Electronic Supplementary Material (ESI) for Dalton Transactions

Carbohydrate-appended photocytotoxic (imidazophenanthroline)-oxovanadium(IV) complexes for cellular targeting and imaging

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Supporting Information

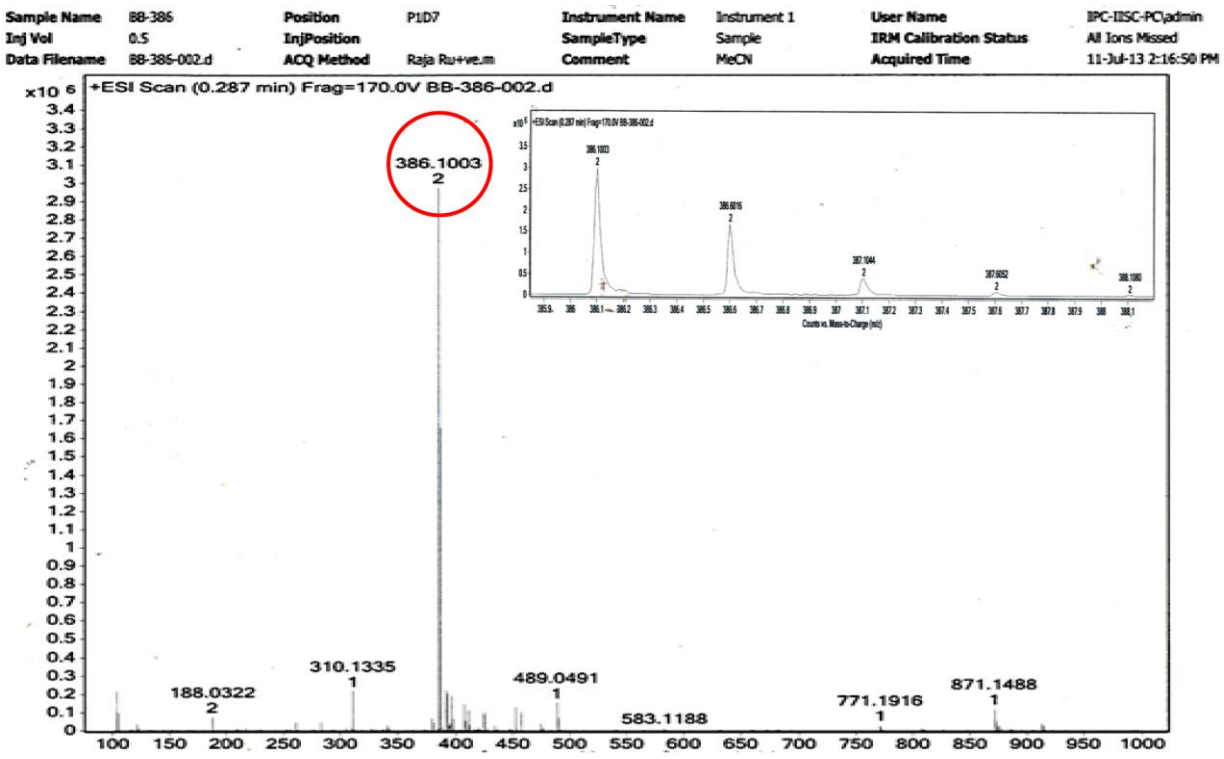

Fig. S1. The ESI-MS spectrum of complex **1** in MeCN showing the peak at 386.1003 that corresponds to $[M]^{2+}$. The inset shows the isotopic distribution of the $[M]^{2+}$ ion peak.

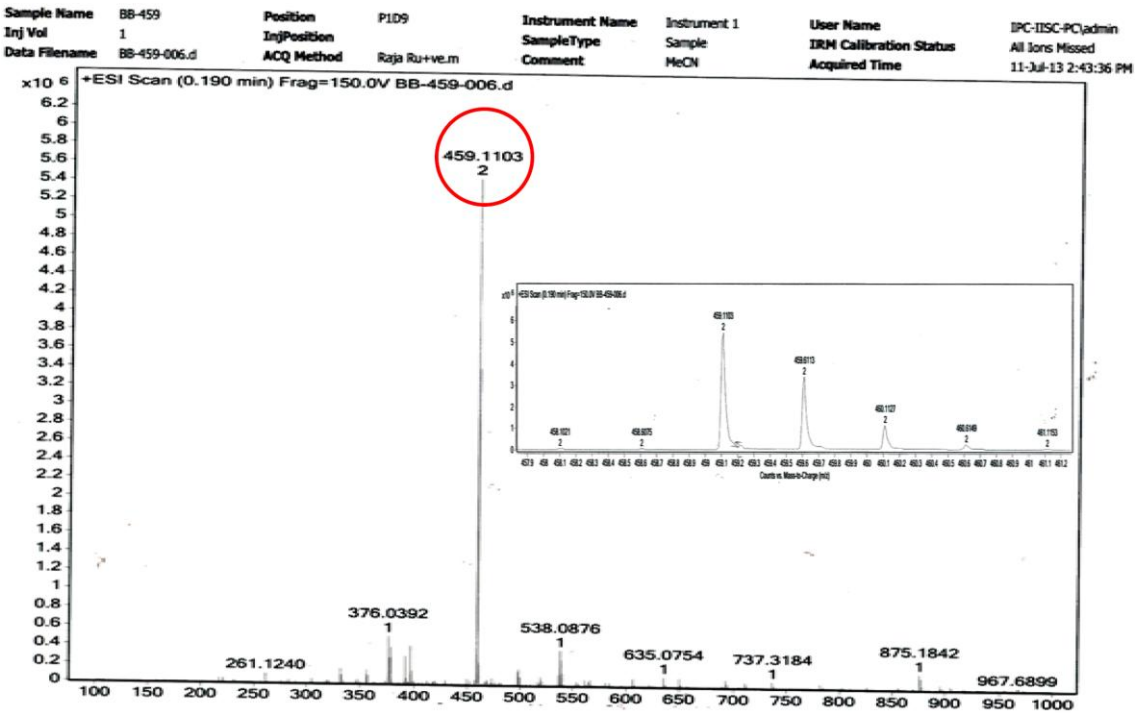

Fig. S2. The ESI-MS spectrum of complex **2** in MeCN showing the peak at 459.1103 (m/z) assignable to $[M]^{2+}$. The inset shows the isotopic distribution of the $[M]^{2+}$ ion peak.

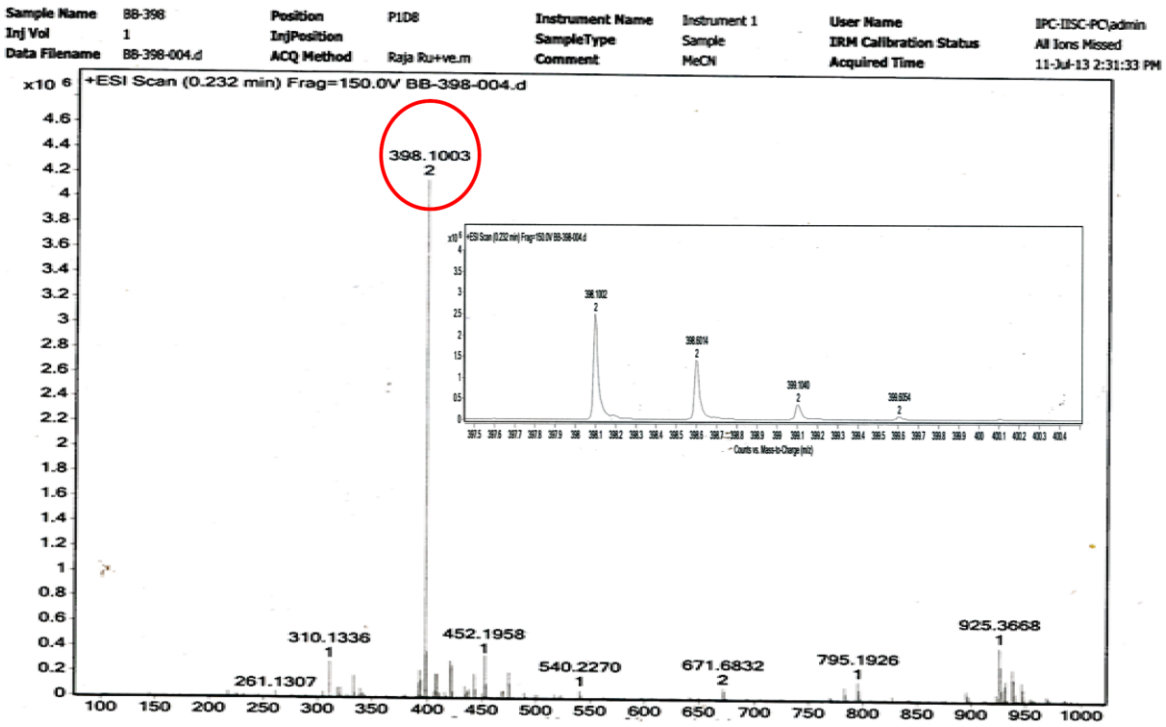

Fig. S3. The ESI-MS spectrum of complex **3** in MeCN showing the peak at 398.1003 that corresponds to $[M]^{2+}$. The inset shows the isotopic distribution of the $[M]^{2+}$ ion peak.

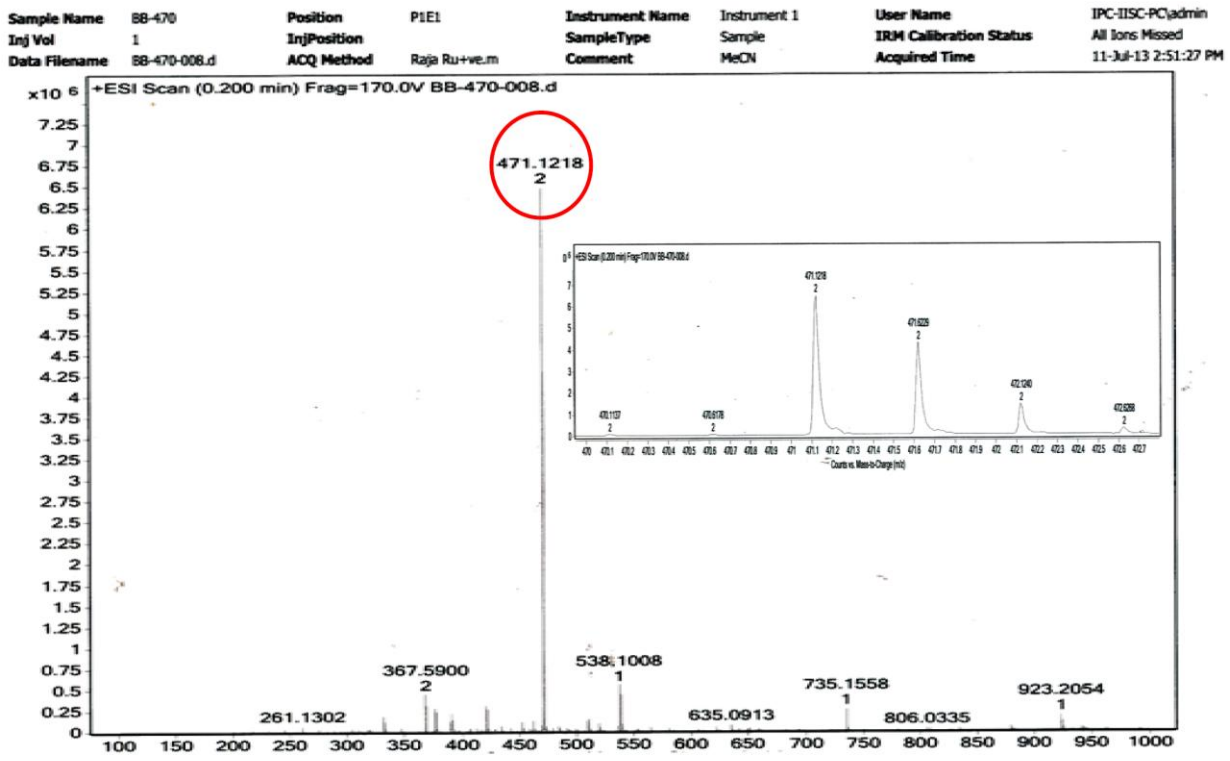

Fig. S4. The ESI-MS spectrum of the complex **4** in MeCN showing a peak at 471.1218 that corresponds to $[M]^{2+}$. The inset shows the isotopic distribution of the $[M]^{2+}$ ion peak.

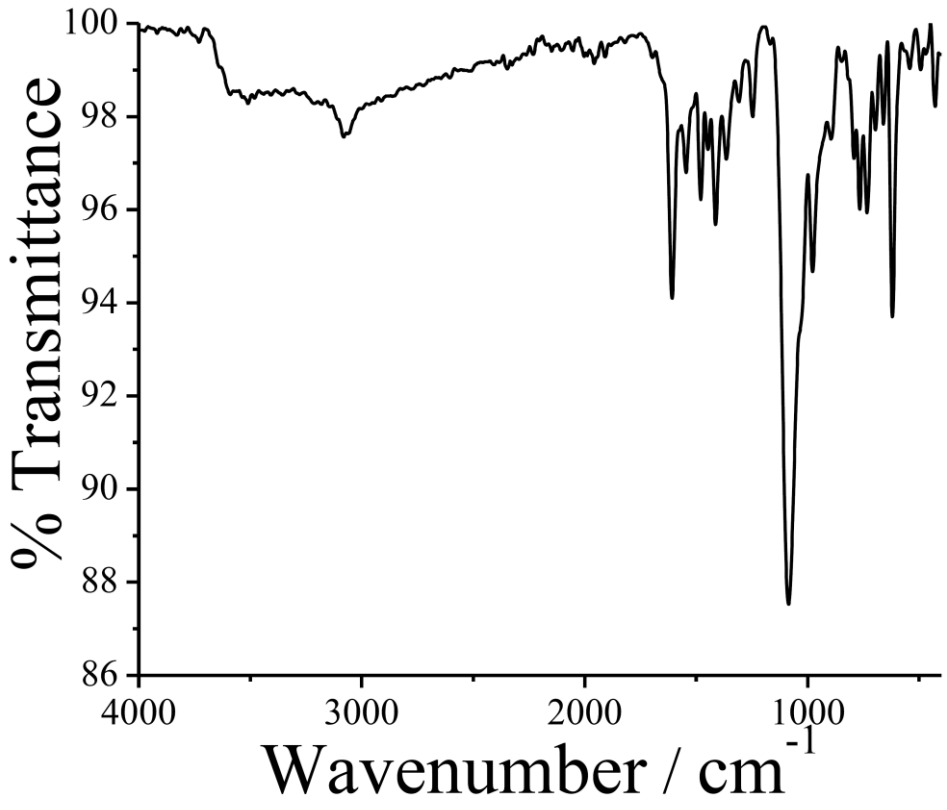

Fig. S5. IR spectra of complex **1**.

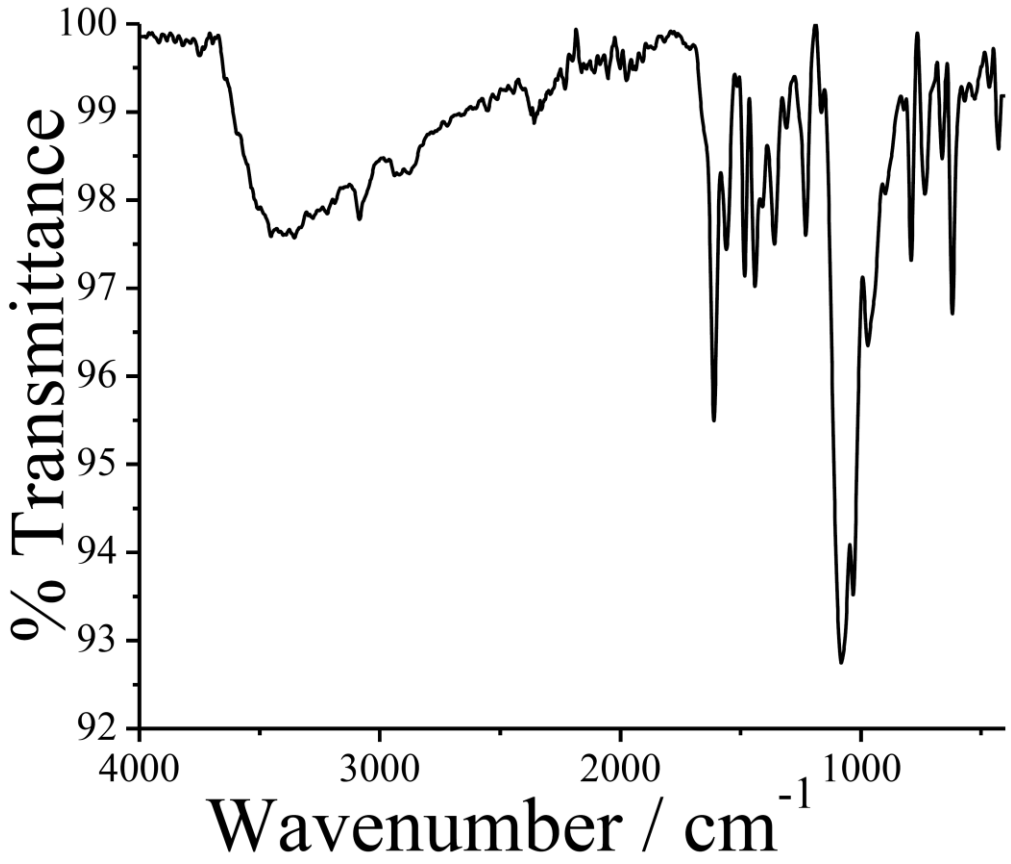

Fig. S6. IR spectra of complex **2**.

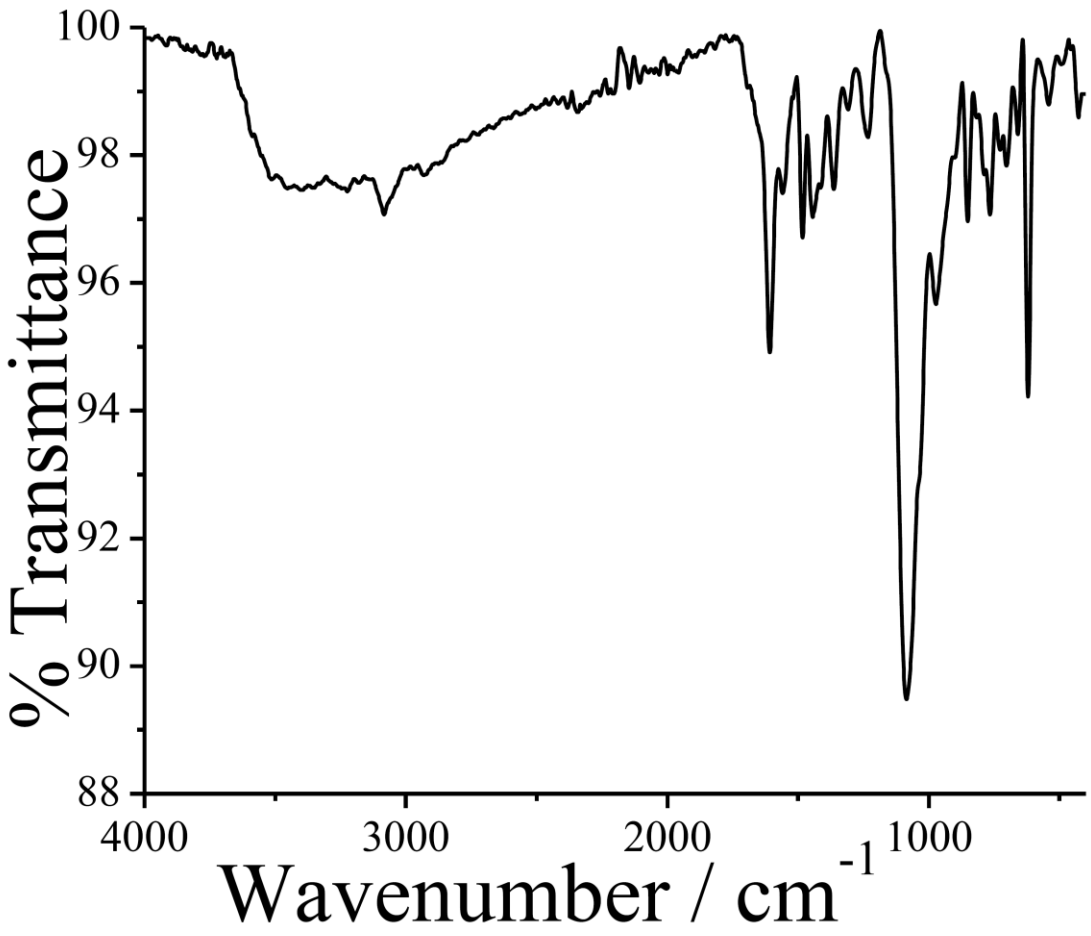

Fig. S7. IR spectra of complex **3**.

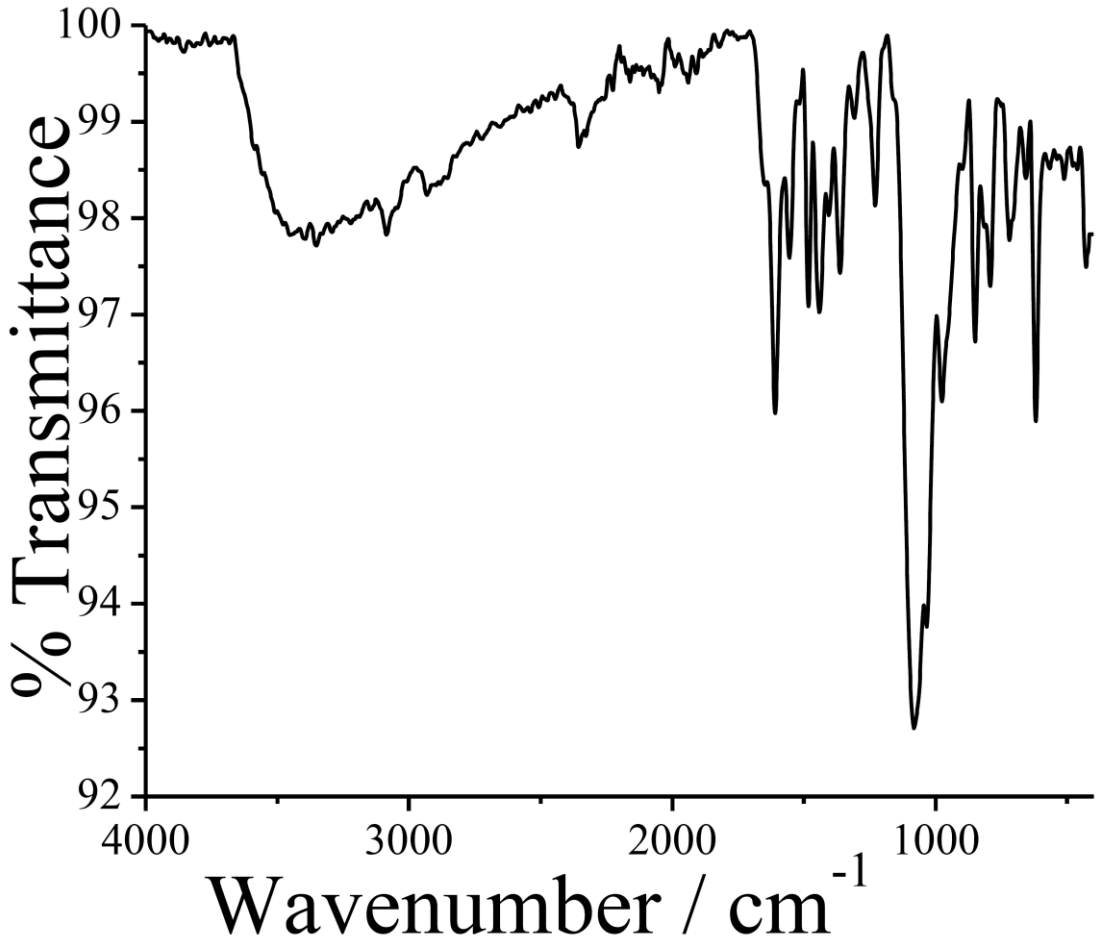

Fig. S8. IR spectra of complex **4**.

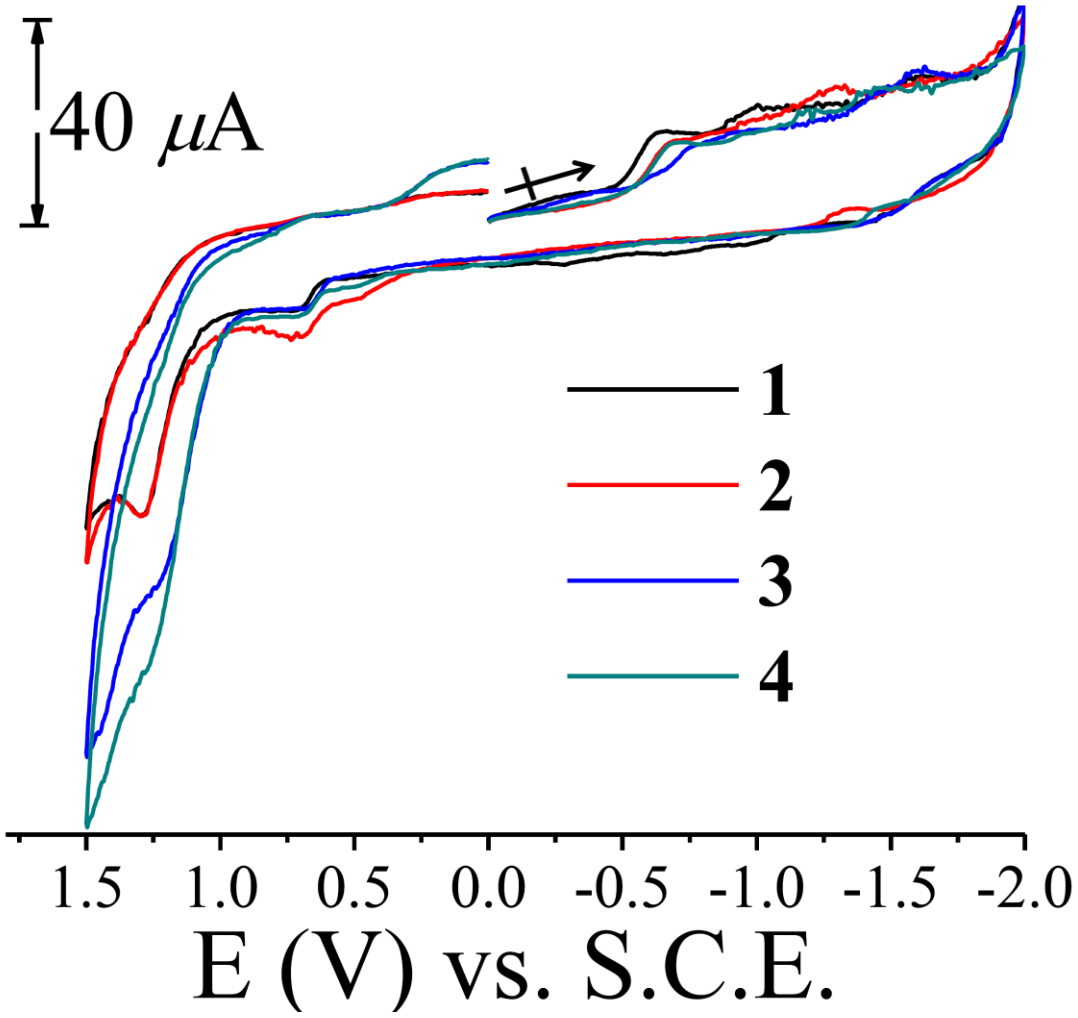

Fig. S9. Cyclic voltammograms of the complexes **1** - **4** in DMF at a scan speed of 50 mV s^{-1} and 0.1 M TBAP as a supporting electrolyte. The V(IV)-V(III) response is irreversible in nature showing only the cathodic peak without having any anodic counterpart.

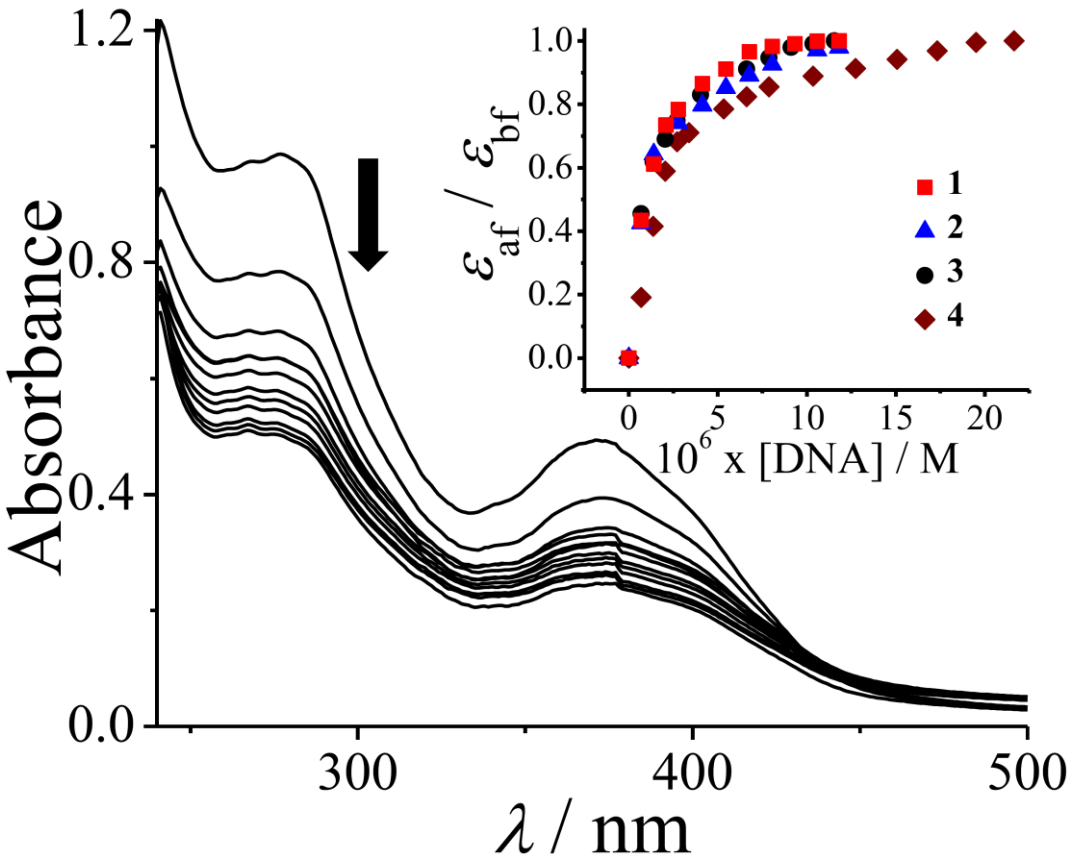

Fig. S10. Absorption spectral traces of complex **4** in 5 mM Tris-HCl buffer (pH 7.2) on increasing the concentration of CT DNA. The inset shows the least-squares fit of $\Delta\varepsilon_{af}/\Delta\varepsilon_{bf}$ vs. [DNA] for **1** - **4** using the MvH equation.

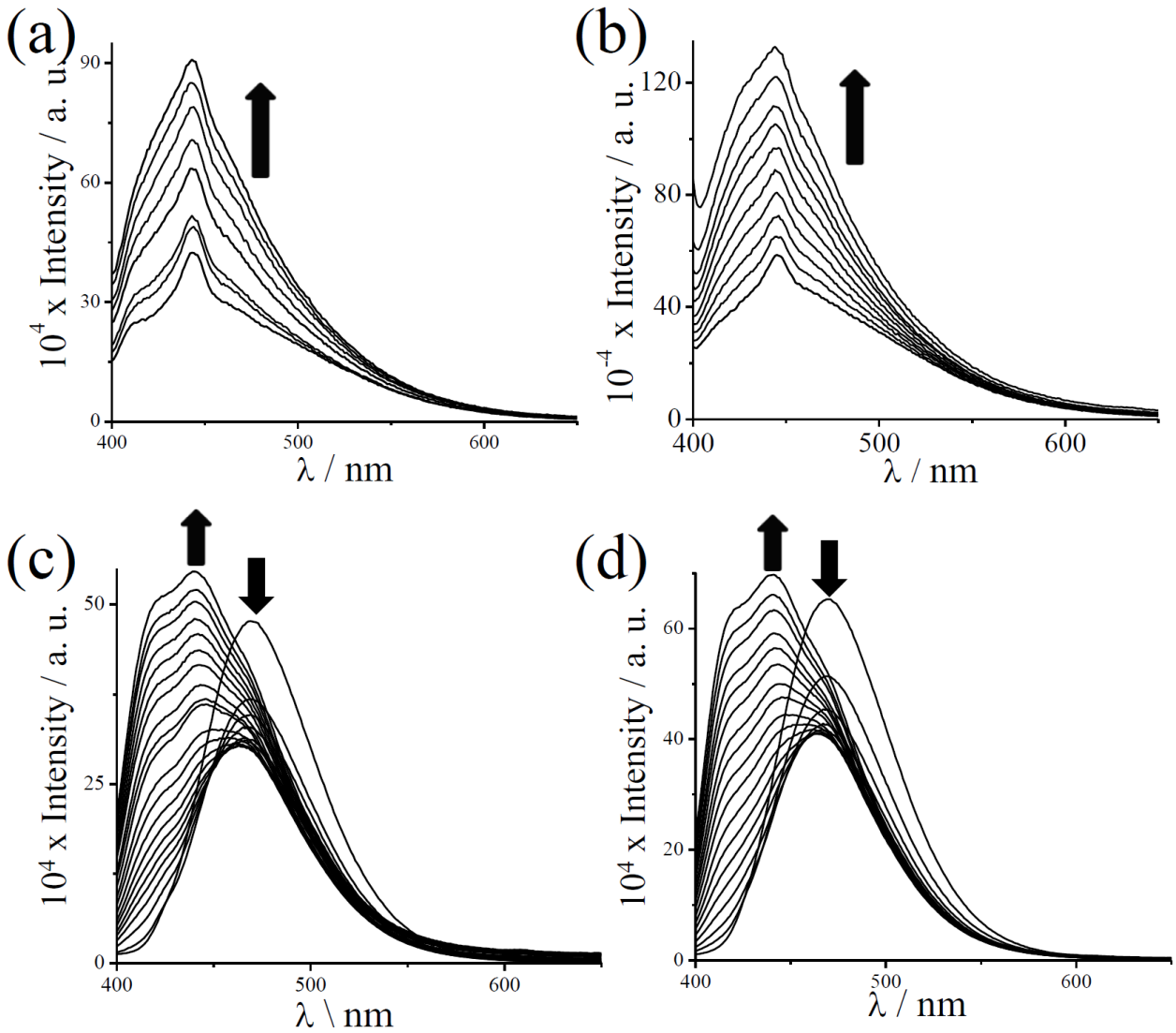

Fig. S11. BSA light switch effect of complexes **1** (a), **2** (b), **3** (c) and **4** (d) in 10% aqueous DMSO.

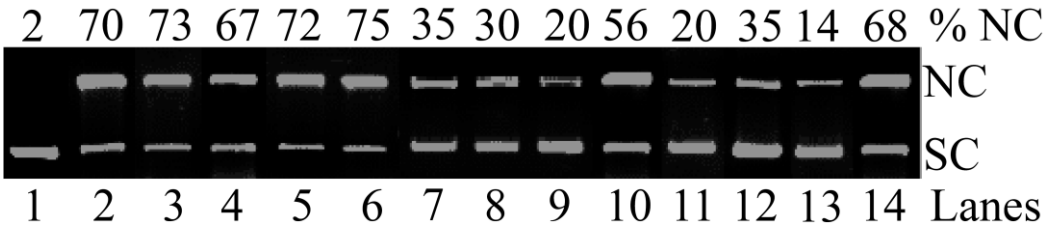

Fig. S12. Cleavage of SC pUC19 DNA (0.2 μg, 30 μM) by the complexes **1**-**4** (50 μM) in the presence of various additives in 50 mM Tris-HCl/NaCl buffer (pH 7.2) containing 1.5% DMF on photo-irradiation at 705 nm for 2 h. The reaction conditions are given below in a tabular form.

Lane No	Reaction conditions
1	DNA control
2	DNA + complex **4**
3	DNA + complex **4** + D_2O
4	DNA + complex **4** + NaN_3
5	DNA + complex **4** + TEMP
6	DNA + complex **4** + DABCO
7	DNA + complex **4** + DMSO
8	DNA + complex **4** + KI
9	DNA + complex **4** + Catalase
10	DNA + complex **4** + SOD
11	DNA + methyl green
12	DNA + methyl green + complex **4**
13	DNA + distamycin-A
14	DNA + distamycin-A + complex **4**

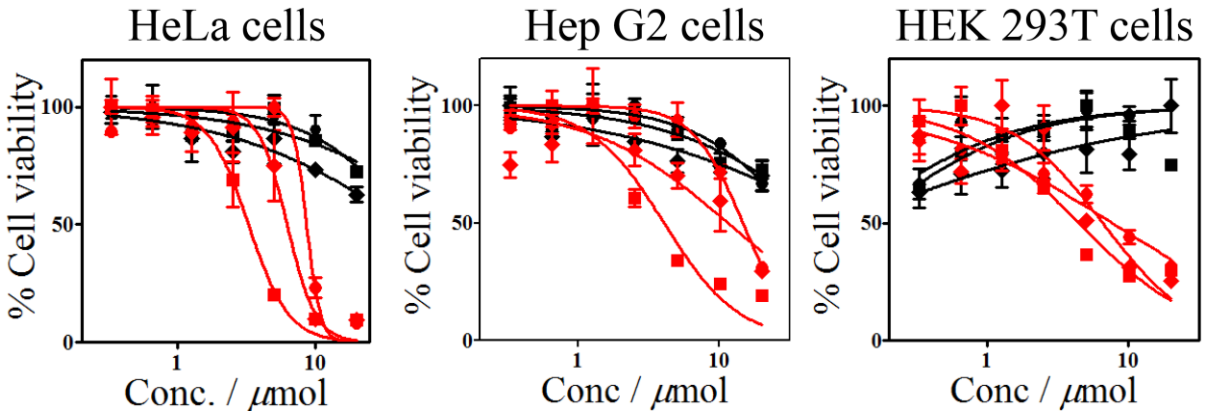

Fig. S13. Photocytotoxicity of complexes **1** (♦), **2** (■) and **3** (●) in HeLa, Hep G2 and HEK 293T cells on 1 h incubation in dark followed by photo-irradiation in visible light (400 to 700 nm) as determined by MTT assay. The traces for photo-exposed and dark-treated cells are shown by red and black curves, respectively.

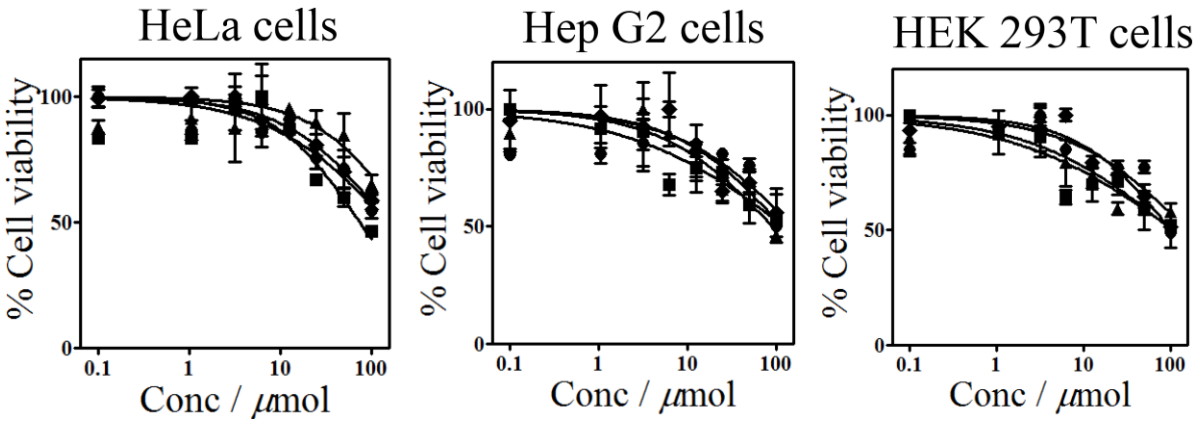

Fig. S14. Cytotoxicity of complexes **1** (♦), **2** (■), **3** (●) and **4** (▲) (upto 100 μM concentration) in HeLa, Hep G2 and HEK 293T cells on 1 h incubation in dark as determined by MTT assay.

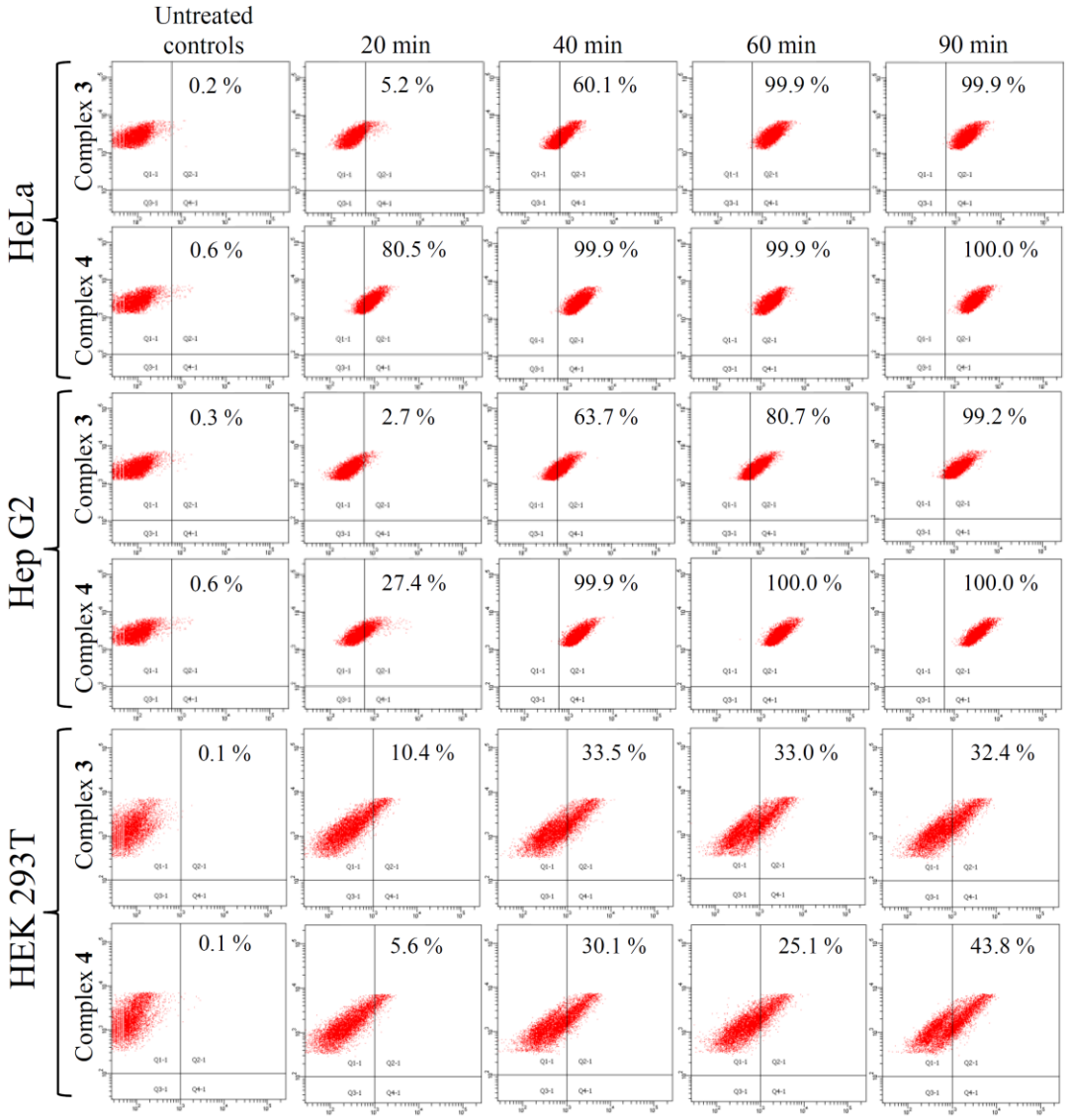

Fig. S15. A comparison of the cellular uptake of the complexes **3** and **4** (0.2 μM) at various time points of incubation with HeLa, Hep G2 and HEK 293T cells as determined from the flow cytometric analysis.

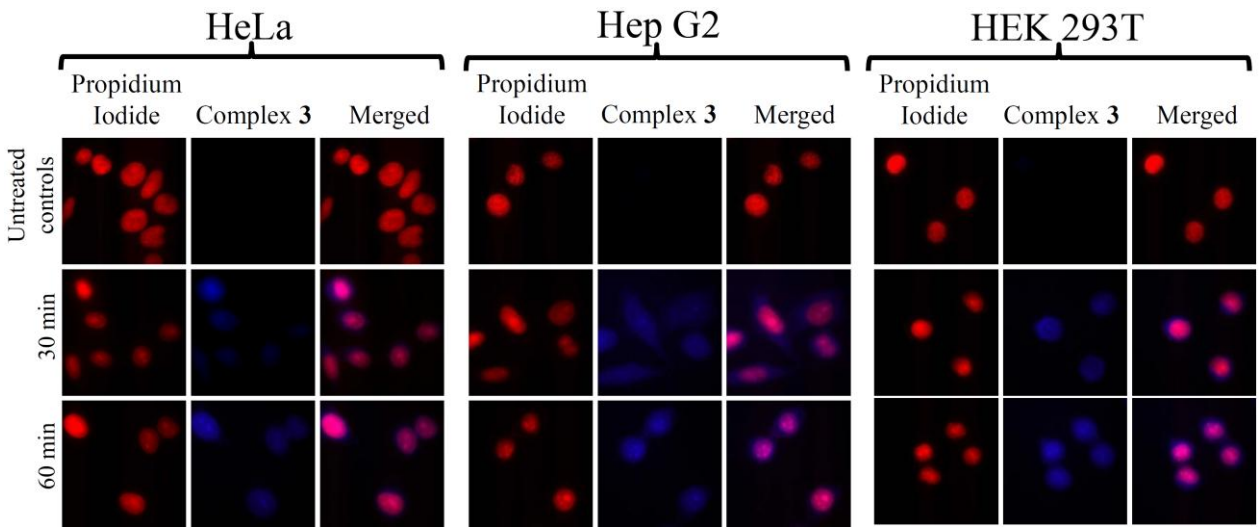

Fig. S16. A time-course collection of the fluorescence microscopic images of the HeLa, Hep G2 and HEK 293T cells treated with complex **3** (1 μM).

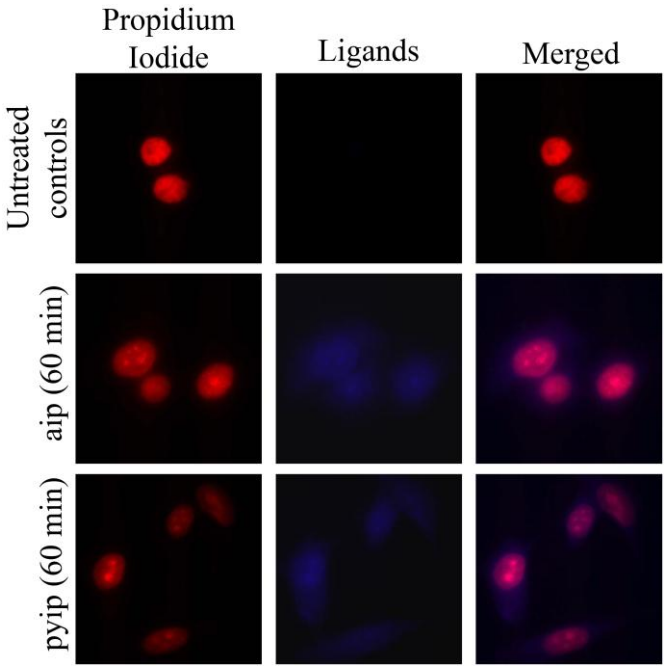

Fig. S17. Fluorescence microscopic images of the HeLa cells treated with the ligands, viz. aip and pyip (5 μM).

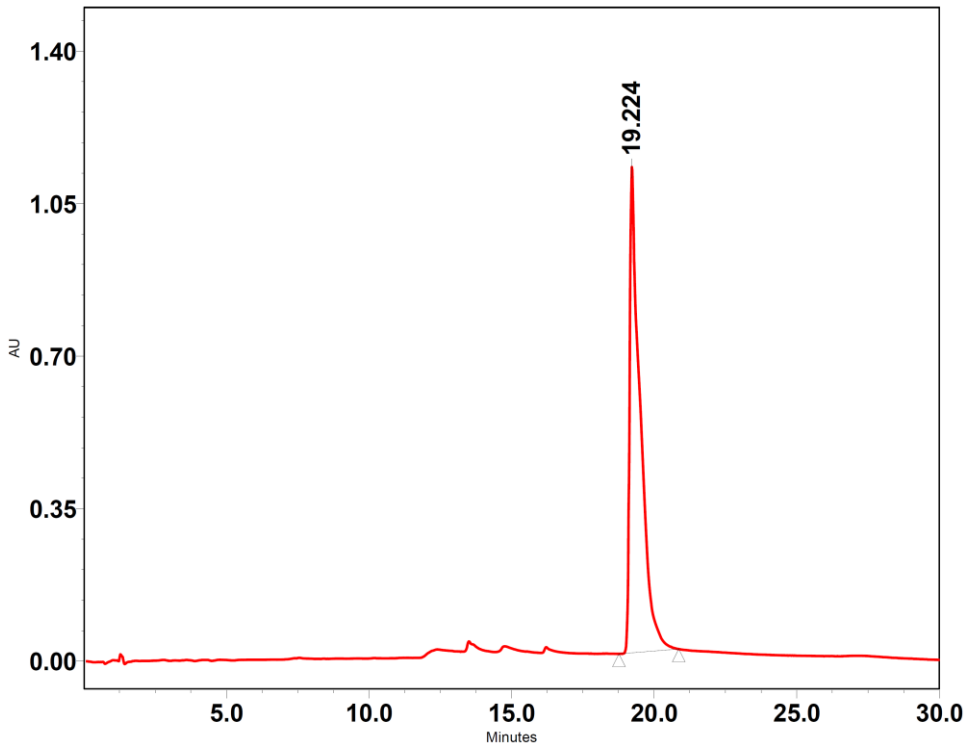

Fig. S18. HPLC chromatogram of the complex **1**.

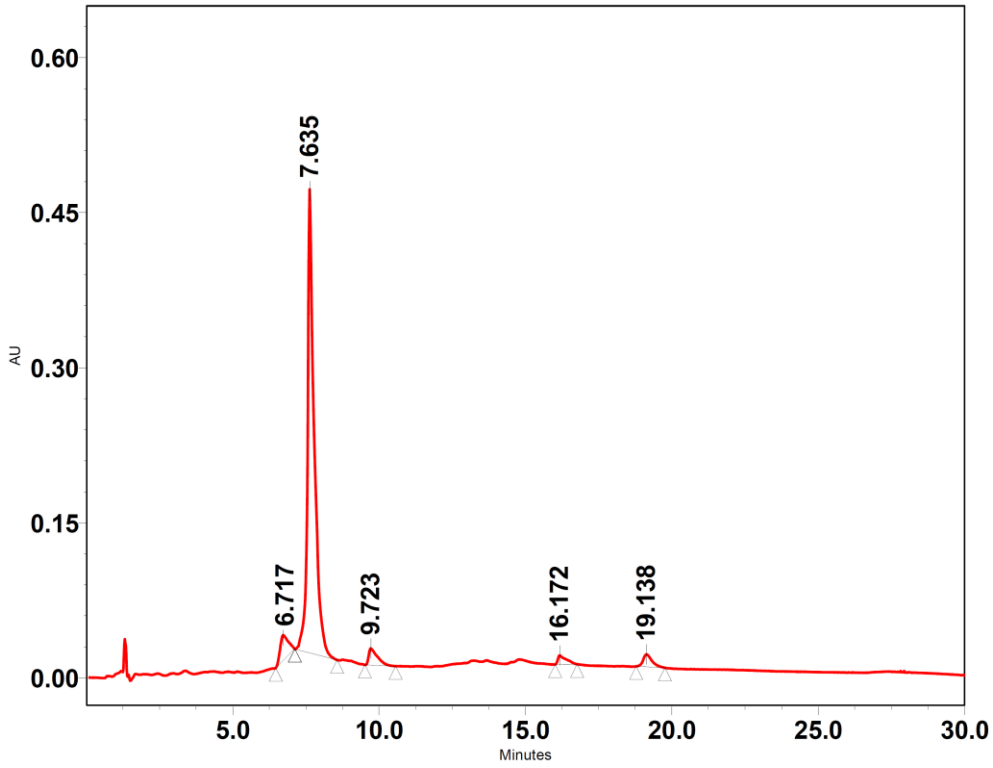

Fig. S19. HPLC chromatogram of the complex **2**.

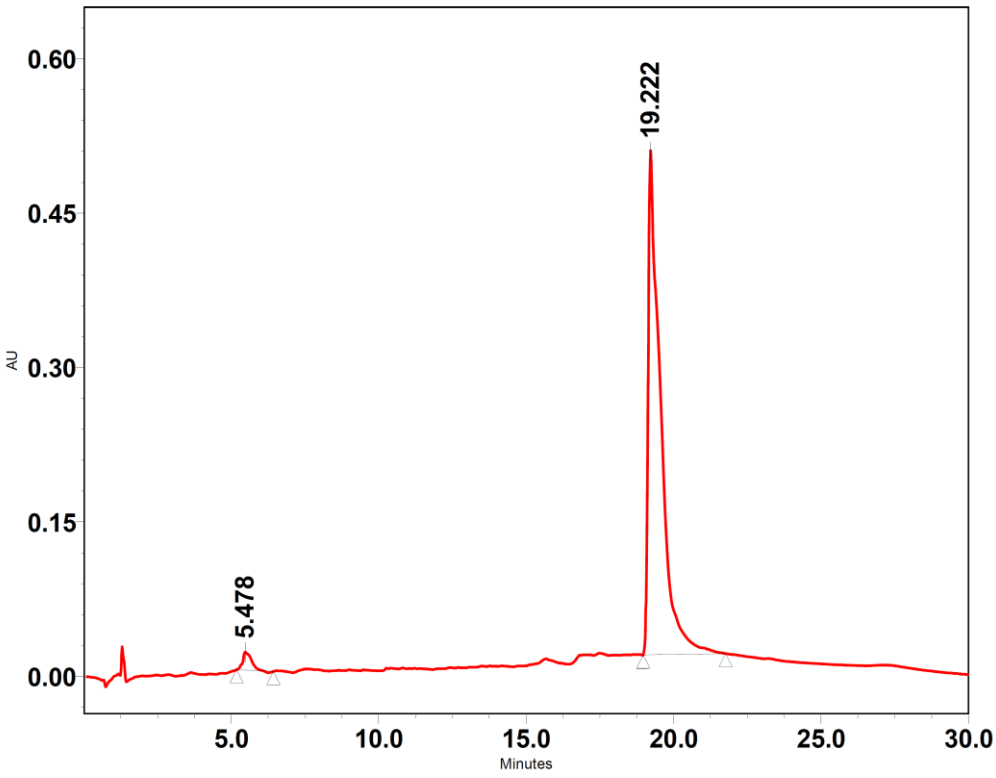

Fig. S20. HPLC chromatogram of the complex **3**.

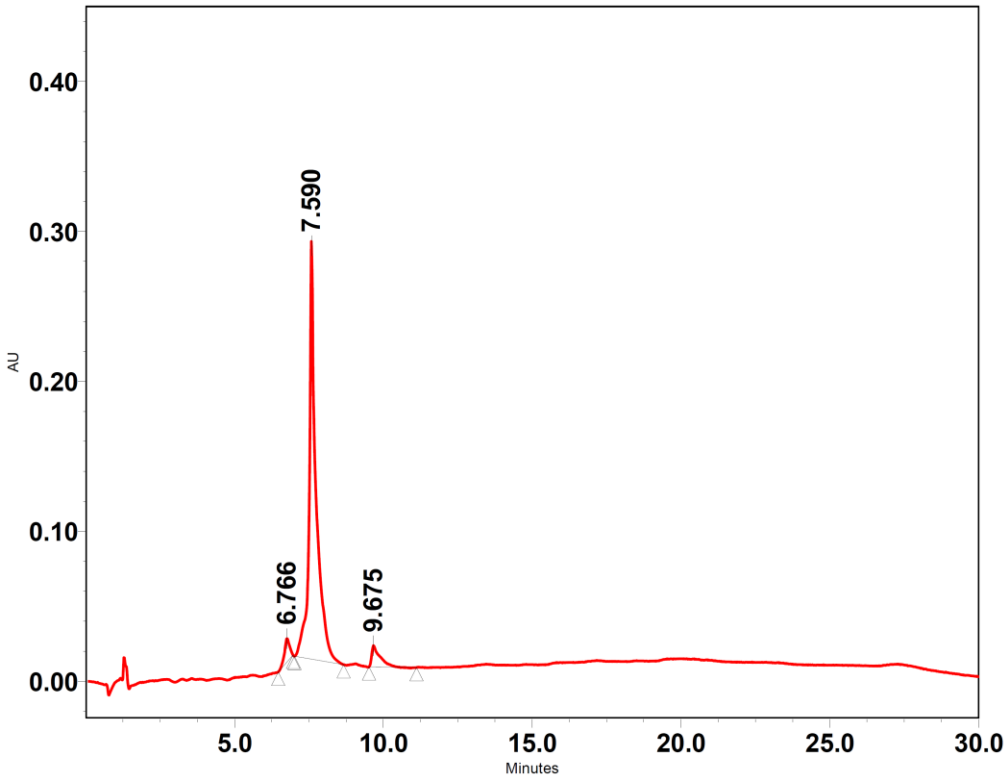

Fig. S21. HPLC chromatogram of the complex **4**.