

## Supporting Information

### Synthesis, X-ray diffraction structure, spectroscopic properties and antiproliferative activity of a novel ruthenium complex with constitutional similarity to cisplatin

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**Figure S1.** Time-dependent UV–vis spectral changes of **1** in dry CH<sub>3</sub>OH: 24 × 2 min (runs 1, 2, 4, 8, 12, 16, 20 and 24), and followed by 24 × 2 h (runs 1, 4, 8, 12, 16, 20 and 24)

**Figure S2.** Time-dependent UV–vis spectral changes of **1** in H<sub>2</sub>O: 24 × 2 min (runs 1, 2, 4, 8, 12, 16, 20 and 24)

**Figure S3.** Time-dependent UV–vis spectral changes of **1** in 0.1 M NaCl: 24 × 2 min (runs 1 and 24), and after 1 h followed by 24 × 10 min (runs 1 and 24), and then 24 × 45 min (runs 1, 4, 8, 12, 16, 20 and 24)

**Figure S4.** Mass spectrum of **1** after 4 days in MeOH (left) with the calculated isotopic pattern for  $[\{(\eta^6\text{-}p\text{-cymene})\text{Ru}\}_2(\mu\text{-OCH}_3)_3]^+$  (right)

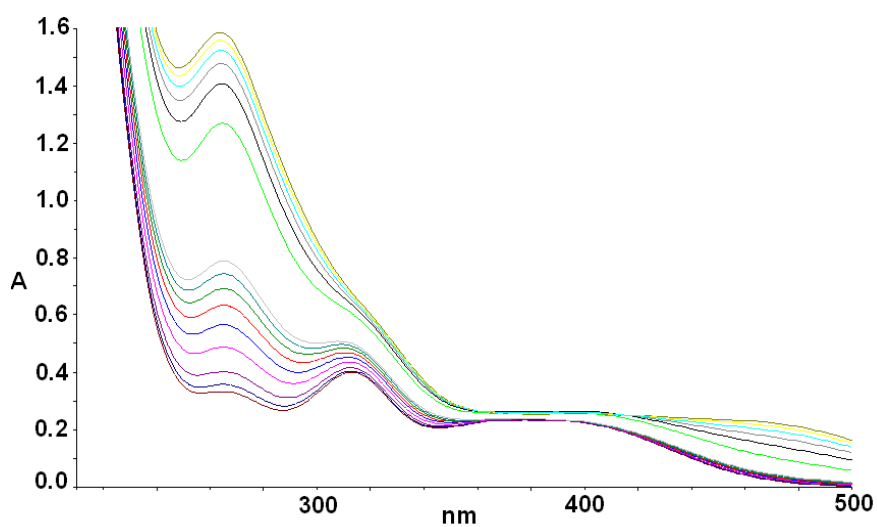
**Figure S5.** Time-dependent UV–vis spectral changes of “[ $(\eta^6\text{-}p\text{-cymene})\text{Ru}(\text{NH}_3)_2(\text{H}_2\text{O})$ ]<sup>2+</sup>” species in H<sub>2</sub>O: 12 × 10 min (runs 1 and 12), followed by 12 × 2 h (run 12)

**Figure S6.** <sup>1</sup>H NMR spectra of **1** in D<sub>2</sub>O (C<sub>6</sub>H<sub>4</sub> region)

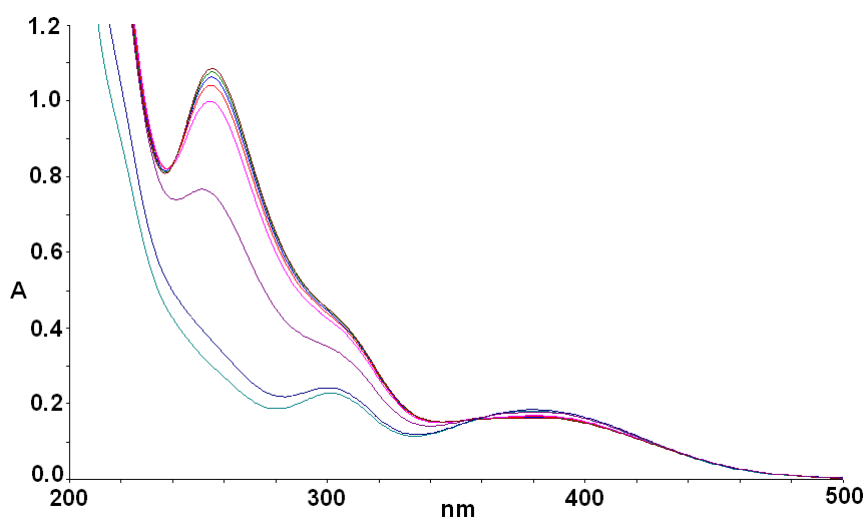
**Figure S7.** <sup>1</sup>H NMR spectra of **1** in D<sub>2</sub>O (CH region)

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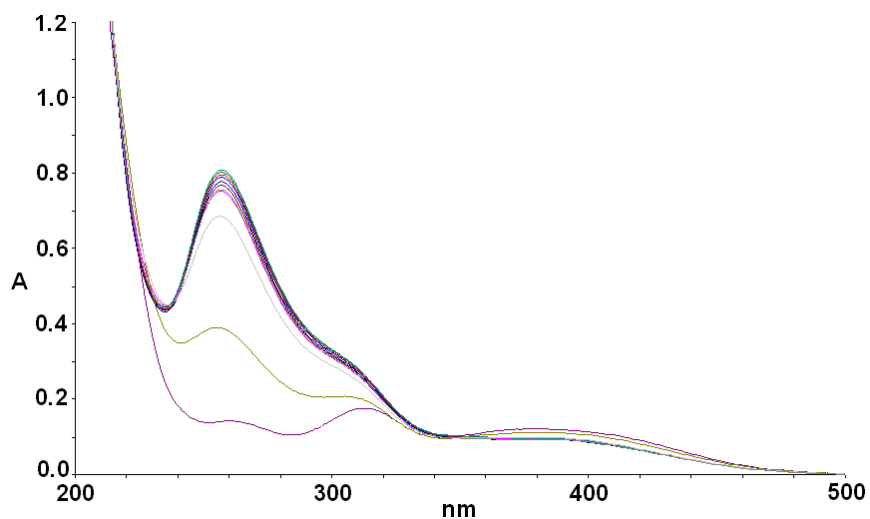
**Figure S9.** <sup>1</sup>H NMR spectra (CH(CH<sub>3</sub>)<sub>2</sub> region) of “[ $(\eta^6\text{-}p\text{-cymene})\text{Ru}(\text{NH}_3)_2(\text{H}_2\text{O})$ ]<sup>2+</sup>” species in D<sub>2</sub>O (the three upper spectra) and **1** after 5 days in D<sub>2</sub>O



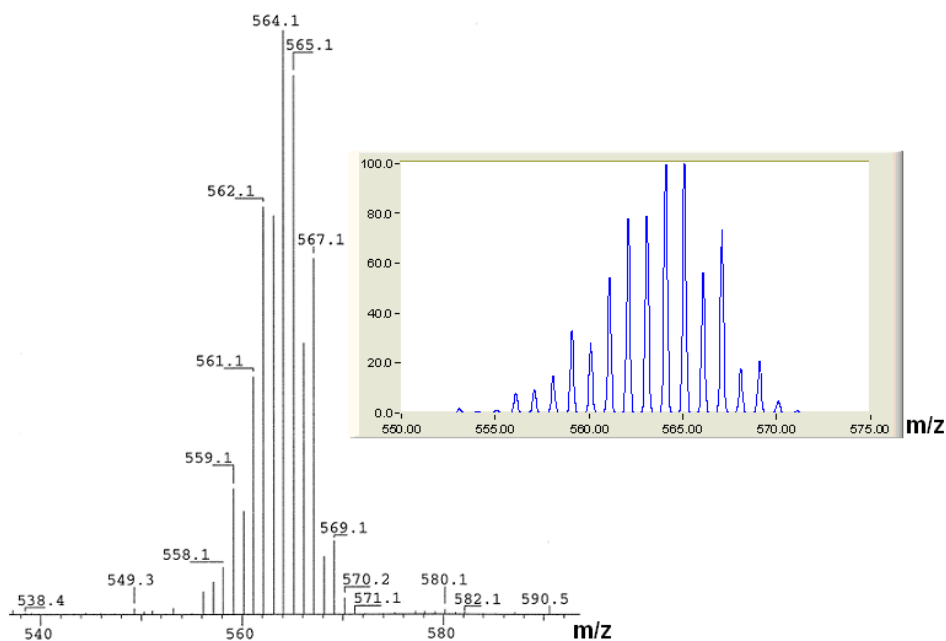
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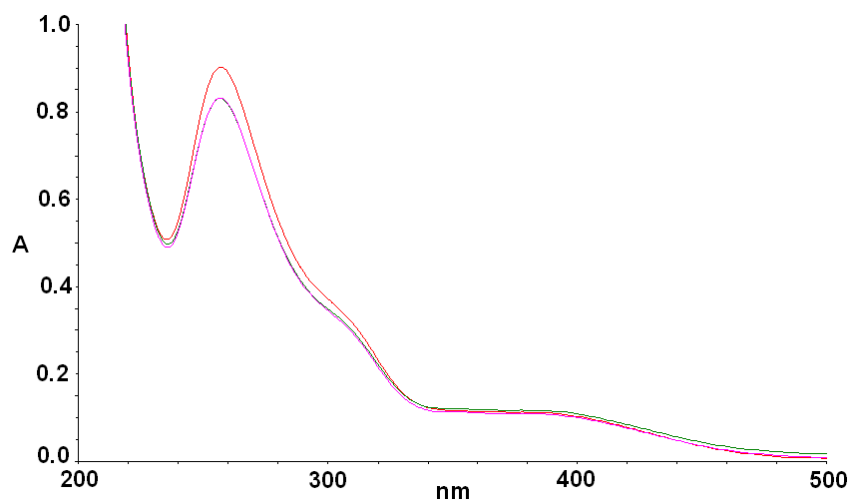
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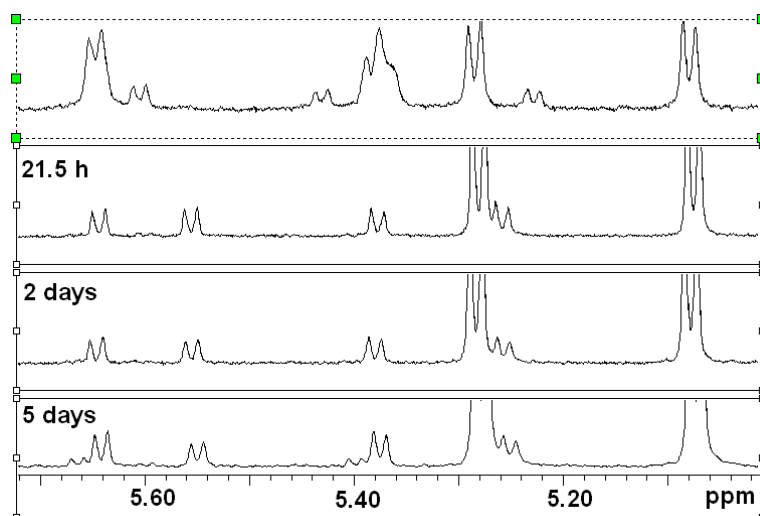
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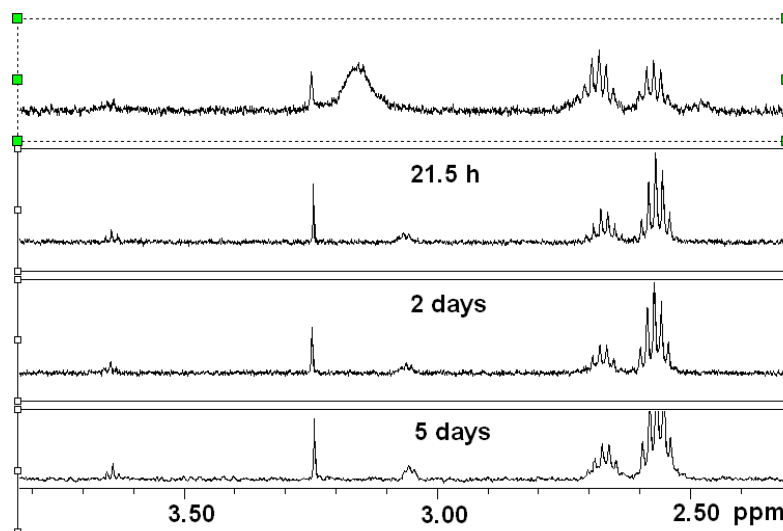
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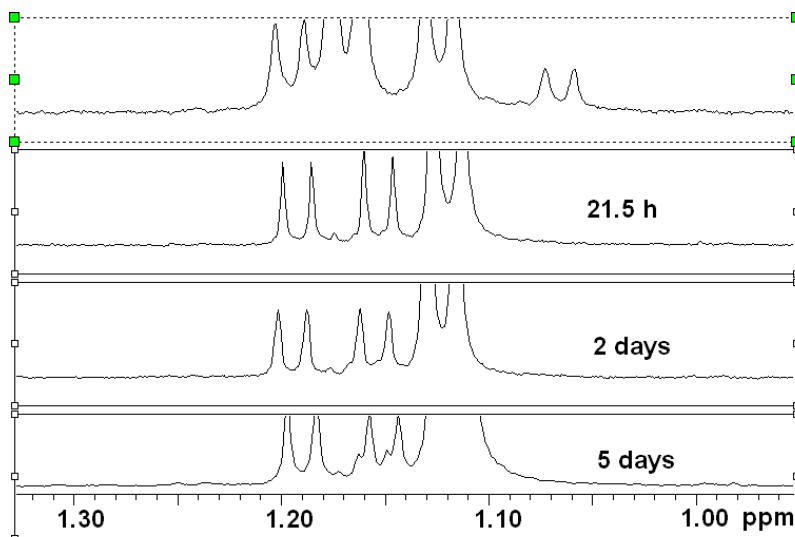
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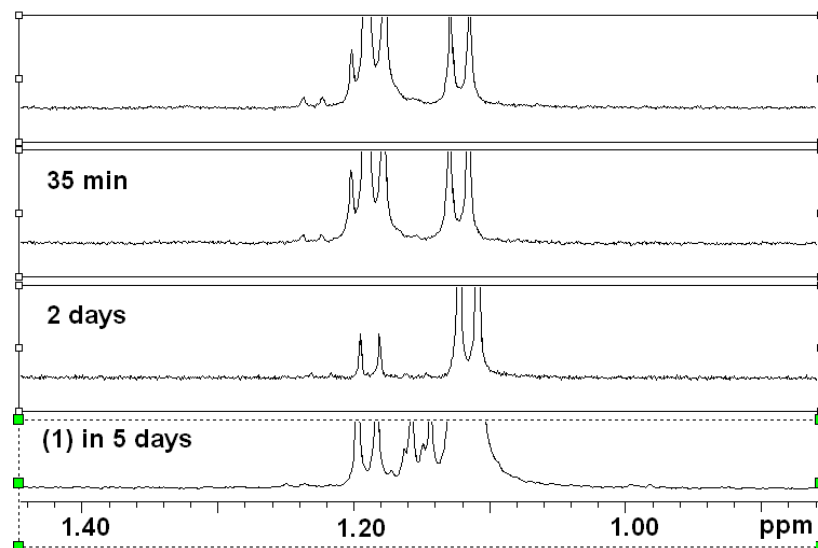
**Figure S6.** <sup>1</sup>H NMR spectra of **1** in D<sub>2</sub>O (C<sub>6</sub>H<sub>4</sub> region).



**Figure S7.**  $^1\text{H}$  NMR spectra of **1** in  $\text{D}_2\text{O}$  (CH region).



**Figure S8.**  $^1\text{H}$  NMR spectra of **1** in  $\text{D}_2\text{O}$  ( $\text{CH}(\text{CH}_3)_2$  region).



**Figure S9.** <sup>1</sup>H NMR spectra (CH(CH<sub>3</sub>)<sub>2</sub> region) of “[ $\eta^6$ -*p*-cymene)Ru(NH<sub>3</sub>)<sub>2</sub>(H<sub>2</sub>O)]<sup>2+</sup>” species in D<sub>2</sub>O (the three upper spectra) and **1** after 5 days in D<sub>2</sub>O.