Electronic Supporting Information

Functionalisation of gold nanoparticles with ruthenium(II) polypyridyl complexes for their application in cellular imaging

Sandra Estalayo-Adrián,*^{ab} Gavin J. McManus,^c Hannah L. Dalton,^a Aramballi J. Savyasachi,^a John M. Kelly ^a and Thorfinnur Gunnlaugsson *^a

^aSchool of Chemistry and Trinity Biomedical Sciences Institute (TBSI), Trinity College Dublin, The University of Dublin, Dublin 2, Ireland. E-mail: <u>estalays@tcd.ie</u>, <u>gunnlaut@tcd.ie</u>

^bAdvanced Materials and BioEngineering Research (AMBER) Centre, Trinity College Dublin, The University of Dublin, Dublin 2, Ireland

^cSchool of Biochemistry and Immunology, Trinity Biomedical Sciences Institute (TBSI), Trinity College Dublin, The University of Dublin, Dublin 2, Ireland

Table of Contents	Page No
Fig. S1. ¹ H NMR spectrum of 3	S2
Fig. S2. ¹³ C NMR spectrum of 3	S 3
Fig. S3. FTIR spectrum of 3	S 3
Fig. S4. ¹ H NMR spectrum of 1	S4
Fig. S5. ¹³ C NMR spectrum of 1	S5
Fig. S6. FTIR spectrum of 1	S5
Fig. S7. ESI ⁺ -HRMS spectrum of 1	S 6
Fig. S8. ¹ H NMR spectrum of 2	S 6
Fig. S9. ¹³ C NMR spectrum of 2	S 7
Fig. S10. FTIR spectrum of 2	S 7
Fig. S11. MALDI ⁺ -HRMS spectrum of 2	S 8
Fig. S12. UV-vis absorption, excitation and emission spectra of 1, 2, 1·AuNP and 2·AuNP	S8
Fig. S13. Confocal fluorescence microscopy images of HeLa cells treated with 1	S9
Fig. S14. Bright field images of HeLa cells treated with 1. AuNP and 2. AuNP	S9
Fig. S15. Toxicity profiles of 1 and 2 in HeLa cells	S10



Fig. S1. ¹H NMR (400 MHz, DMSO- d_6) spectrum of ligand 3.





Fig. S3. FTIR spectrum of ligand 3.



Fig. S4. ¹H NMR (400 MHz, DMSO- d_6) spectrum of complex 1. Signals corresponding to **phen** ligands are in green and signals assigned to ligand **3** are in red.



Fig. S5. ¹³C NMR (101 MHz, DMSO- d_6) spectrum of complex 1.





Fig. S7. Comparison between the calculated (blue) and experimental (black) isotopic distribution pattern for complex **1** from matrix-assisted laser desorption/ionisation (positive mode) high resolution mass spectrometry analysis.



Fig. S8. ¹H NMR (400 MHz, DMSO- d_6) spectrum of complex 2. Signals corresponding to TAP ligands are in green and signals assigned to ligand 3 are in red.







Fig. S11. Comparison between the calculated (blue) and experimental (black) isotopic distribution pattern for complex **2** from matrix-assisted laser desorption/ionisation (positive mode) high resolution mass spectrometry analysis.



Fig. S12. UV-vis absorption, excitation and emission spectra of (a) 1, (b) 2, (c) 1·AuNP and (d) 2·AuNP in 10 mM sodium phosphate-buffered aqueous solution at pH 7.4, at 298 K.



Fig. S13. Confocal fluorescence microscopy images of HeLa cells showing the nuclear uptake of 1 (red) at 20 μ M after 24 h incubation. The nucleus is stained blue with Hoechst 33258.



Fig. S14. Bright field images of HeLa cells showing the uptake of $1 \cdot AuNP$ and $2 \cdot AuNP$ at *ca.* 20 μ M Ru(II) complex concentration after 2, 4 and 24 h incubation.



Fig. S15. Toxicity profiles of (a) 1 and (b) 2 in HeLa cells.