

**Electronic Supporting Information (ESI)** 

Figure S1. <sup>1</sup>H NMR spectra of complex **1** CD<sub>3</sub>CN. The chemical shifts are expressed in ppm. The chemical structures represented belong to the coordinating ligands 2,2'-bipyridine (bipy) and bathocuproine (BC). The hydrogens are labeled by numbers and are assigned to the peaks on the spectra. \* represents the hydrogens on the phenyl groups which are detected as a multiplets on the spectrum and † represents the solvent residual peaks. The peak at 0 corresponds to TMS.



Figure S2. <sup>13</sup>C NMR spectra of complex **1** in CD<sub>3</sub>CN. The chemical shifts are expressed in ppm and the characteristic peaks for the complex are at  $\delta = 167.36$ , 158.62, 158.34, 153.86, 152.76, 150.40, 150.23, 138.77, 138.60, 136.73, 130.66, 130.55, 130.03, 128.78, 128.42, 128.32, 128.24, 125.78, 125.46, 125.37, 26.39.



Figure S3. HRMS of complex 1. The m/z value is assigned to the peaks and the y axis represents the percent abundance of the signals (%). The exact mass of the counter-ion free complex  $[M-2(PF_6)]^{2+}$  was found to 387.1034 as compared to 387.1029 which is the theoretical mass.

TOF/TOF<sup>™</sup> Reflector Spec #1 MC[BP = 773.1, 29350]



Figure S4. MALDI spectrum of complex 1. The m/z value is assigned to the peaks and the y axis represents the percent intensity of the signals (%). The complex was detected as  $[Ru(bipy)_2(BC) - H^+]^+$  at m/z = 773.1.



Figure S5. LC-MS/MS calibration curve of [Ru(bipy)<sub>2</sub>BC]Cl<sub>2</sub>.



Figure S6. LC-MS/MS calibration curve of  $[Ru(bipy)_2phen]Cl_2$ . y = 5.16E-08x + 6.55E-04;  $R^2 = 0.998$ .



Figure S7. LC-MS/MS calibration curve of BC. y = 7.07E-07x - 8.12E-03;  $R^2 = 0.988$ .



Figure S8. ESI-MS full scan spectrum of 1:1 bipy:BC mixture. bipy:  $m/z [M + H^+]^+ = 157.11$ , BC:  $m/z [M + H^+]^+ = 361.22$ .



Figure S9. LC-MS/MS analysis for the uptake of complex 1 (a), BC (a, inset), and complex 2 (b) by A549 cells. Results are averages of four different experiments ( $\pm$ SEM) and are expressed in nmol/ 10<sup>6</sup> cells, as estimated from the calibration curves (Figures S5, S6, and S7).



Figure S10. Effect of complex 1 on the survival of MSCs. Treatment was performed with 3-fold dilutions of the complex starting at 120  $\mu$ M. Cytotoxicity was evaluated in both dark and light conditions (blue LED at a power of 100 mW/cm<sup>2</sup>) and the experiment was repeated three times, with measurements performed in triplicates. IC<sub>50</sub> (Dark) = 52 ± 13  $\mu$ M, IC<sub>50</sub> (Light) = 0.024 ± 0.002  $\mu$ M, p < 0.05. The graph shown here corresponds to a single representative trial.