

# CHEMISTRY

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### Supporting Information

#### **Heteropentanuclear Oxalato-Bridged $nd-4f$ ( $n = 4, 5$ ) Metal Complexes with NO Ligand: Synthesis, Crystal Structures, Aqueous Stability and Antiproliferative Activity**

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**Figure S1.** Phosphorescence emission spectrum of complex **4**.

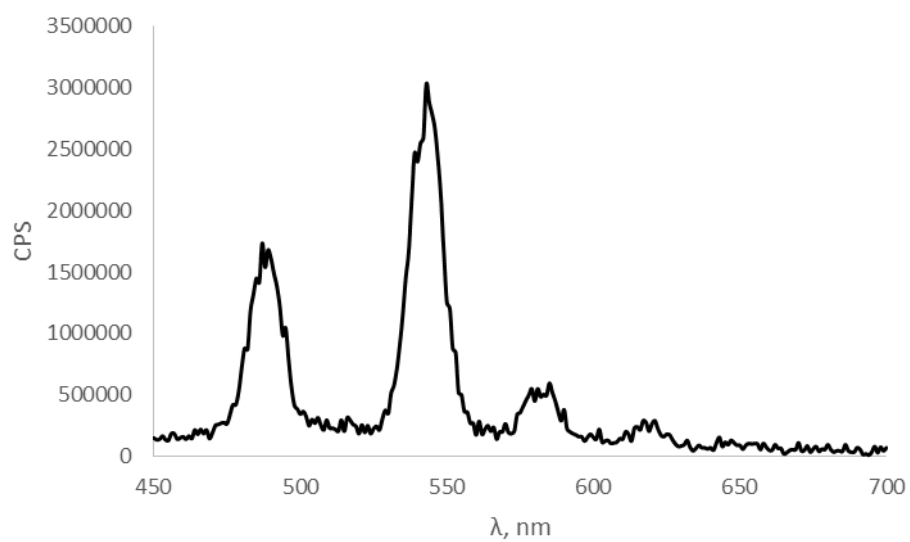
**Figure S2.** Structural formulas of the model compounds.

**Figure S3.** UV–vis spectra of **5** (0.35 mM) in aqueous solution measured directly after dissolution (black dashed trace) and 96 h thereafter (red trace).

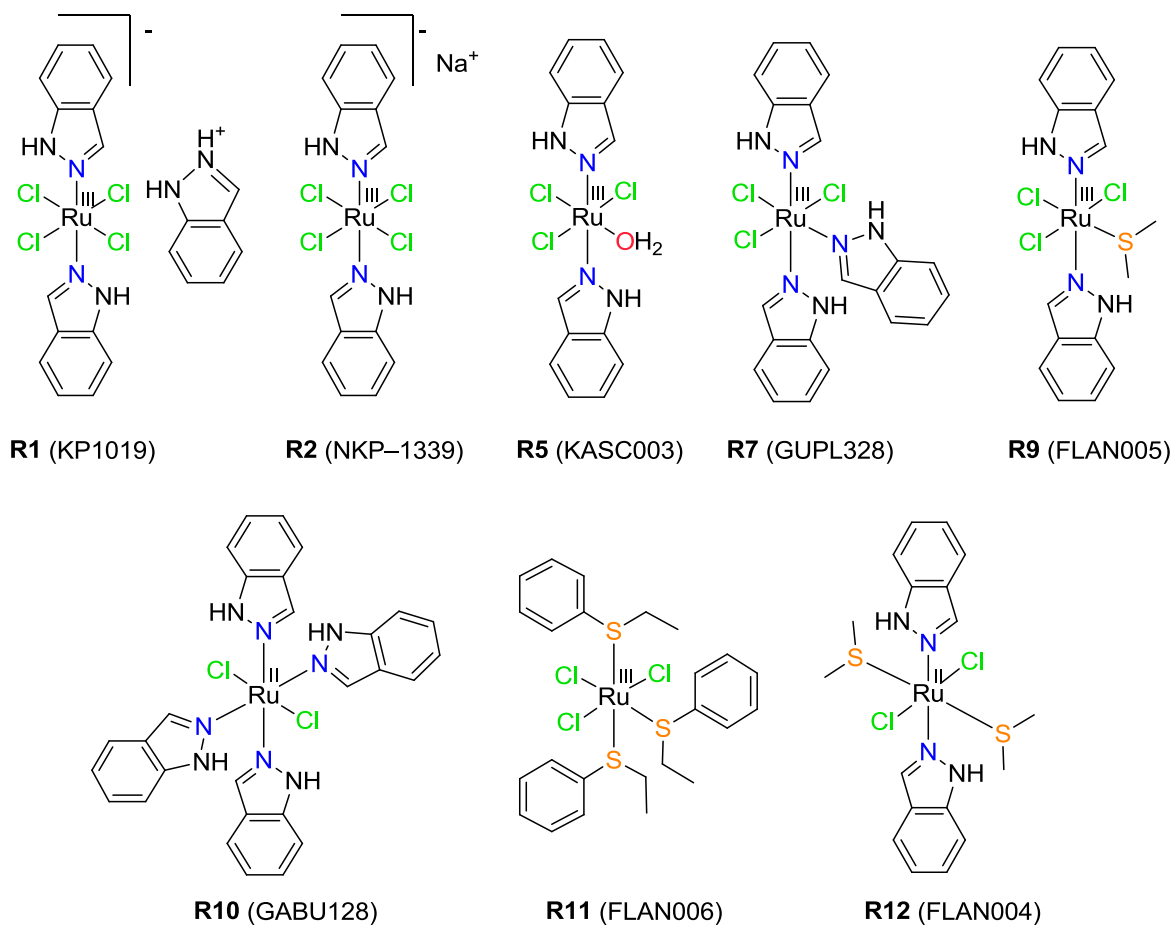
**Figure S4.** UV–vis spectrum of **9** (0.34 mM) in aqueous solution measured directly after dissolution (black line) and 96 h thereafter (red line).

**Figure S5.** Concentration-effect curves of complexes **1–9**.

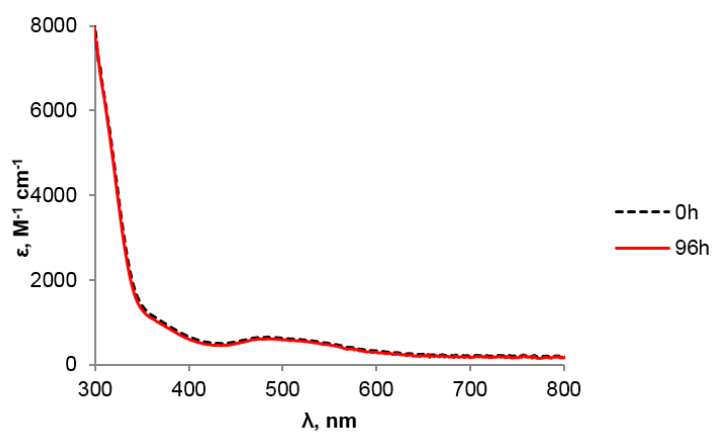
**Table S1.** Unit cell parameters for **3** and **4**.



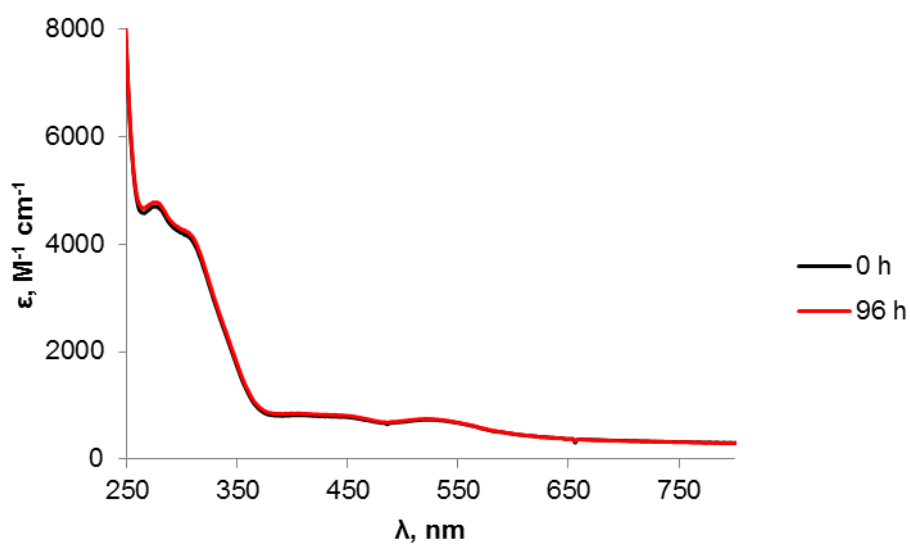
**Figure S1.** Phosphorescence emission spectrum ( $\lambda_{\text{ex}} = 365$  nm) of complex **4**.



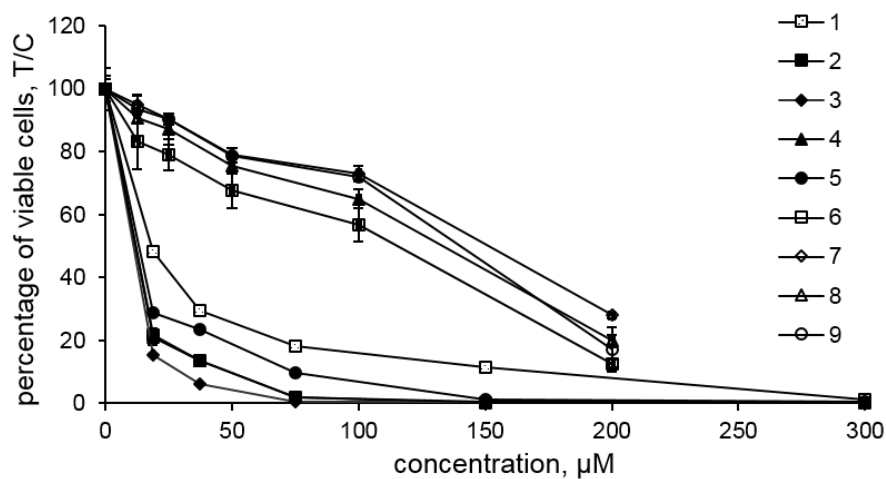
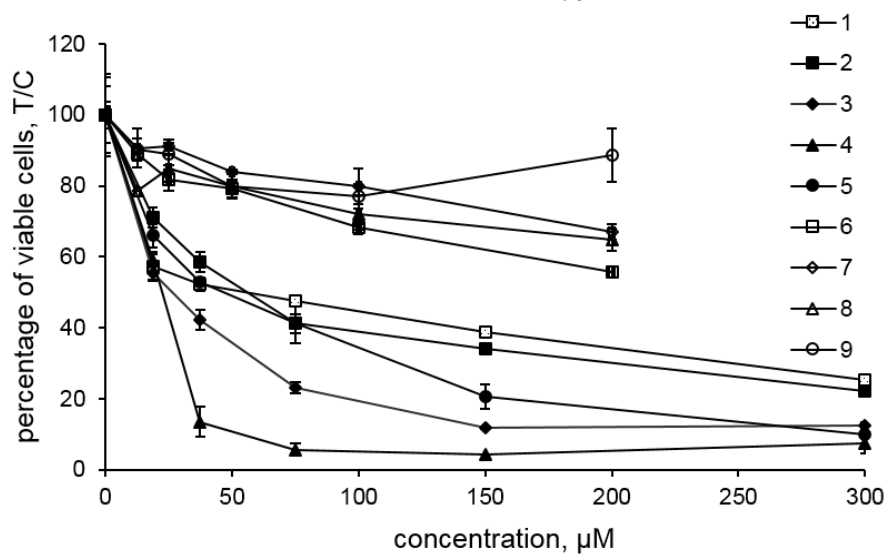
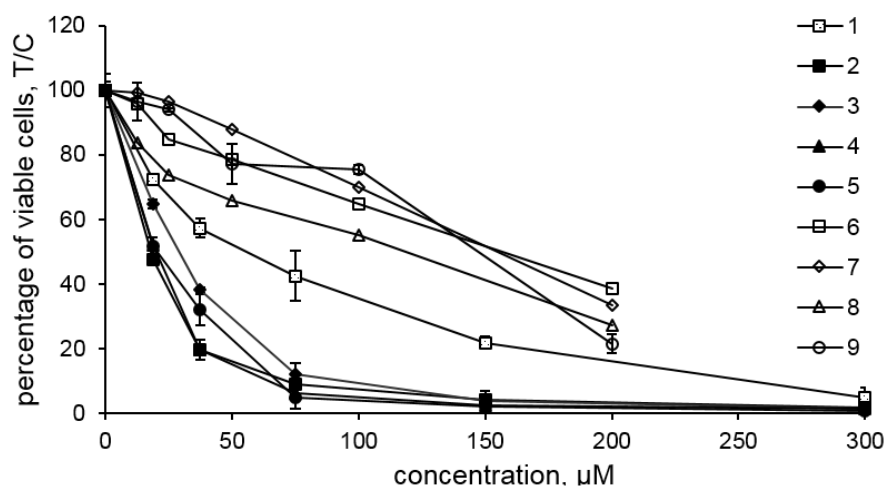
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**Figure S4.** UV-vis spectrum of **9** (0.34 mM) in aqueous solution measured directly after dissolution (black line) and 96 h thereafter (red line).



**Figure S5.** Concentration-effect curves of complexes 1–9 in the two human cancer cell lines HeLa and A549 and in the noncancerous cell line MRC-5, obtained by the MTT assay (48 h exposure).

**Table S1.** Crystal parameters for **3**, **4** and **4'**.

Compound	<b>3</b>	<b>4</b>	<b>4'</b>
Space group	<i>Cc</i>	<i>Cc</i>	<i>P-42<sub>1</sub>c</i>
$a$ , Å	17.9318	18.0098	18.4046
$b$ , Å	27.1662	27.233	18.4046
$c$ , Å	26.8678	26.9135	18.4366
$\alpha$ , °			
$\beta$ , °	92.721	92.529	
$\gamma$ , °			