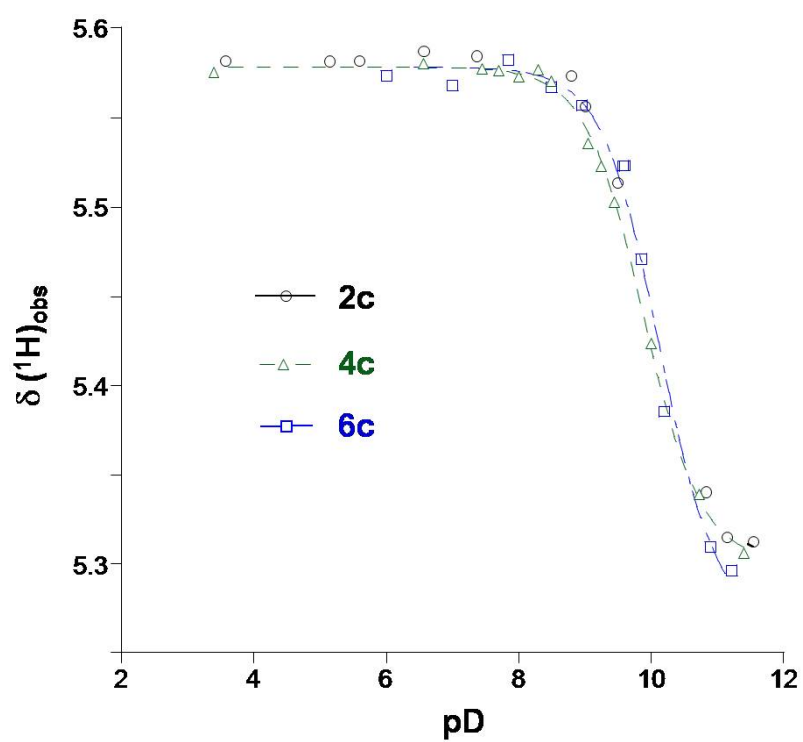


Figure S4. Observed ^1H -NMR chemical shift (δ_{obs}) vs. pD values for **2c**, **4c**, and **6c**.

1.4. Structures of 7 and 8

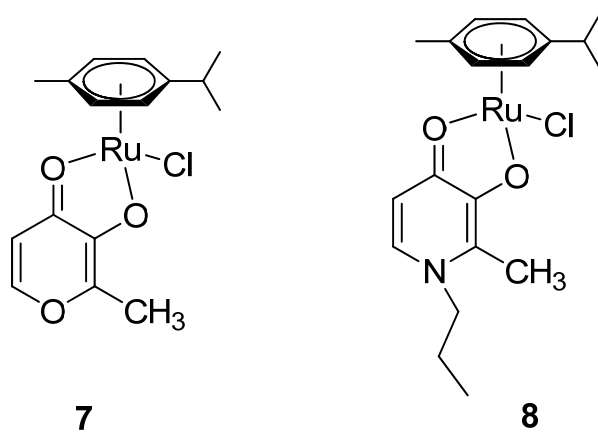


Figure S5. Structures of 7 and 8