Synthesis, characterization and antitumor properties of two highly cytotoxic ruthenium(III) complexes with bulky triazolopyrimidine ligands

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† Electronic supplementary information (ESI) available: CIF files and crystals packing of both ruthenium(III) compounds 1,2; CV and EPR spectra; comparison of X–X distances and X–M–X angles in the studied octahedral ruthenium complexes. CCDC 787821 1 and 901853 2. For ESI and crystallographic data in CIF or other electronic format see DOI: 10.1039/c2dt32216a.

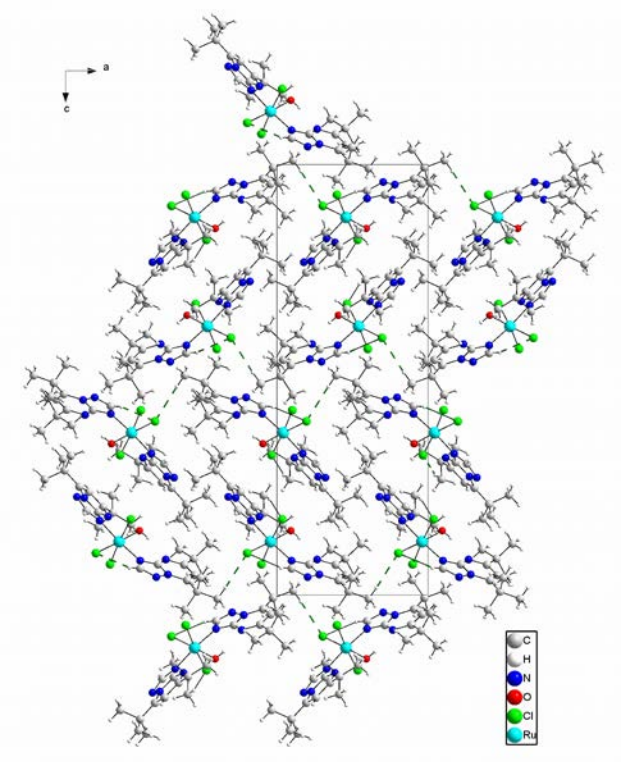

Figure S1. Packing of **1**.

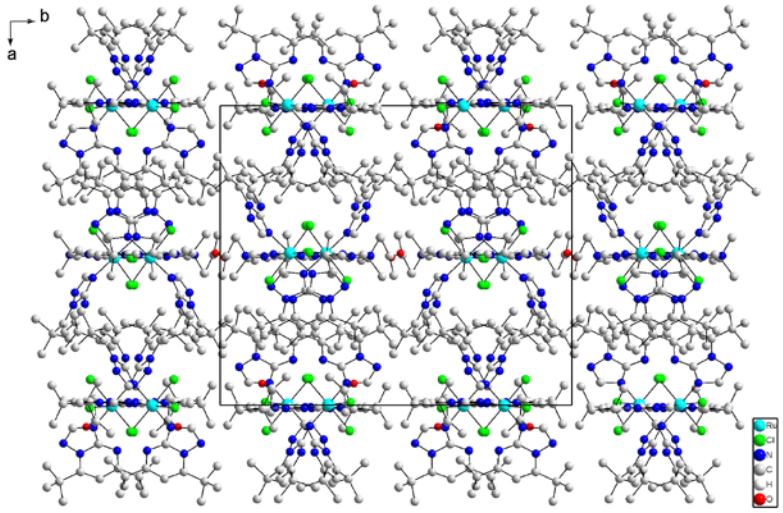

Figure S2. Packing of **2** with omitted hydrogen atoms and acetone molecule occurring only in one orientation (alternate structure was omitted for the clarity of the picture) along *c* axis reveals *bc* layers.

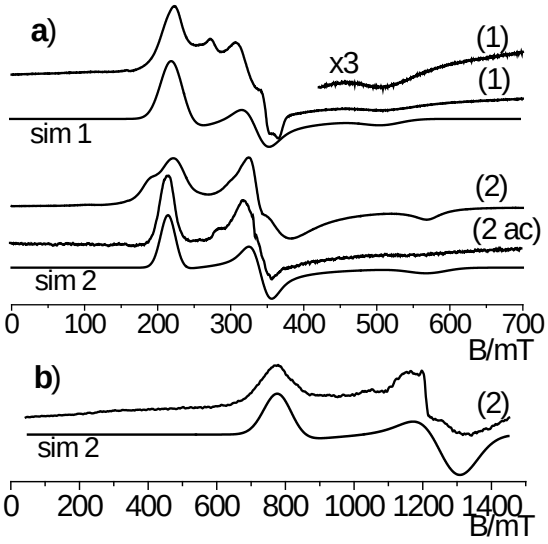

Figure 3S. The EPR spectra, (1) and (2), of powdered **1** and **2** complexes, respectively, and (2 ac) of the acetone solution of 2, measured a) at X-band (9.581GHz) and b) at Q-band (33.98 GHz) and at 77 K, together with computer simulated spectra (sim **1** and sim **2**, respectively) using the spin Hamiltonian parameters given in the text.

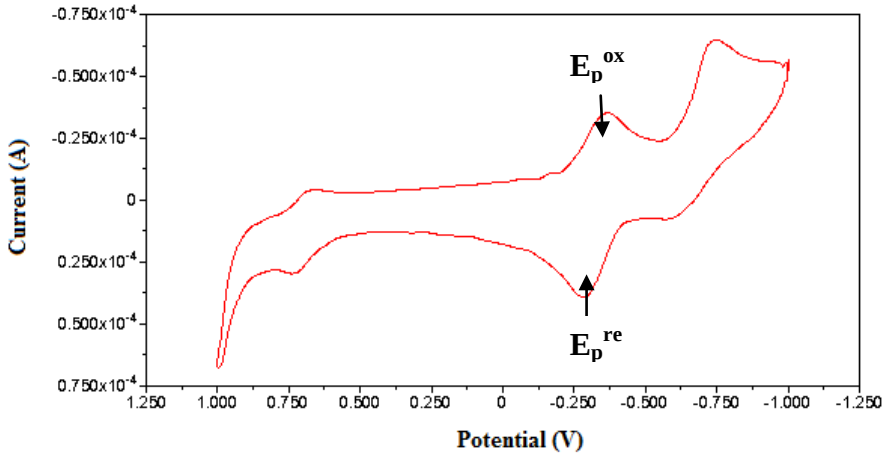

Fig. 4a

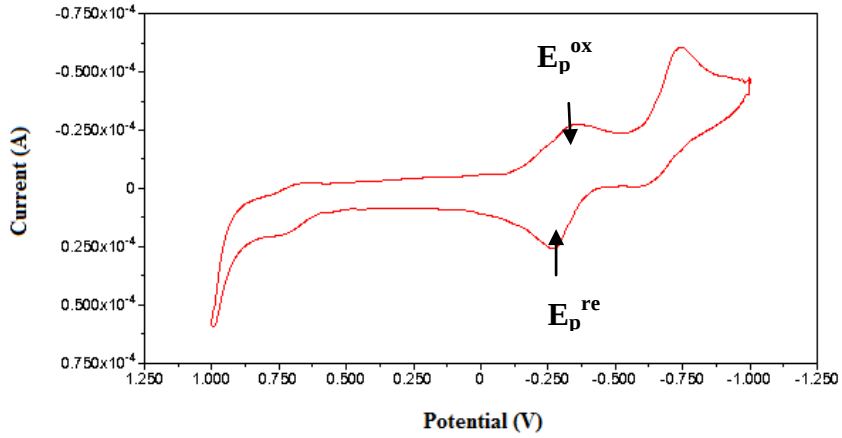

Fig. 4b

Figure 4S. Cyclic voltammograms of 10^3 M DMF solutions of complex **1** (**Fig. 3a**) (E_p^{ox} = -0.36 V and E_p^{red} = -0.29 V), and complex **2** (**Fig. 3b**) (E_p^{ox} = -0.36 V and E_p^{red} = -0.27 V) in 0.1 M $[nBu_4N](PF_6)$ at a scan rate of 0.1 Vs^{-1}.

Table 1S. Comparison of X-X distance and X-M-X angle in selected octahedral ruthenium complexes with halogen atoms and triazolopyrimidine as ligands.

Compound	M-N [Å]	M-X [Å]	X-X [Å]	X-M-X [º]	REF.
trans-[$RuCl_3(H_2O)(dbtp)_2$]	2.074 and 2.075	2.3118, 2.3182, 2.3291	3.323, 3.348, 4.644	91.74, 92.33 175.36	This paper
mer-[$RuCl_3(dbtp)_3$]·0.829$OCMe_2$	2.050, 2.067, 2.076, 2.085, 2.093, 2.094	2.350, 2.3520, 2.3551, 2.363, 2.364, 2.3723	3.340, 3.342, 3.375, 3.390, 4.707, 4.713	89.97, 90.00, 91.10, 91.98, 177.99, 178.52,	This paper
trans-[$RuCl_3(dmtp)_2$(9-methyladenine)]·½CH_2Cl_2	2.035 (adn) 2.090 and 2.083	2.333, 2.377, 2.385	3.364, 3.366, 4.710,	89.89, 91.03, 178.64	9
trans-[$RuCl_3(H_2O)(dmtp)_2$]	2.092(4) 2.092(4) 2.101(4) (Ru1-O1)*	2.306(2) 2.331(2) 2.388(2)	3.331 3.342 4.693	91.8(1) 90.1(1) 178.0(2)	5a
mer-[$RuCl_3(H_2O)$(dmso)(dmtp)]·H_2O	2.137(2) 2.267(1) (Ru1-S1) 2.094(2) (Ru1-O2)	2.313(1) 2.332(1) 2.337(1)	3.360 3.407 4.659	94.22 92.66 172.77	4
(Hdmtp)*trans*-[$RuCl_4$(dmso)(dmtp)]·¼Et_2O	2.121(8) 2.255(2) (Ru1-S1)	2.329(2) 2.346(3) 2.349(2) 2.364(3)	3.442 3.262 3.295 3.273 4.691 4.692	94.73 87.62 89.62 88.04 175.22 177.63	4