

SUPPORTING INFORMATION FILE

Ruthenium (II)/(III) complexes of 4-hydroxy-pyridine-2, 6-dicarboxylic acid with PPh₃/AsPh₃ as co-ligand: Impact of oxidation state and co-ligands on anticancer activity in vitro

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Table of Contents

1. Characterization of the complex by ^1H NMR spectroscopy
2. Cyclic voltammetry
3. Single crystal X-Ray diffraction analysis data
4. DNA Binding studies
5. Antioxidant activity
6. *in vitro* anticancer studies

1. Characterization of the complex [Ru^{II}-hpa-P] by ¹H NMR spectroscopy

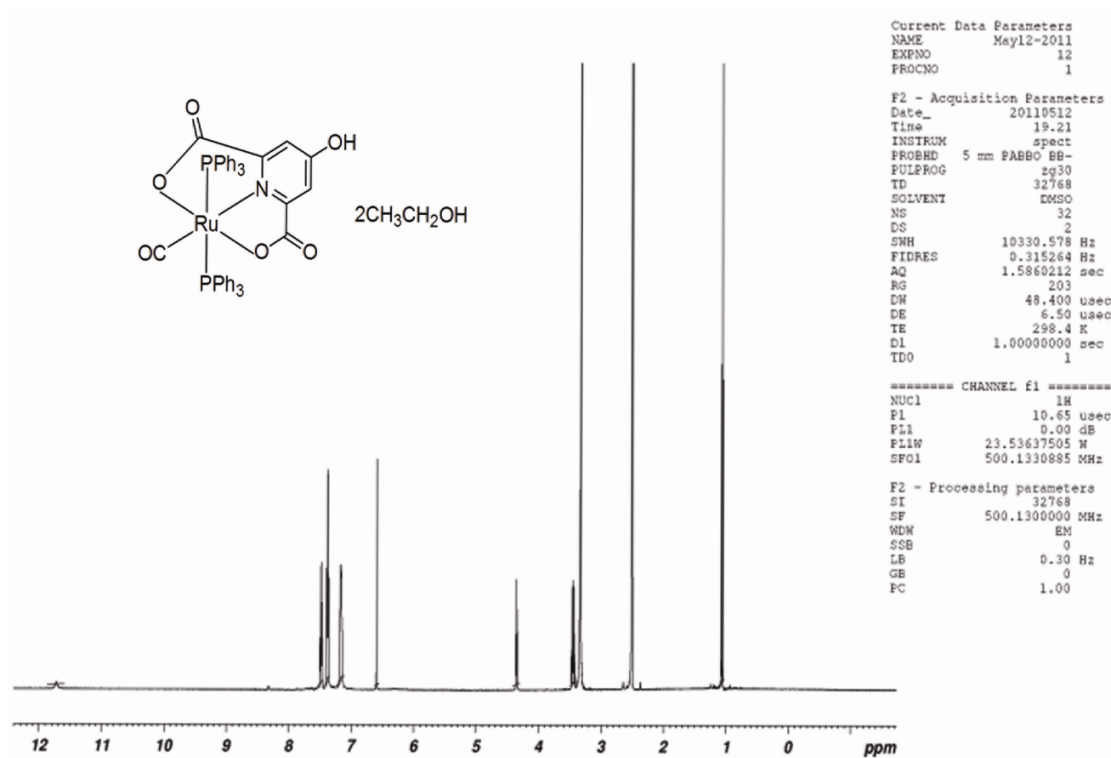


Fig. S1 ¹H NMR Spectrum of the complex [Ru^{II}-hpa-P]

2. Cyclic Voltammetry

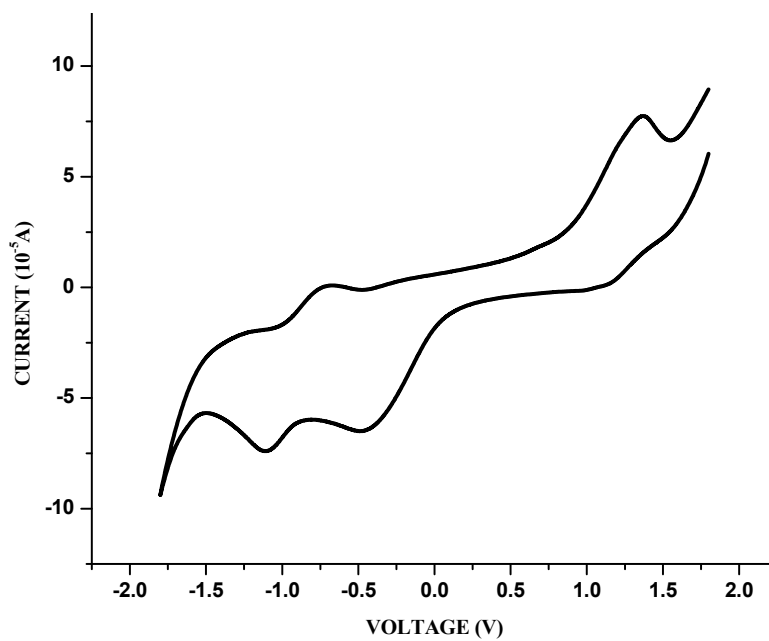


Fig. S2 Cyclic voltammetric response of [Ru^{II}-Hpa-P]

3. X-ray crystallography

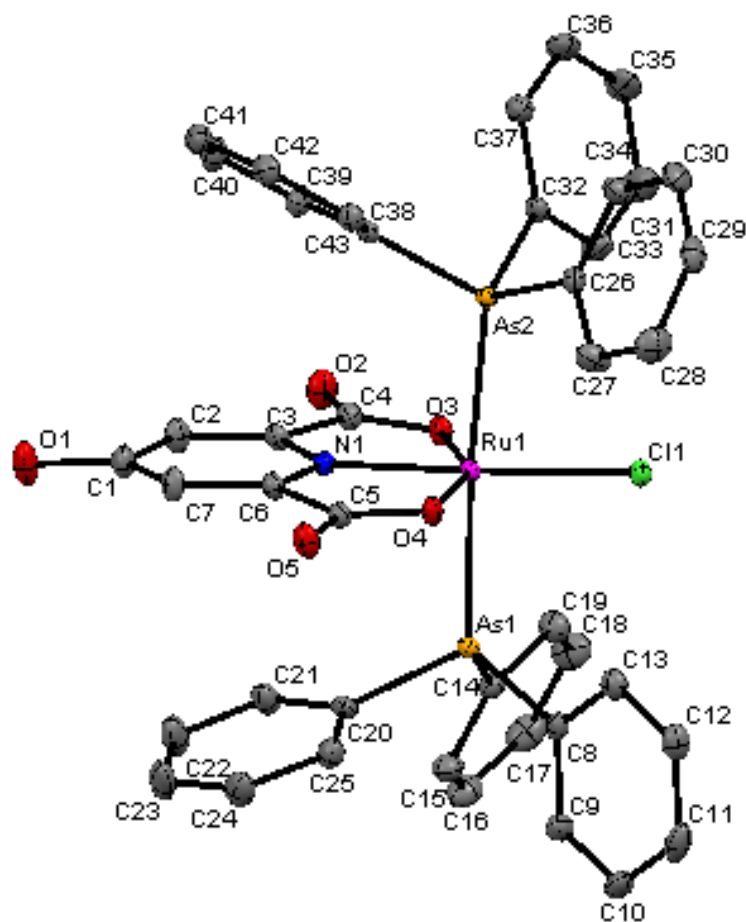


Fig. S3 X-ray crystal structure and atom numbering scheme for $[\text{Ru}^{\text{III}}\text{-hpa-As}]$ as thermal ellipsoids at 50% probability level. The hydrogen atoms have been omitted for clarity.

Table S1 Hydrogen-bonding distances (Å) and angles (°)

Complex	D-H...A	D-H	H...A	D...A	D-H...A
	O8-H8...O5	0.840(3)	1.902(1)	2.733(3)	170.0(2)
$[\text{Ru}^{\text{II}}\text{-hpa-P}]$	O1-H1...O7	0.840(1)	1.728(1)	2.558(2)	169.3(1)
	O7-H7A-O2	0.840(1)	1.834(1)	2.644(2)	161.3(1)
$[\text{Ru}^{\text{III}}\text{-hpa-P}]$	O1-H1...O5	0.820(2)	1.932(2)	2.735(3)	166.3(2)
$[\text{Ru}^{\text{III}}\text{-hpa-As}]$	O1-H1...O5	0.841(2)	1.926(2)	2.729(2)	159.6(1)

4. DNA Binding studies

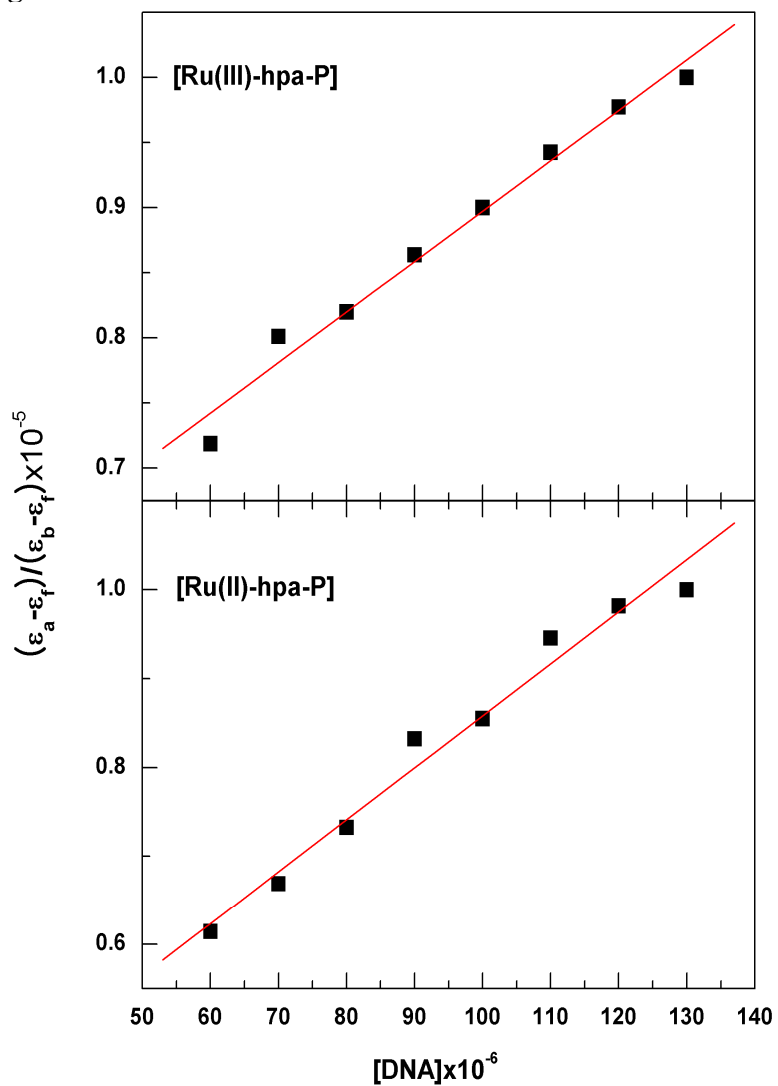


Fig. S4 Plot of $(\epsilon_a - \epsilon_f) / (\epsilon_b - \epsilon_f)$ vs $[\text{DNA}]$ for the titration of DNA with complexes and solid line is linear fitting of the data.

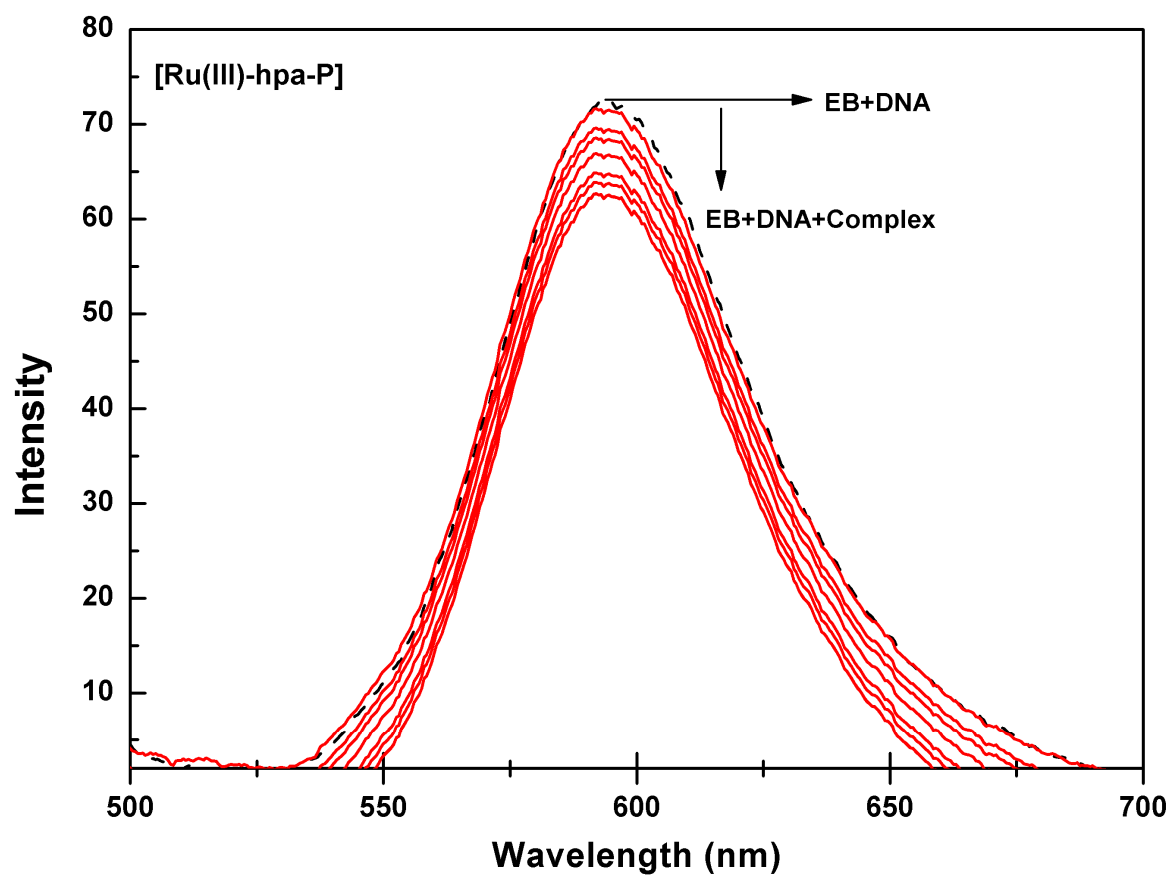


Fig. S5 Emission spectra of EB bound to DNA in the absence (- - -) and in the presence of [Ru^{III}-hpa-P], [EB] = 3 μ M, [DNA] = 12.5 μ M, [Complex] = 0.75 -2 μ M

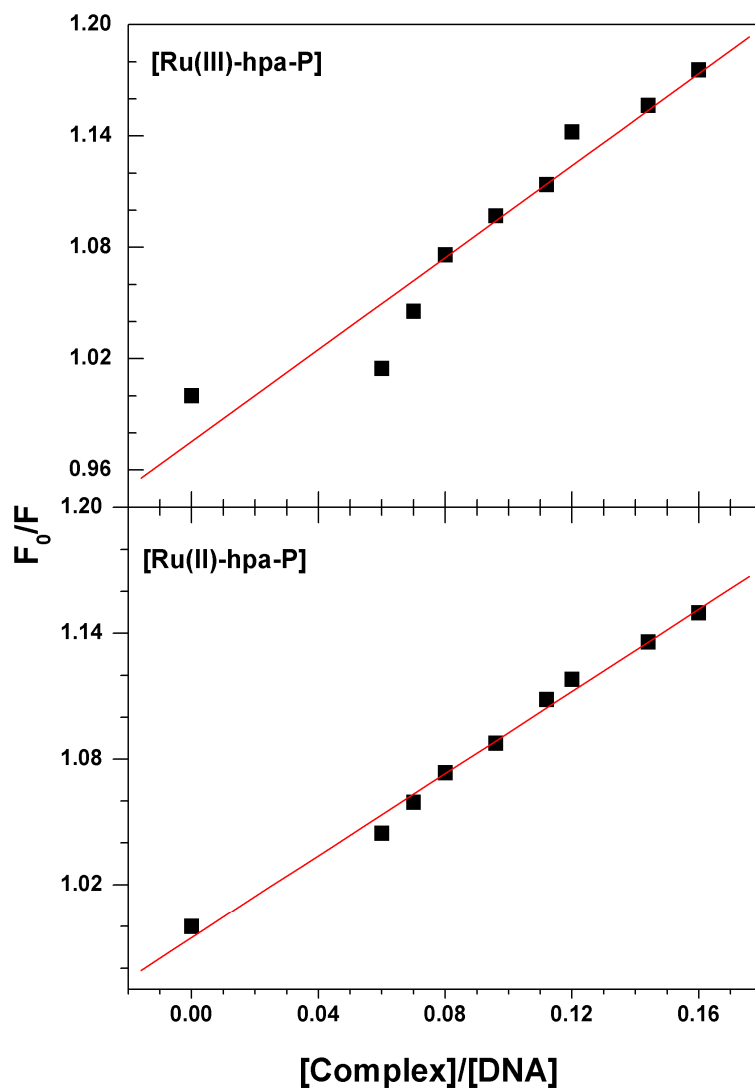


Fig. S6 Stern–Volmer quenching plot of EB bound to CT-DNA by ruthenium complexes [EB] = $3\mu\text{M}$, [DNA] = $12.5\mu\text{M}$, [Complex] = $0.75-2\mu\text{M}$

5. Antioxidant activity

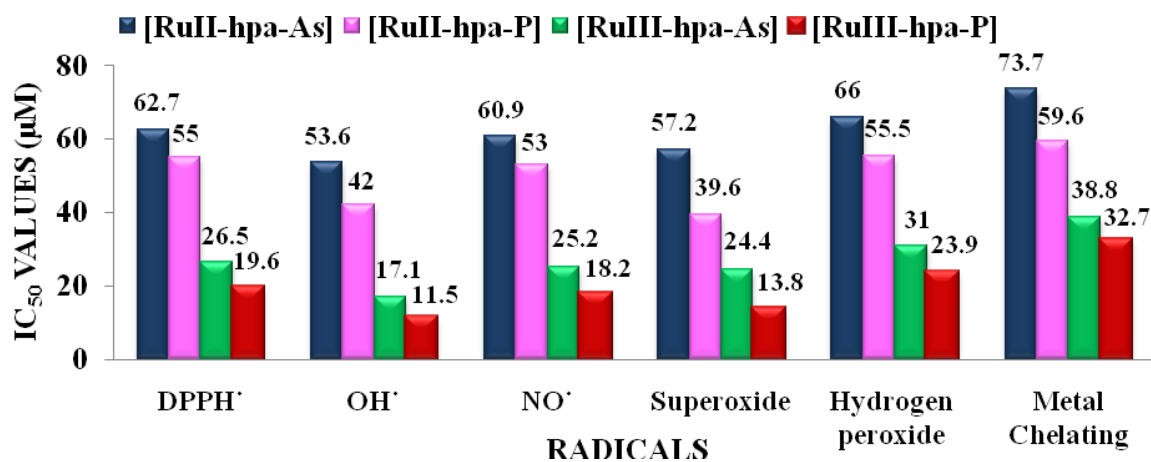


Fig. S7 Antioxidant activity of all the complexes against various radicals

6. *in vitro* anticancer studies

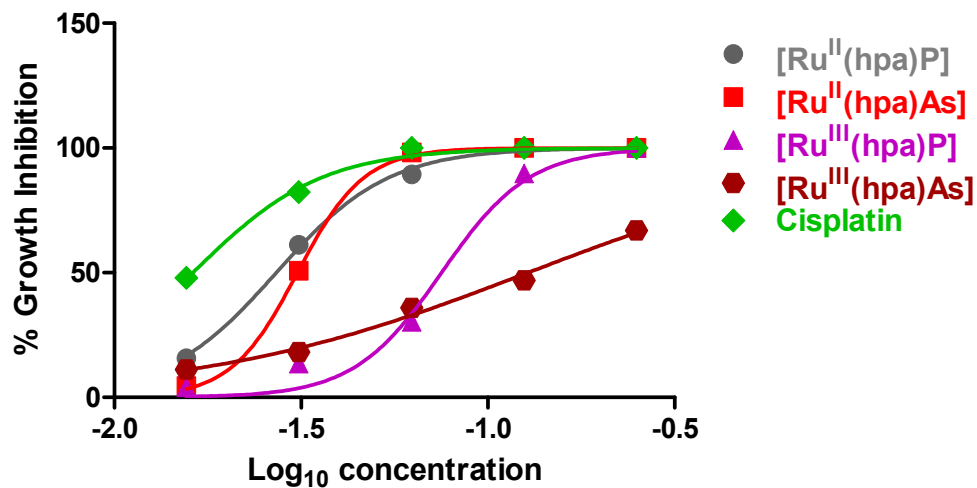


Fig. S8 Concentration effect curve of the complexes against HeLa cell line

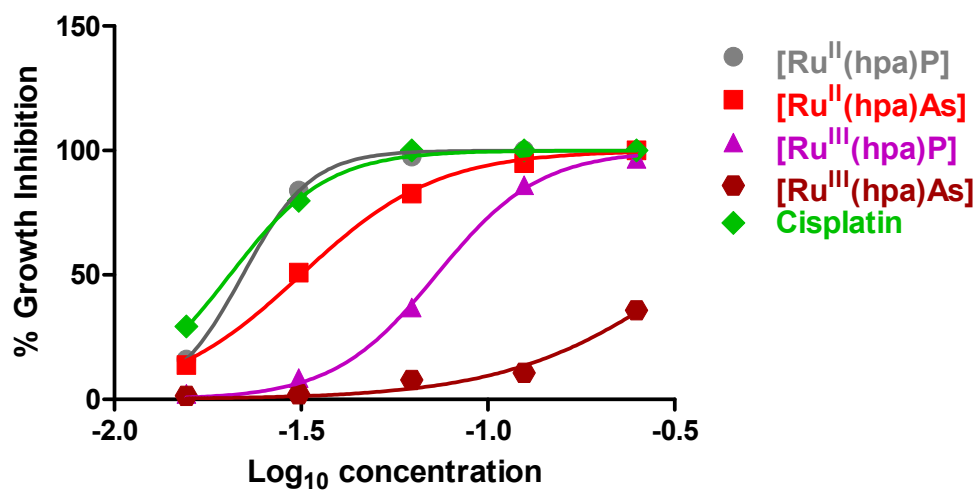


Fig. S9 Concentration effect curve of the complexes against HepG2 cell line

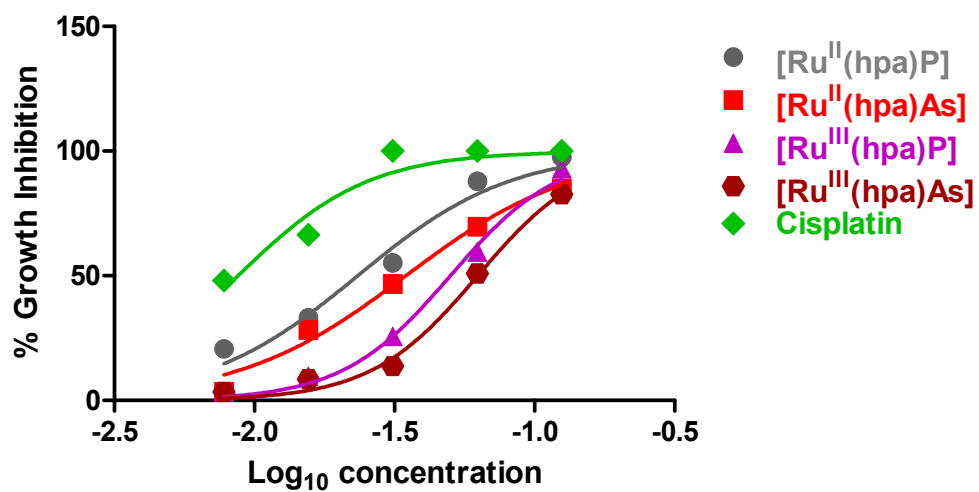


Fig. S10 Concentration effect curve of the complexes against HEP-2 cell line

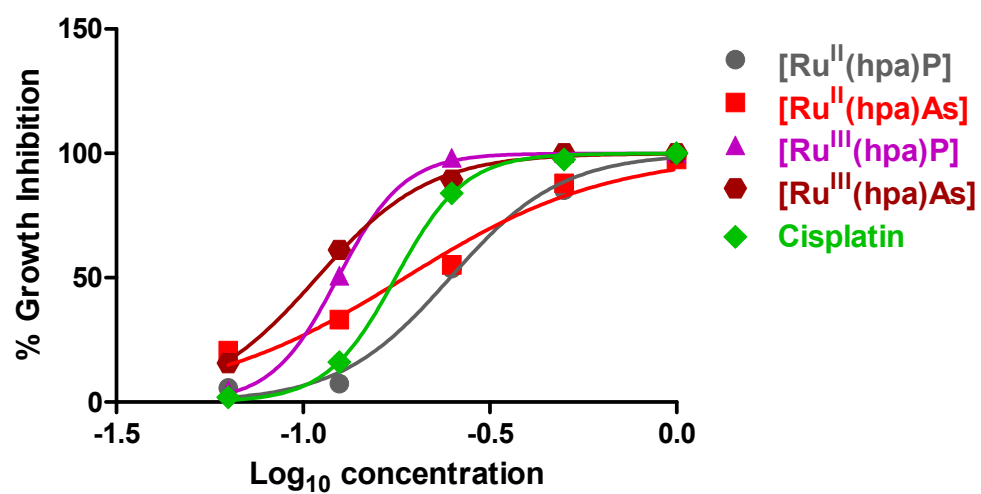


Fig. S11 Concentration effect curve of the complexes against NIH 3T3 cell line