

Metal-arene complexes with indolo[3,2-*c*]-  
quinolines: effects of Ru vs Os and modifications of  
the lactam unit on intermolecular interactions,  
anticancer activity, cell cycle and cellular  
accumulation

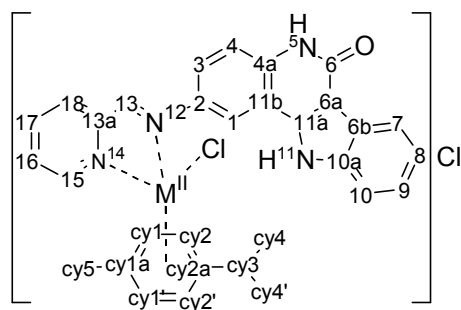
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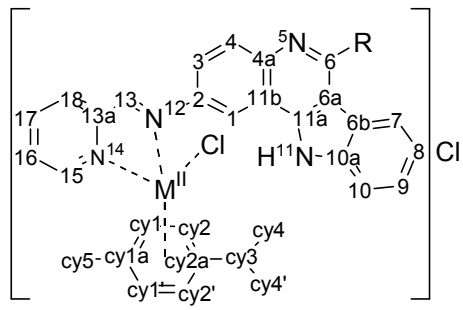
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**1a:** M = Ru  
**1b:** M = Os



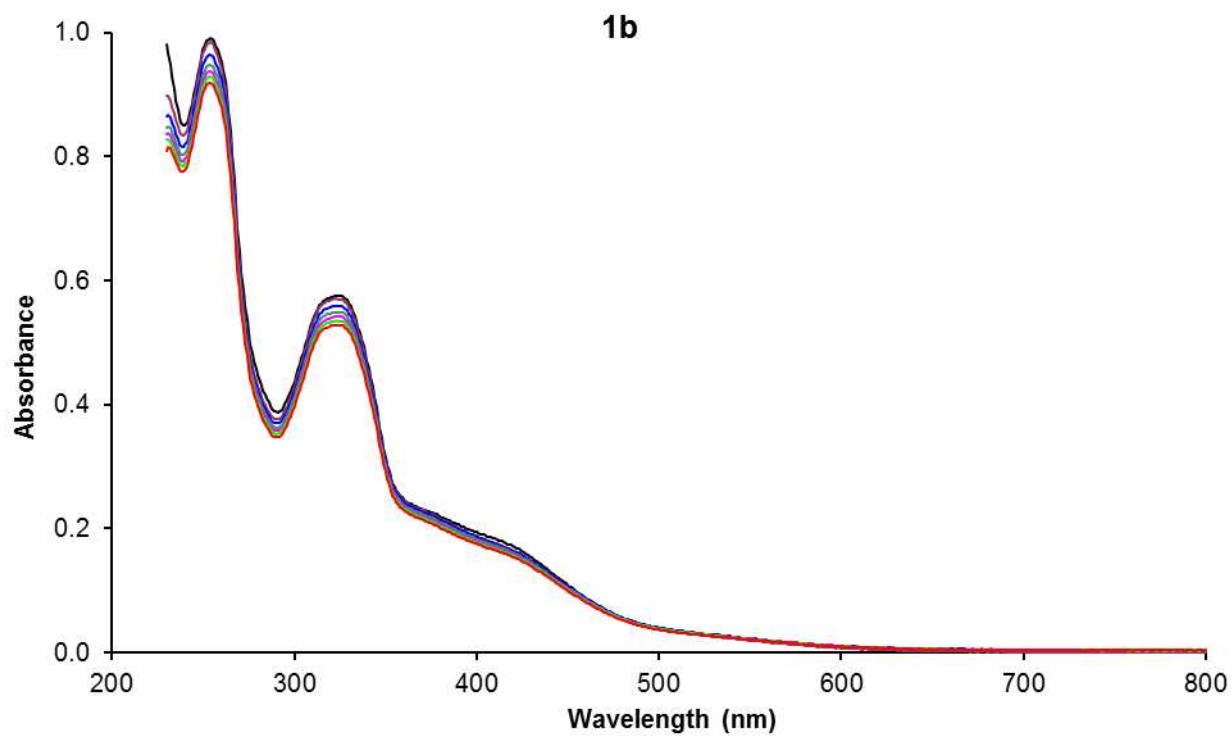
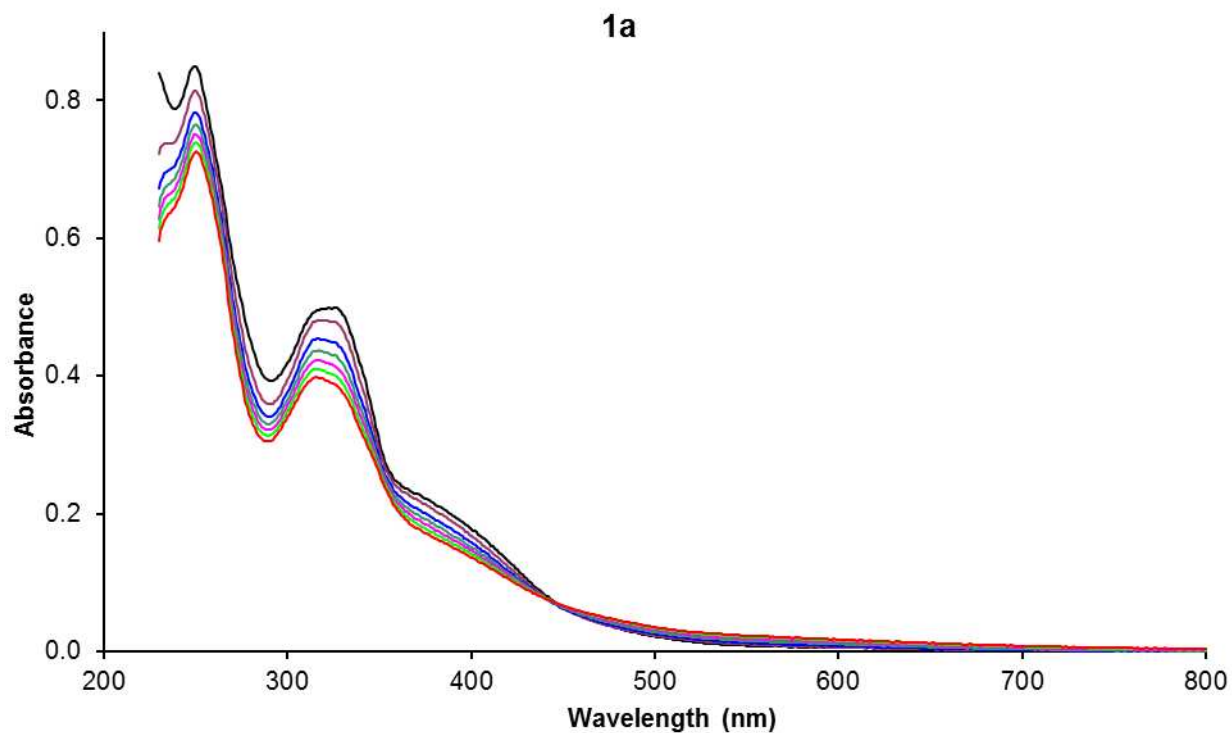
**2a:** M = Ru, R = H  
**2b:** M = Os, R = H  
**3a:** M = Ru, R = Cl  
**3b:** M = Os, R = Cl

Chart S1. Atom numbering scheme used for NMR assignment for the complexes **1a,b**, **2a,b**, and **3a,b**.

**Table S1.** Crystal data and details of data collection for **1a**·C<sub>2</sub>H<sub>5</sub>OH·H<sub>2</sub>O, **1b**·C<sub>2</sub>H<sub>5</sub>OH·H<sub>2</sub>O, **2a**·CH<sub>3</sub>OH·H<sub>2</sub>O and **3a**·4H<sub>2</sub>O.

	<b>1a</b> ·C <sub>2</sub> H <sub>5</sub> OH·H <sub>2</sub> O	<b>1b</b> ·C <sub>2</sub> H <sub>5</sub> OH·H <sub>2</sub> O	<b>2a</b> ·CH <sub>3</sub> OH·H <sub>2</sub> O	<b>3a</b> ·4H <sub>2</sub> O
empirical formula	C <sub>33</sub> H <sub>36</sub> Cl <sub>2</sub> N <sub>4</sub> O <sub>3</sub> Ru	C <sub>33</sub> H <sub>36</sub> Cl <sub>2</sub> N <sub>4</sub> O <sub>3</sub> Os	C <sub>32</sub> H <sub>36</sub> Cl <sub>2</sub> N <sub>4</sub> O <sub>3</sub> Ru	C <sub>31</sub> H <sub>35</sub> Cl <sub>3</sub> N <sub>4</sub> O <sub>4</sub> Ru
Fw	708.63	797.76	696.62	735.05
space group	<i>P</i> 2 <sub>1</sub> / <i>n</i>	<i>P</i> 2 <sub>1</sub> / <i>n</i>	<i>P</i> 2 <sub>1</sub> / <i>c</i>	<i>P</i> -1
<i>a</i> [Å]	17.7577(11)	17.7341(18)	11.998(3)	9.8541(7)
<i>b</i> [Å]	9.4186(5)	9.5157(9)	21.243(4)	12.9200(10)
<i>c</i> [Å]	18.9531(12)	19.070(2)	12.307(2)	13.3236(10)
$\alpha$ [°]				107.902(5)
$\beta$ [°]	90.097(2)	90.096(2)	90.084(7)	104.282(5)
$\gamma$ [°]				94.798(5)
<i>V</i> [Å <sup>3</sup> ]	3170.0(3)	3218.2(6)	3136.9(11)	1540.7(2)
<i>Z</i>	4	4	4	2
$\lambda$ [Å]	0.71073	0.71073	0.71073	0.71073
$\rho_{\text{calcd}}$ [g cm <sup>-3</sup> ]	1.485	1.647	1.475	1.584
crystal size [mm <sup>3</sup> ]	0.18 × 0.06 × 0.02	0.22 × 0.20 × 0.03	0.20 × 0.15 × 0.03	0.25 × 0.18 × 0.10
<i>T</i> [K]	100(2)	100(2)	150(2)	100(2)
$\mu$ [mm <sup>-1</sup> ]	0.703	4.168	0.709	0.813
<i>R</i> <sub>1</sub> <sup>[a]</sup>	0.0449	0.0395	0.0756	0.0566
<i>wR</i> <sub>2</sub> <sup>[b]</sup>	0.1148	0.0950	0.2118	0.1283
GOF <sup>[c]</sup>	1.028	1.027	1.053	0.988

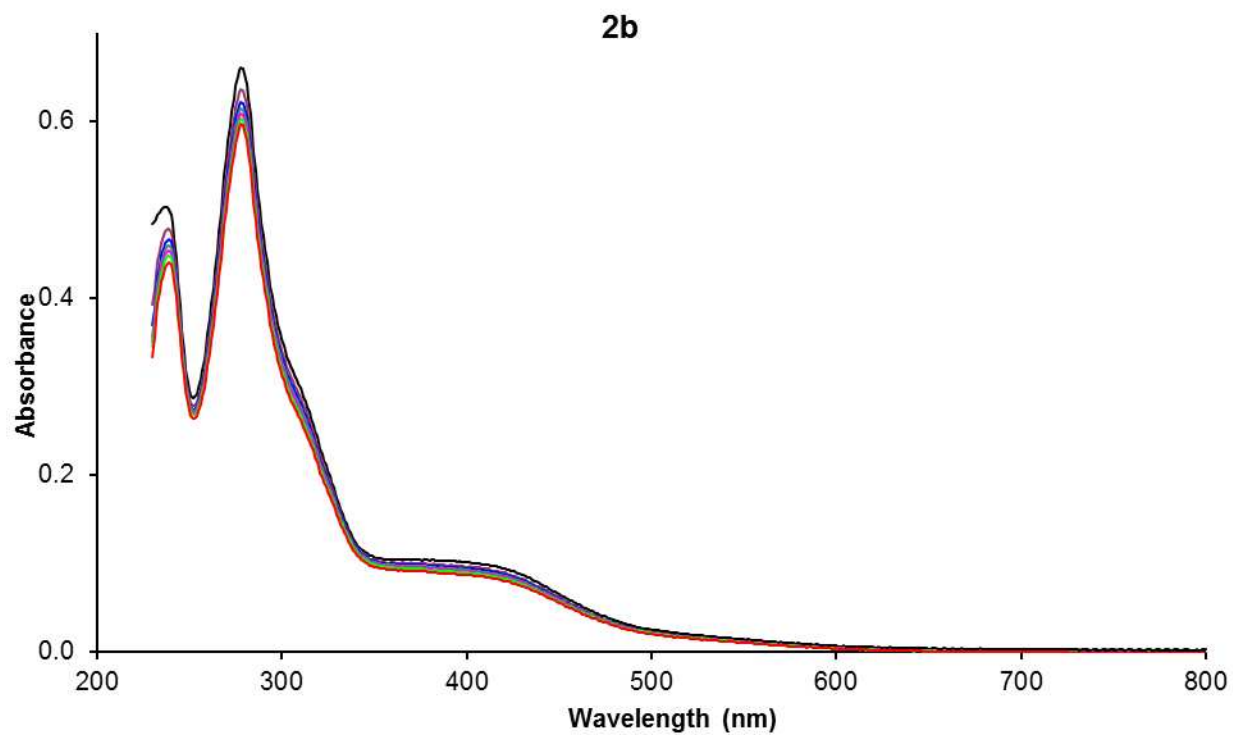
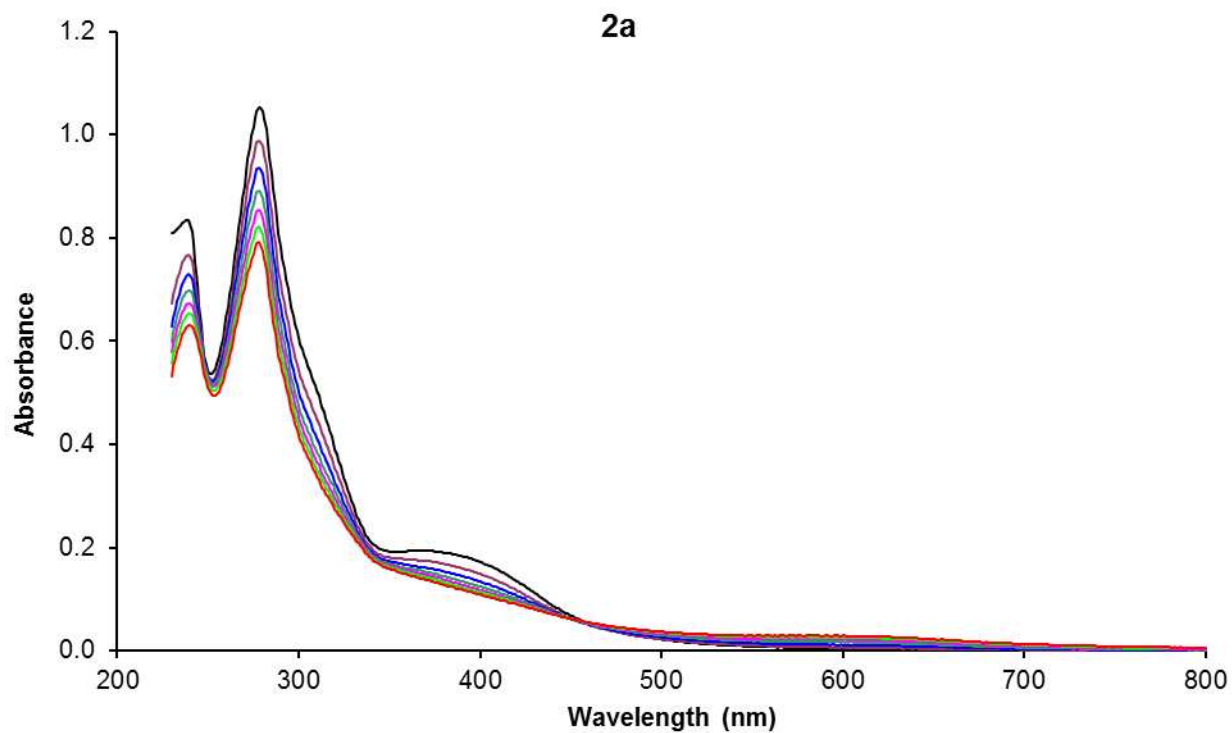
<sup>a</sup> $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$ . <sup>b</sup> $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$ . <sup>c</sup> GOF =  $\{\Sigma[w(F_o^2 - F_c^2)^2]/(n-p)\}^{1/2}$ , where *n* is the number of reflections and *p* is the total number of parameters refined.



**Figure S1.** UV-vis spectra of complexes **1a** and **1b** in 1% DMSO/water. Spectra were recorded after 0 h, black; 4 h, violet; 8 h, blue; 12 h, dark green; 16 h, pink; 20 h, light green; 24

h,

red.



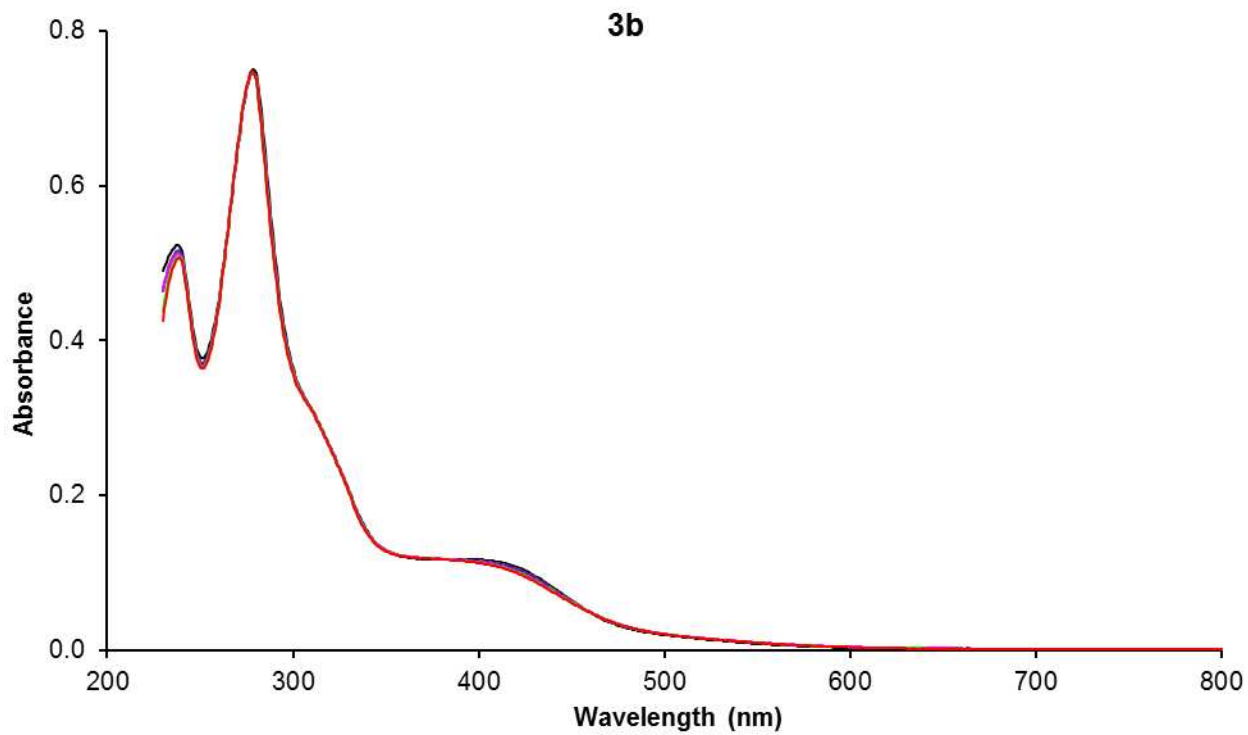
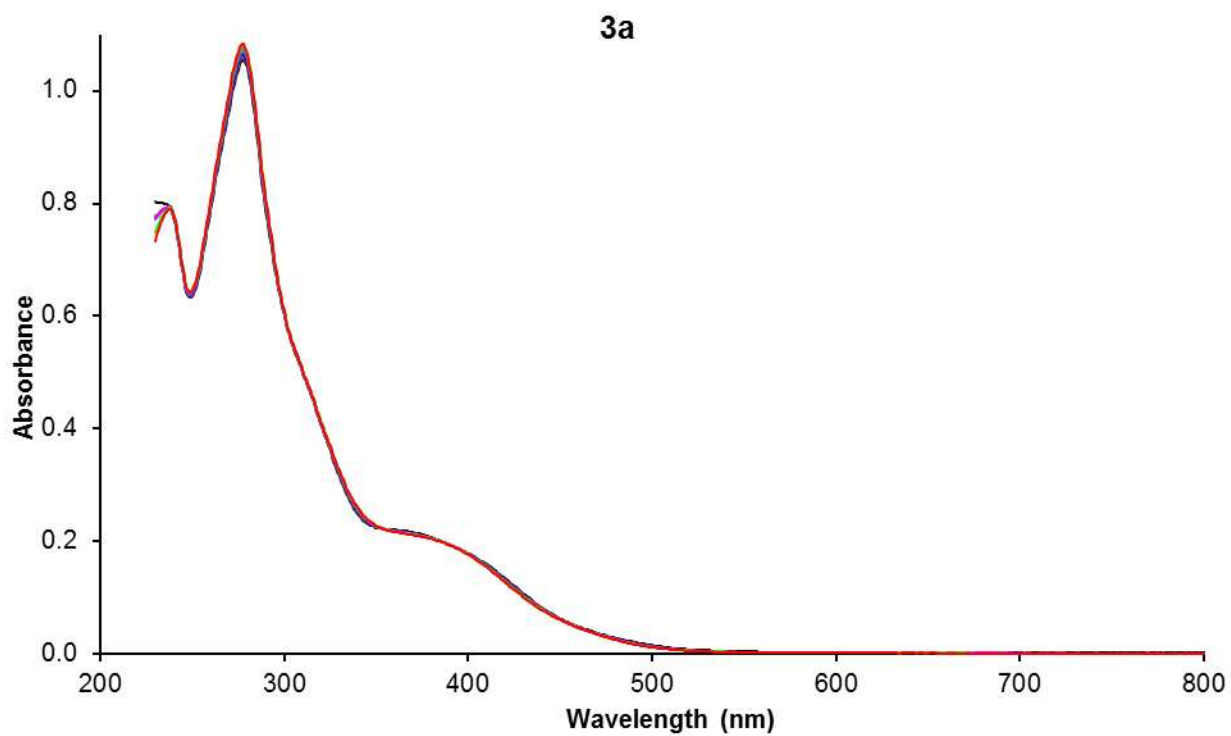
**Figure S1 (continued).** UV-vis spectra of complexes **2a** and **2b** in 1% DMSO/water. Spectra were recorded after 0 h, black; 4 h, violet; 8 h, blue; 12 h, dark green; 16 h, pink; 20 h, light

green;

24

h,

red.



**Figure S1 (continued).** UV-vis spectra of complexes **3a** and **3b** in 1% DMSO/water. Spectra were recorded after 0 h, black; 4 h, violet; 8 h, blue; 12 h, dark green; 16 h, pink; 20 h, light

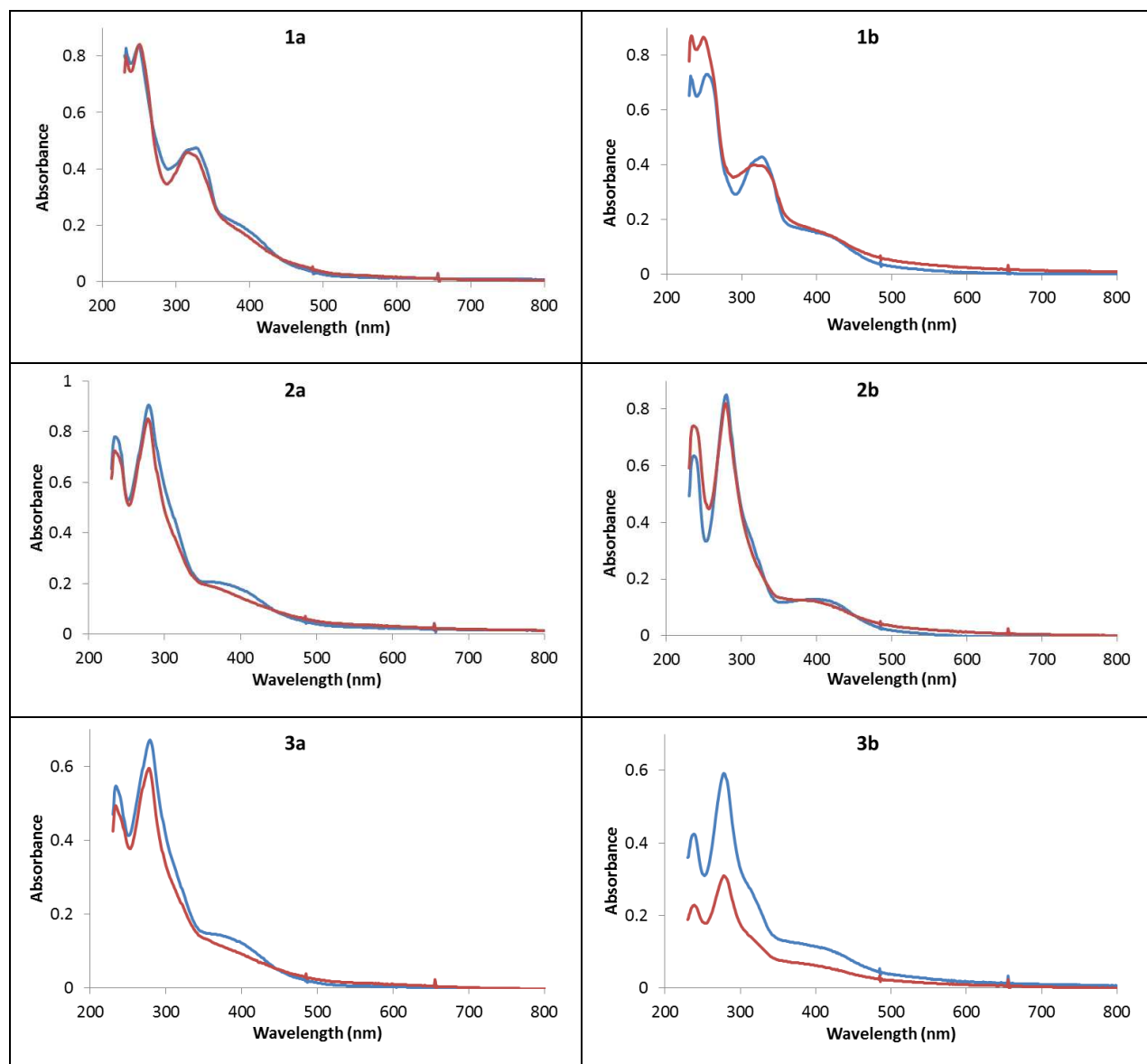


green;

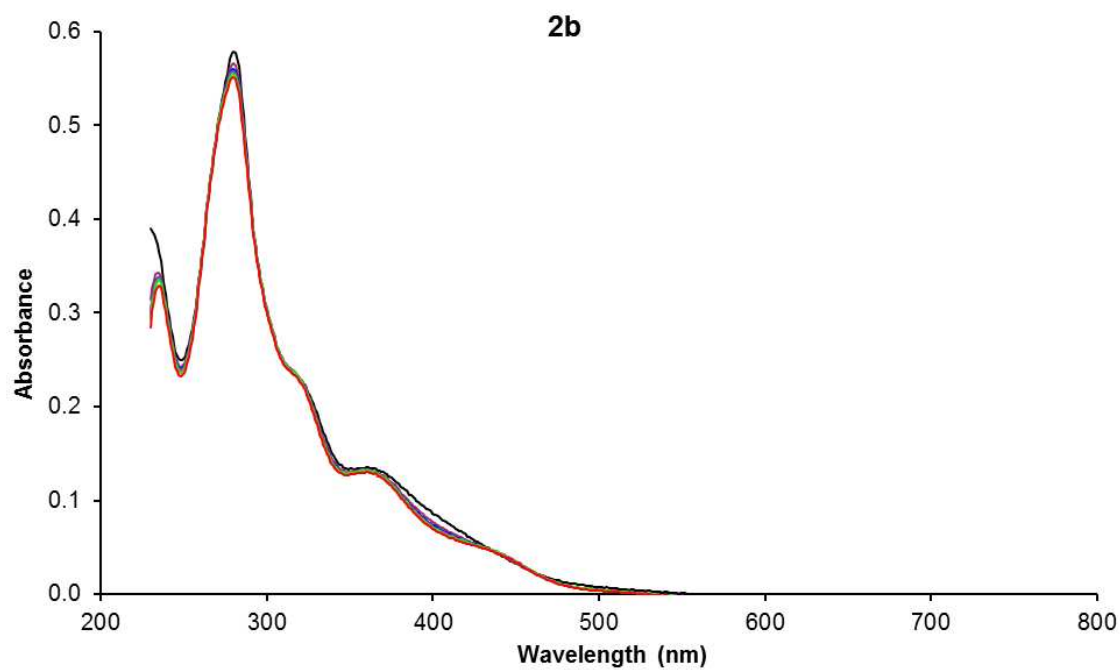
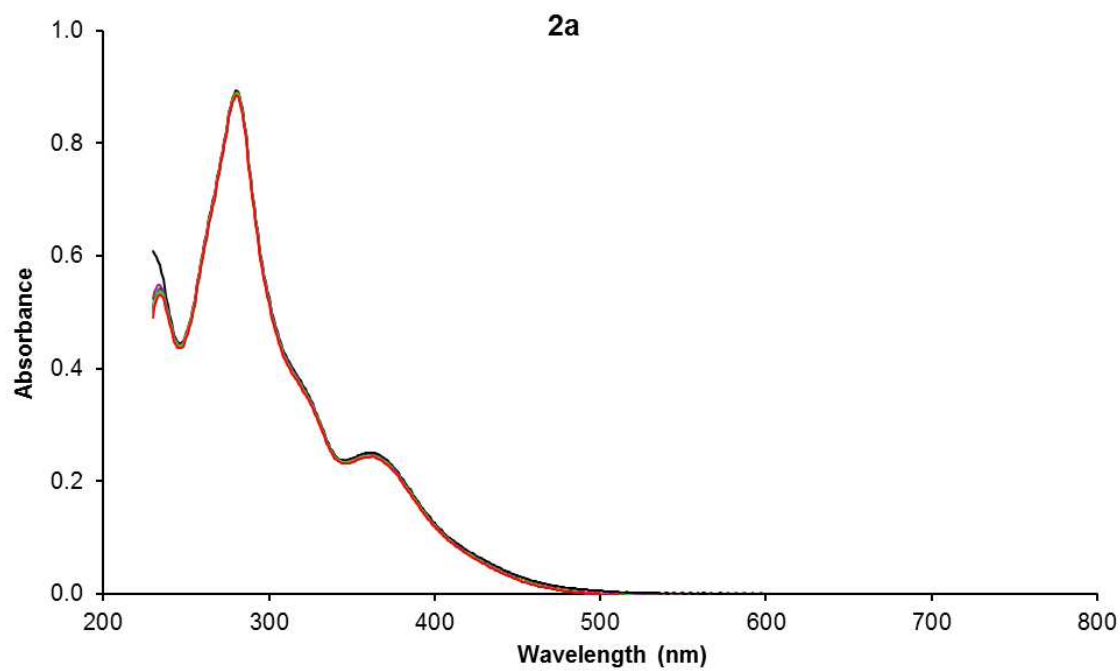
24

h,

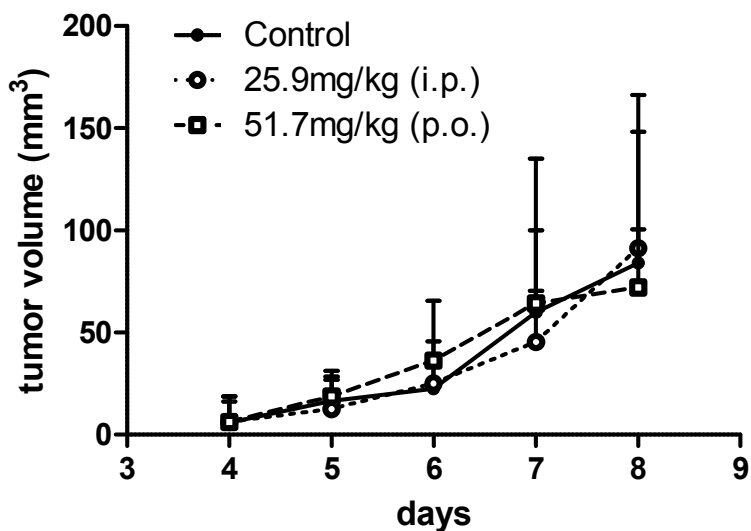
red.



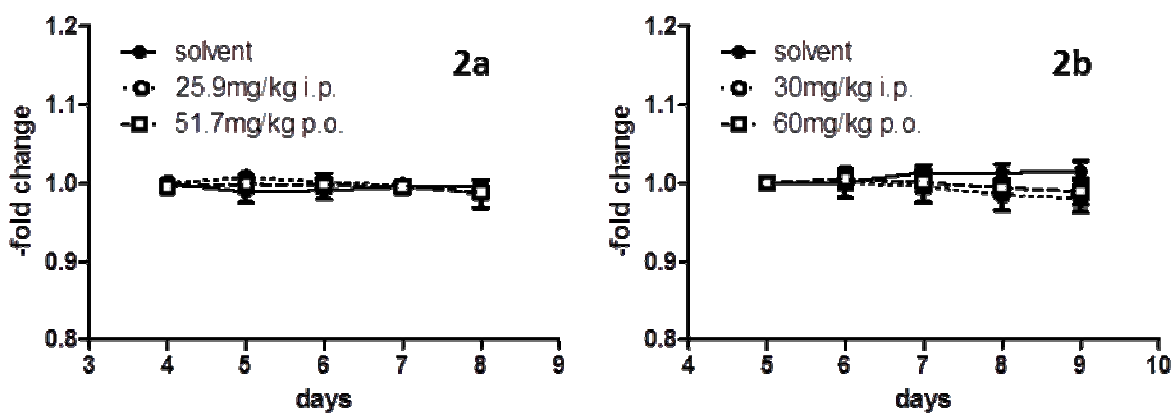
**Figure S2.** UV-vis spectra of complexes **1a,b**, **2a,b** and **3a,b** in 1%DMSO in modified MEM (without phenyl red and *L*-glutamine). Spectra were recorded at 0 h (blue line) and 24 h (red line).



**Figure S3.** UV-vis spectra of complexes **2a** and **2b** in 1% DMSO/water at pH 3.4. The pH was set by addition of conc. HCl to the dissolved complex. The pH was chosen in order to resemble that of the pH of mouse stomach. Spectra were recorded after 0 h, black; 4 h, violet; 8 h, blue; 12 h, dark green; 16 h, pink; 20 h, light green; 24 h, red.



**Figure S4.** Anticancer activity of **2a** in vivo. CT-26 cells were injected subcutaneously in the right flank of BALB/c mice. After the tumor was palpable, mice were treated for 5 days (day 4-8) with 25.9 mg/kg (i.p.) and 51.7 mg/kg (p.o.) of **2a**, respectively. Tumor volumes were calculated as described in *Materials and Methods*. Each experimental group contained four animals. Data are means  $\pm$  S.D.



**Figure S5.** Change of body weight during treatment. Data are means  $\pm$  S.D.