Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Information

Cytotoxic *cis*-ruthenium(III) bis(amidine) complexes

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Table S1 Crystallographic data of **[6](CF$_3$SO$_3$)**.

Empirical formula	C_{27} $H_{50.23}$ F_3 N_4 $O_{7.11}$ Ru S
Formula weight	734.91
Temperature	100.00 K
Wavelength	1.54184 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 11.1355(2) A alpha = 105.416(2) deg. b = 17.8642(3) A beta = 99.450(2) deg. c = 19.5372(4) A gamma = 106.518(2) deg.
Volume	3469.04(12) A^3
Z, Calculated density	4, 1.407 Mg/m^3
Absorption coefficient	4.760 mm^-1
F (000)	1537
Crystal size	0.15 x 0.12 x 0.1 mm
Theta range for data collection	2.429 to 77.205 deg.
Limiting indices	-14<=h<=11, -21<=k<=22, -23<=l<=24
Reflections collected / unique	48026 / 13744 [R(int) = 0.0670]
Completeness to theta = 67.684	99.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.75222
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	13744 / 0 / 804
Goodness-of-fit on F^2	1.049
Final R indices [I>2sigma(I)]	R1 = 0.0591, wR2 = 0.16
R indices (all data)	R1 = 0.0710, wR2 = 0.1744
Extinction coefficient	n/a
Largest diff. peak and hole	2.115 and -1.987 e.A^-3

Table S2. Selected bond distances (Å) and angles (deg) for **6**.

Bond distances			
Ru(1)-O(3)	2.007(3)	Ru(2)-O(6)	2.007(3)
Ru(1)-O(4)	2.030(3)	Ru(2)-O(8)	2.015(3)
Ru(1)-O(1)	2.019(3)	Ru(2)-O(5)	2.029(3)
Ru(1)-O(2)	2.040(3)	Ru(2)-O(7)	2.042(3)
Ru(1)-N(1)	2.034(3)	Ru(2)-N(7)	2.025(3)
Ru(1)-N(3)	2.038(4)	Ru(2)-N(5)	2.045(4)
Bond angles			
O(3)-Ru(1)-O(4)	93.15(11)	O(6)-Ru(2)-O(8)	178.76(11)
O(3)-Ru(1)-O(1)	179.49(11)	O(6)-Ru(2)-O(5)	93.30(11)
O(3)-Ru(1)-O(2)	87.86(12)	O(6)-Ru(2)-O(7)	87.44(11)
O(3)-Ru(1)-N(1)	84.82(13)	O(6)-Ru(2)-N(7)	85.12(13)
O(3)-Ru(1)-N(3)	91.49(13)	O(6)-Ru(2)-N(5)	91.02(13)
O(4)-Ru(1)-O(2)	87.93(12)	O(8)-Ru(2)-O(5)	87.86(11)
O(4)-Ru(1)-N(1)	177.58(12)	O(8)-Ru(2)-O(7)	93.03(12)
O(4)-Ru(1)-N(3)	92.72(13)	O(8)-Ru(2)-N(7)	93.73(12)
O(1)-Ru(1)-O(4)	87.22(12)	O(8)-Ru(2)-N(5)	88.51(13)
O(1)-Ru(1)-O(2)	92.51(12)	O(5)-Ru(2)-O(7)	88.11(11)
O(1)-Ru(1)-N(1)	94.83(12)	O(5)-Ru(2)-N(5)	92.09(12)
O(1)-Ru(1)-N(3)	88.13(13)	O(7)-Ru(2)-N(5)	178.45(12)
N(1)-Ru(1)-O(2)	90.69(12)	N(7)-Ru(2)-O(5)	178.07(12)
N(1)-Ru(1)-N(3)	88.64(14)	N(7)-Ru(2)-O(7)	90.72(13)
N(3)-Ru(1)-O(2)	179.11(12)	N(7)-Ru(2)-N(5)	89.04(14)

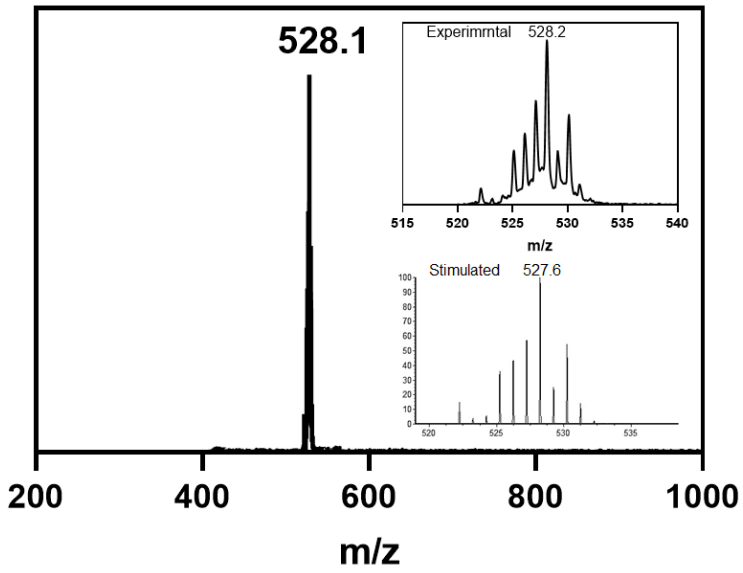

Figure S1. MALDI-TOF mass spectrum of complex **1**.

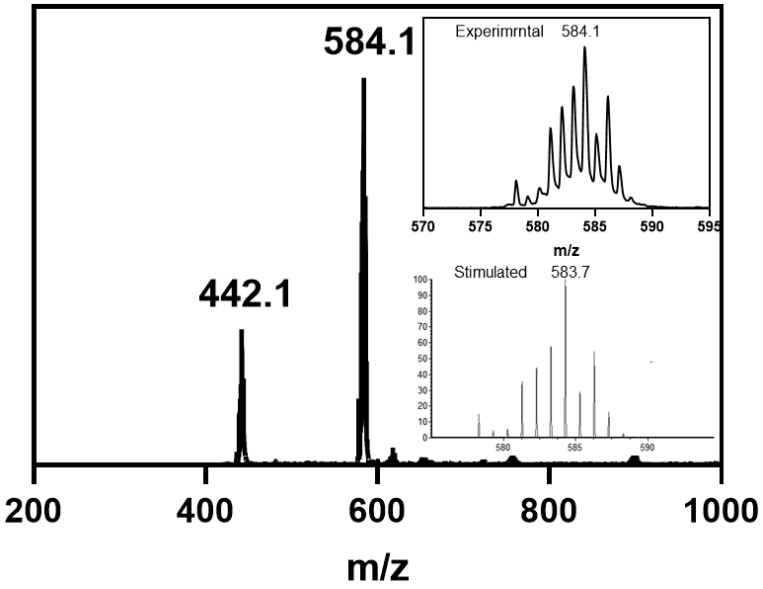

Figure S2. MALDI-TOF mass spectrum of complex **2**.

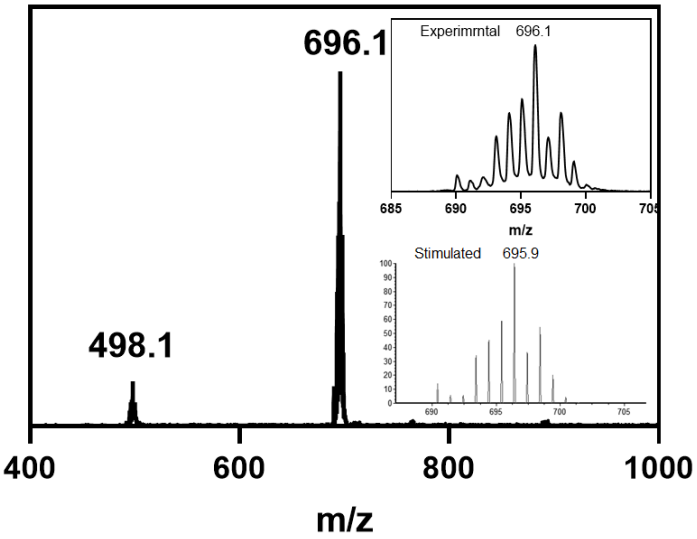

Figure S3. MALDI-TOF mass spectrum of complex **3**.

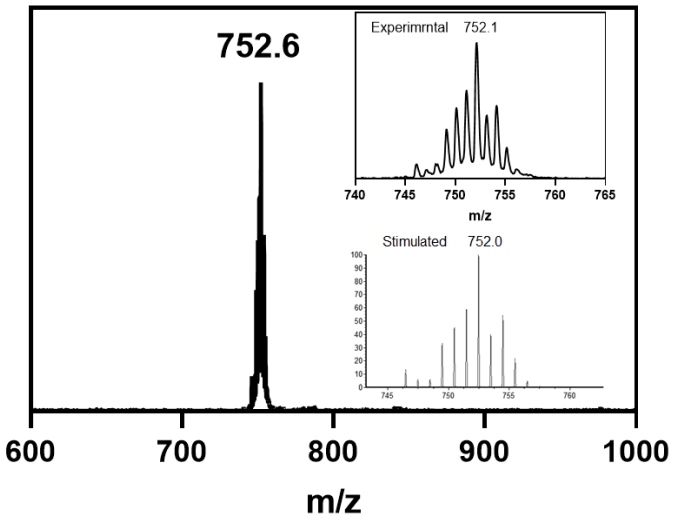

Figure S4. MALDI-TOF mass spectrum of complex **4**.

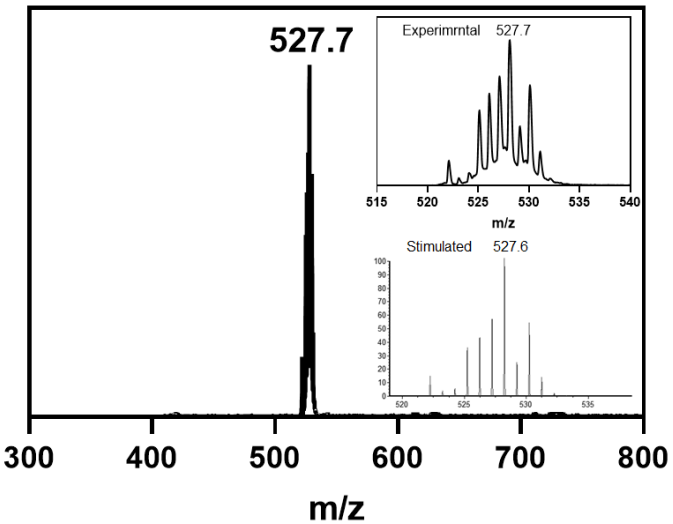

Figure S5. MALDI-TOF mass spectrum of complex **5**.

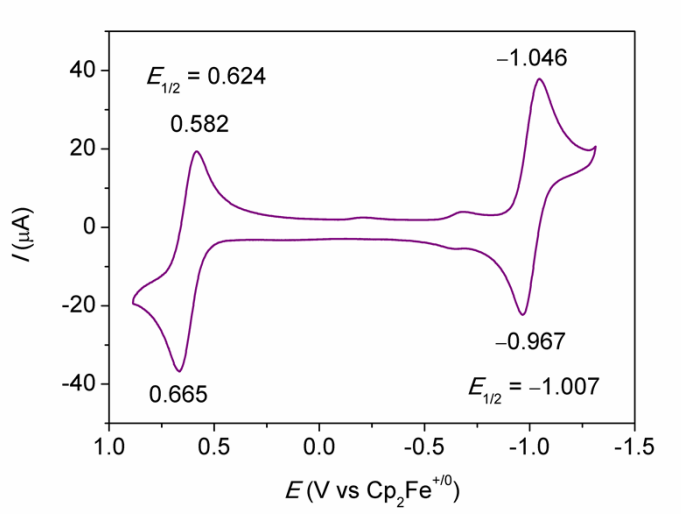

Figure S6. Cyclic voltammogram of **5** in CH_3CN.

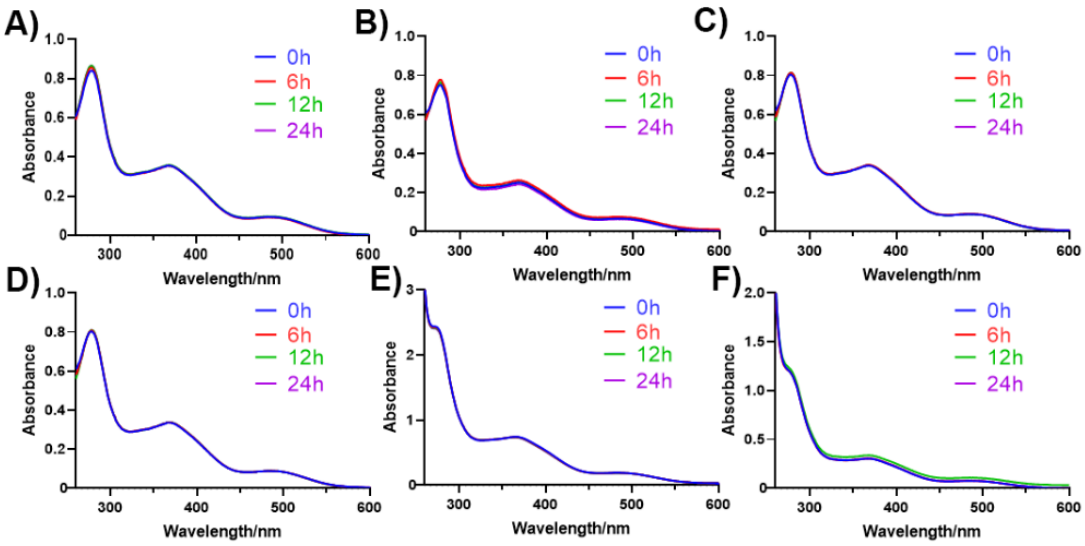

Figure S7. UV-vis spectra of complexes **1**–**6** in DMSO at different time intervals. (A) **1**, 50 µM (B) **2**, 50 µM (C) **3**, 50 µM (D) **4**, 50 µM (E) **5**, 100µM and (F) **6**, 40 µM.

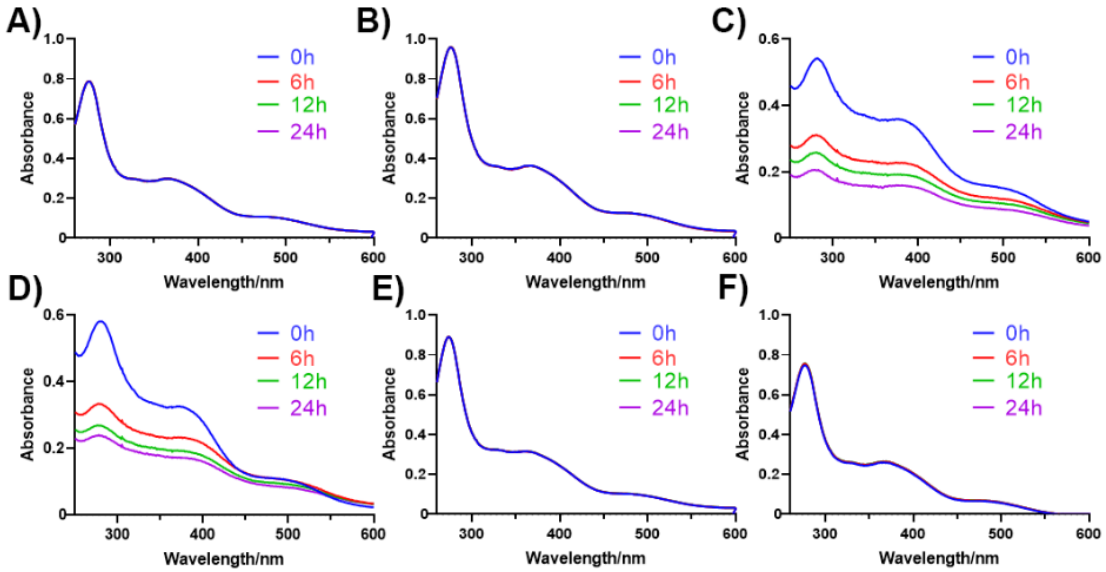

Figure S8. UV-vis spectra of 40 μM complexes **1**–**6** in PBS (1% DMSO) at different time intervals. A-F for **1**–**6**.

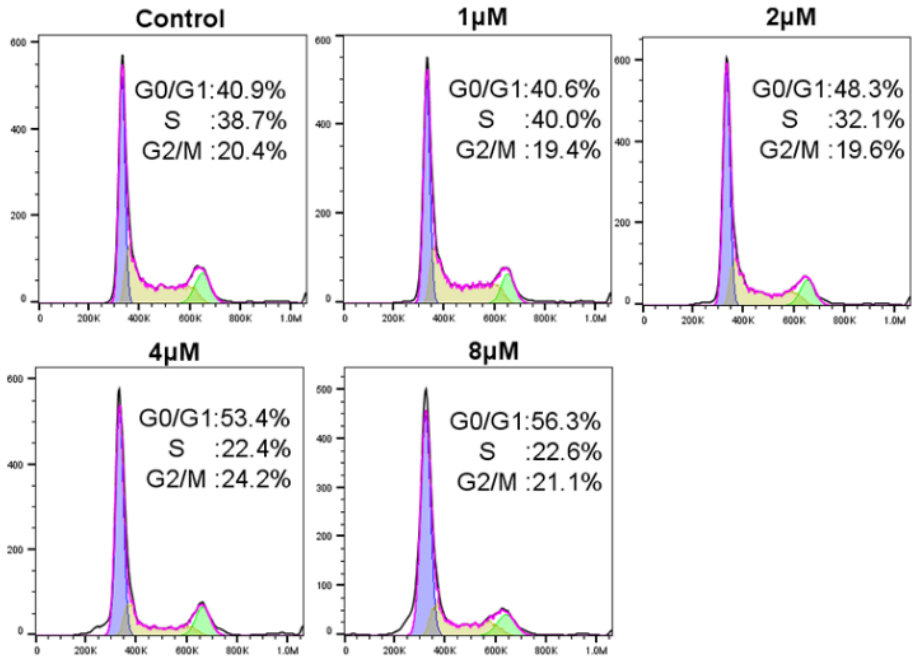

Figure S9. Effects of complex **6** treatment on cell-cycle phases in NCI-H460 cells as detected by propidium iodide (PI) staining with the flow cytometry. Cells were exposed to **6** for 24 h at indicated concentrations.

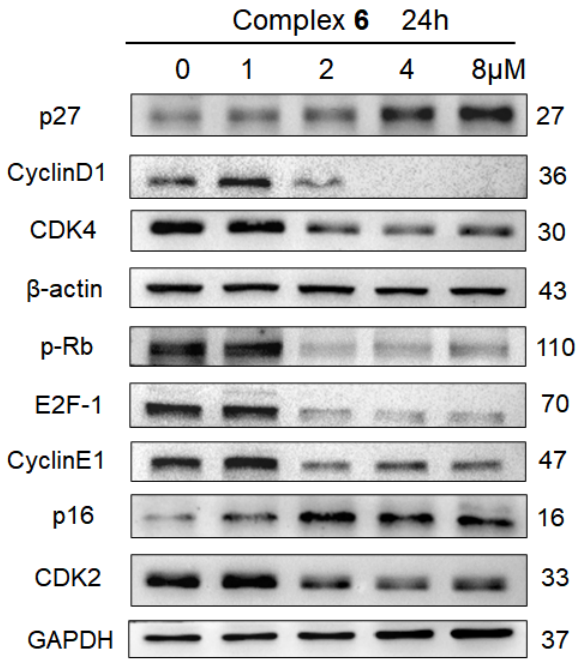

Figure S10. A western blot assay assessed the expression levels of G0/G1 cell phase arrest relevant protein in NCI-H460 cells after incubation with 6 at various concentrations for 24 h.

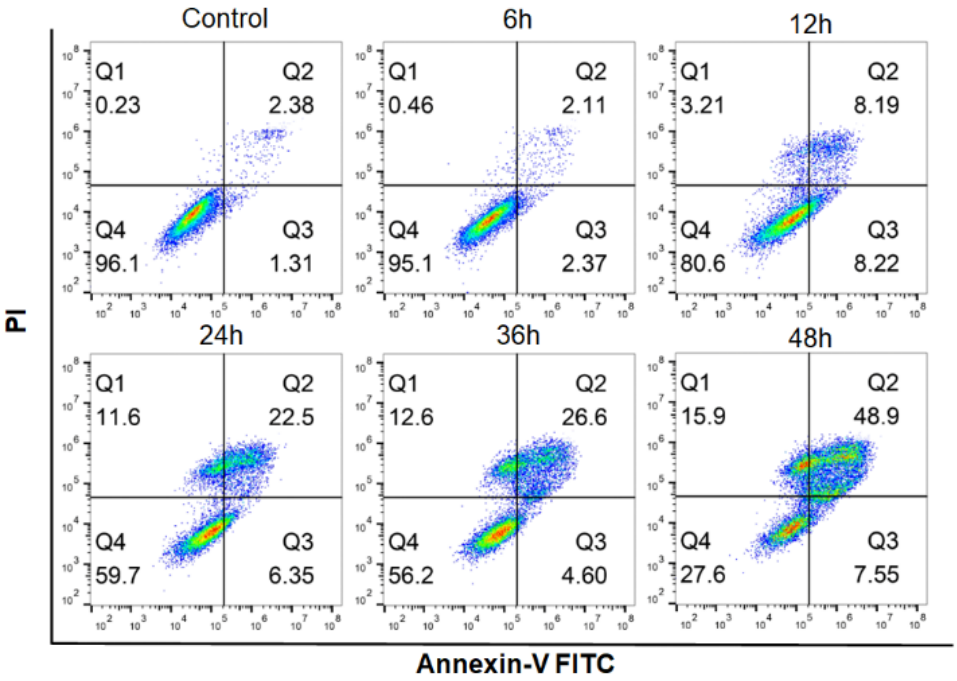

Figure S11. Time-dependent apoptosis detection in NCI-H460 cells with treatment of 8μM complex **6** using Annexin V-FITC and Propidium Iodide (PI) double staining.

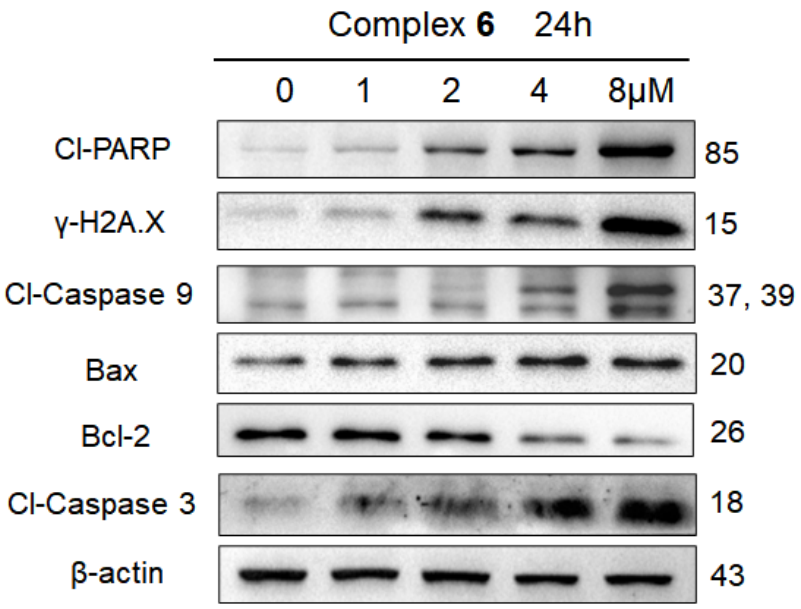

Figure S12. A western blot assay assessed the expression levels of apoptosis and DNA damage of the relevant proteins in NCI-H460 cells after incubation with various concentrations of **6** for 24 h.