

Electronic Supporting Information (ESI†)

for

Significant photocytotoxic effect of an iron(III) complex of a Schiff base ligand derived from vitamin B₆ and thiosemicarbazide in visible light

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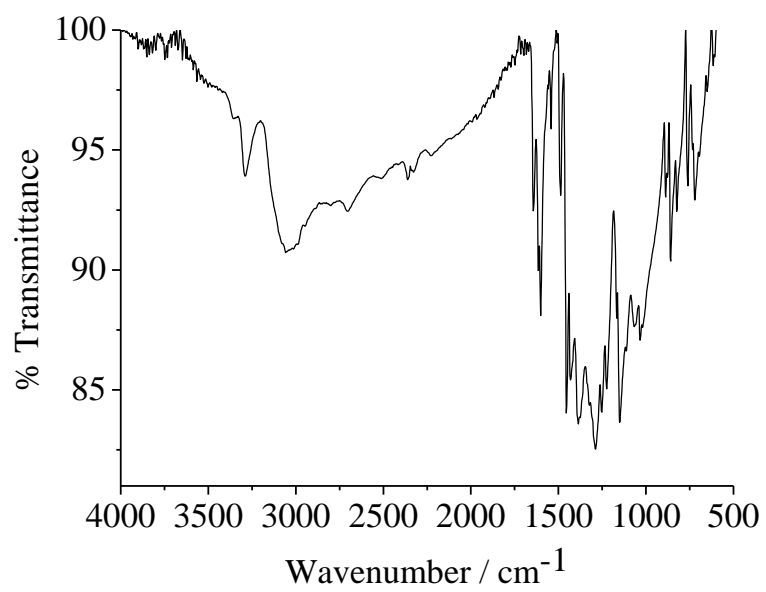


Fig. S1 The IR spectrum of [Fe(tsc-py)₂](NO₃) (complex **1**).

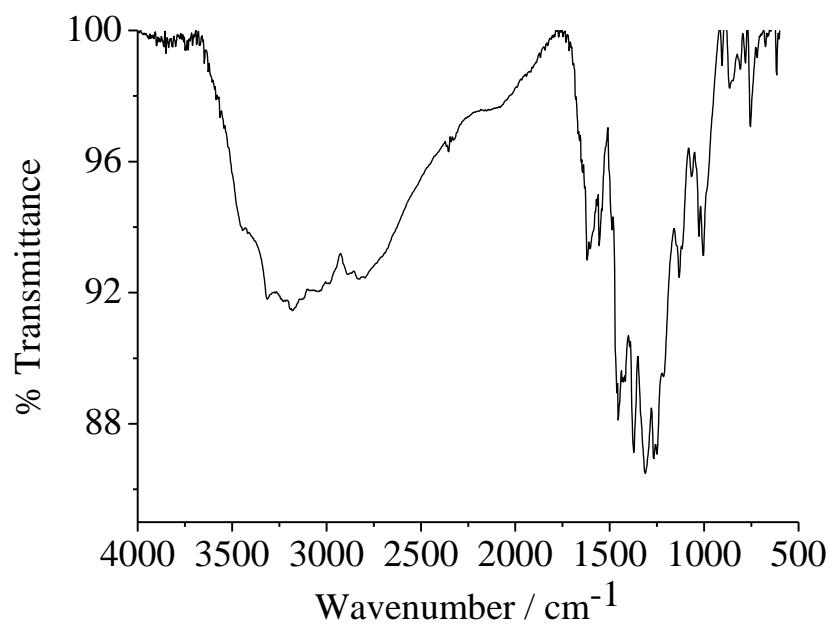


Fig. S2 The IR spectrum of $[\text{Fe}(\text{tsc-acpy})_2](\text{NO}_3)$ (complex **2**).

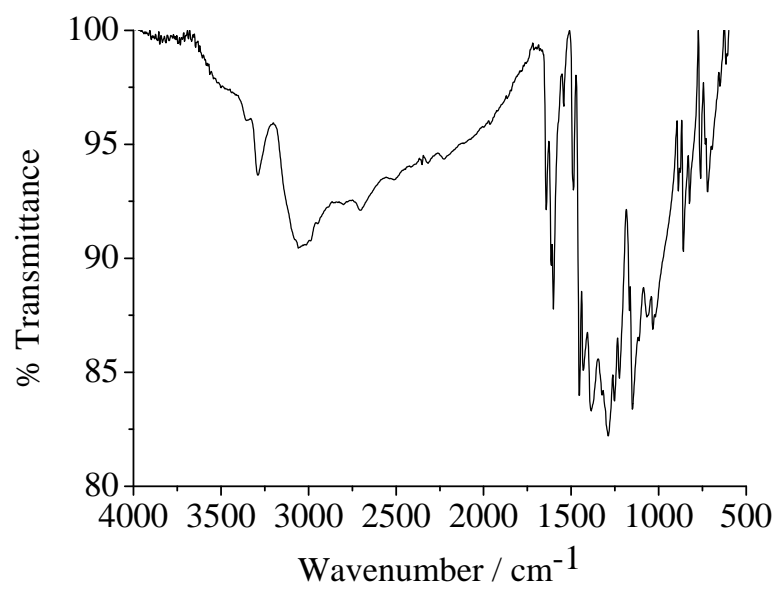


Fig. S3 The IR spectrum of $[\text{Fe}(\text{tsc-VB}_6)_2](\text{NO}_3)$ (complex **3**).

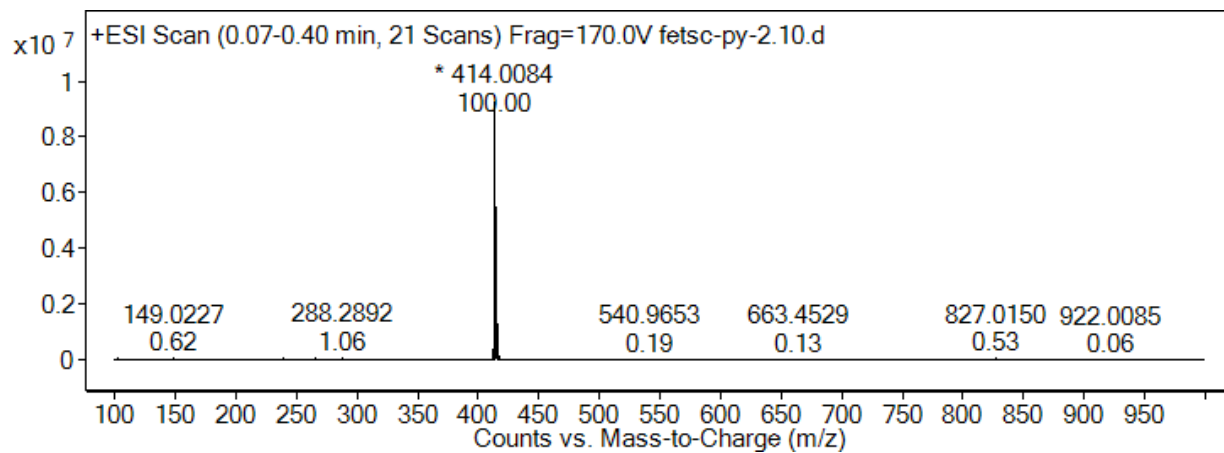


Fig. S4 The ESI-MS spectrum of $[\text{Fe}(\text{tsc-py})_2](\text{NO}_3)$ (complex **1**) in 10% aqueous methanol showing the $[\text{M}-(\text{NO}_3)]^+$ peak.

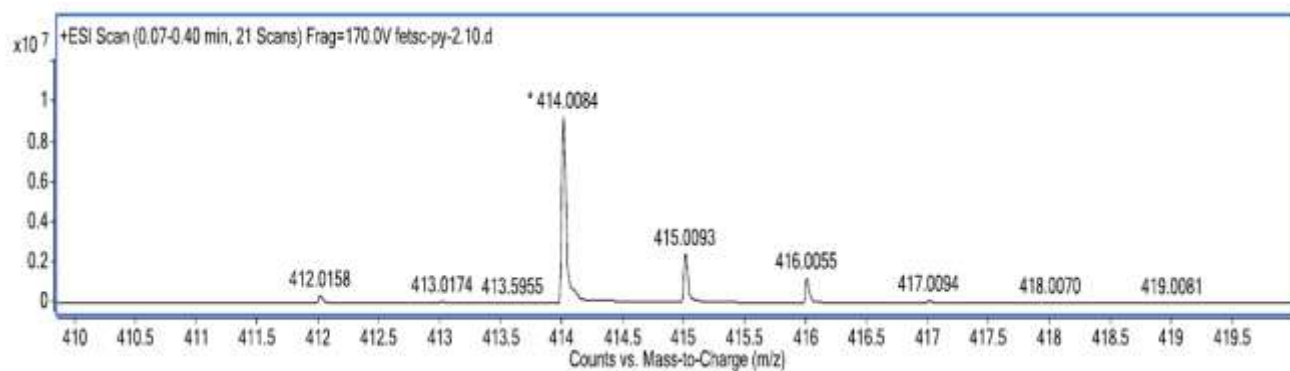


Fig. S5 The isotopic distribution pattern for the $[M-(NO_3^-)]^+$ peak of $[Fe(tsc-py)_2](NO_3)$ (complex **1**) in the ESI-MS spectrum shown in Fig. S4.

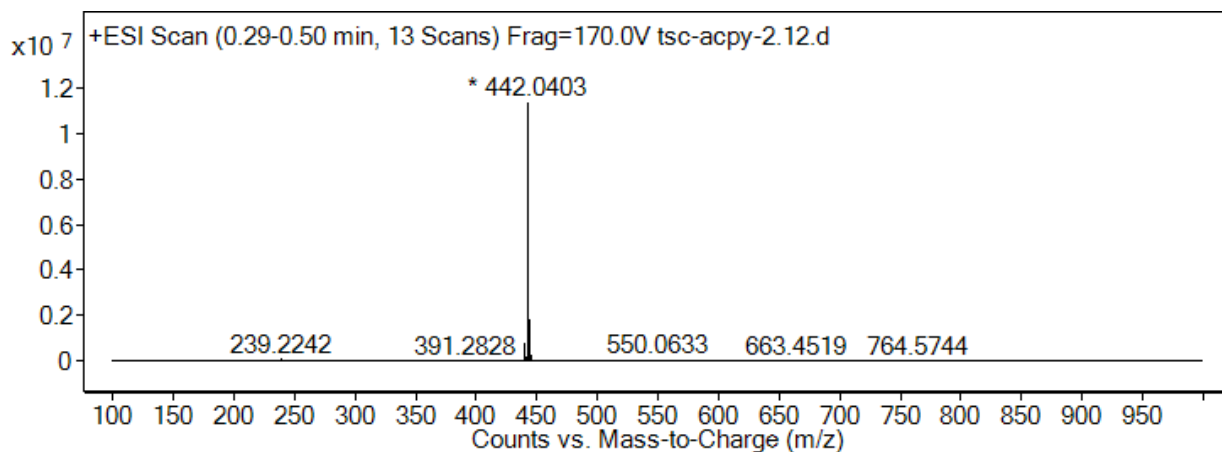


Fig. S6 The ESI-MS spectrum of $[\text{Fe}(\text{tsc-acpy})_2](\text{NO}_3)$ (complex **2**) in 10% aqueous methanol showing the $[\text{M}-(\text{NO}_3)]^+$ peak.

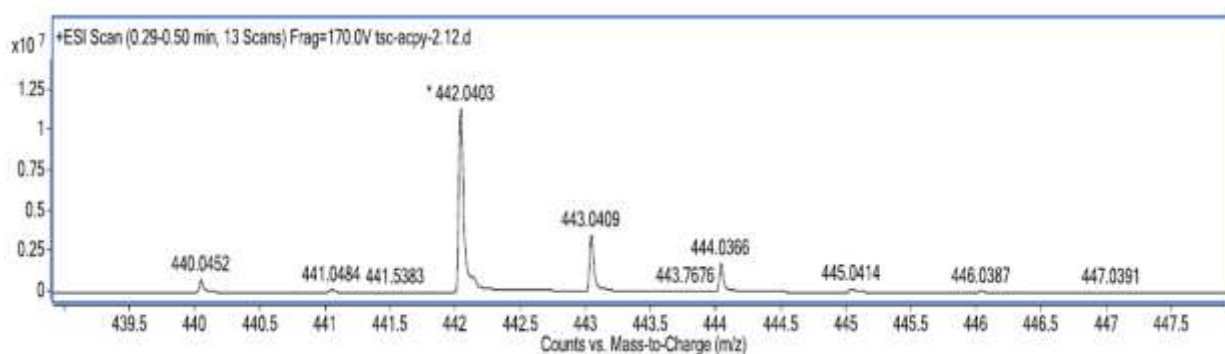


Fig S7 The isotopic distribution pattern for the $[\text{M}-(\text{NO}_3)]^+$ peak of $[\text{Fe}(\text{tsc-acpy})_2](\text{NO}_3)$ (complex **2**) in the ESI-MS spectrum shown in Fig. S6.

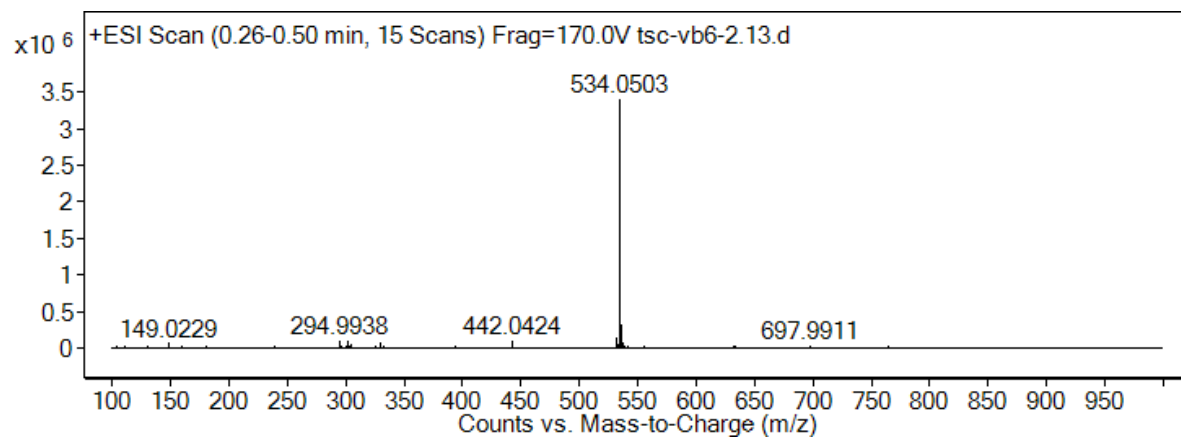


Fig. S8 The ESI-MS spectrum of $[\text{Fe}(\text{tsc-VB}_6)_2](\text{NO}_3)$ (complex **3**) in 10% aqueous methanol showing the $[\text{M}-(\text{NO}_3)]^+$ peak.

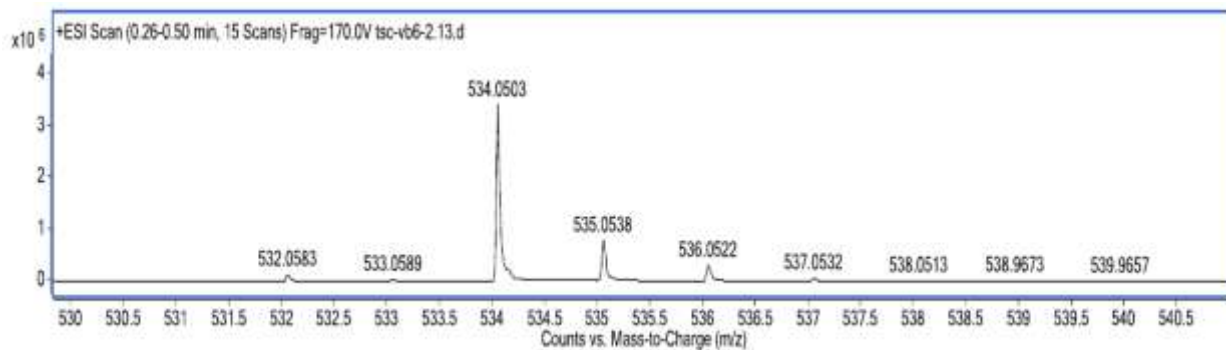


Fig. S9 The isotopic distribution pattern for the $[M-(NO_3)]^+$ peak of $[Fe(tsc-VB_6)_2](NO_3)$ (complex **3**) in the ESI-MS spectrum shown in Fig. S8.

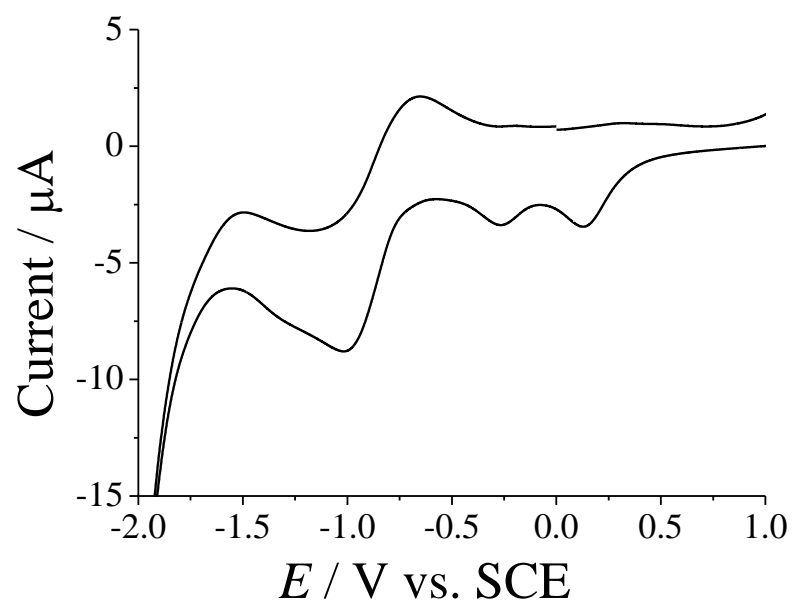


Fig. S10 The cyclic voltammogram of complex **2** in DMF (0.1 M TBAP) showing the cathodic and anodic peaks.

Table S1 Cathodic and anodic peak potentials (Volt vs SCE) for complexes **1-3**.

Complex	E_{pc1}	E_{pc2}	E_{pa1}	E_{pa2}	E_{pa3}
1	-1.51	-0.66	-1.01	-0.27	0.13
2	-0.74	-0.14	-1.14	-0.23	0.19
3	-0.89	0.49	-1.27	0.21	-0.52

Note: E_{pc} and E_{pa} are the cathodic and anodic peak potentials, respectively.

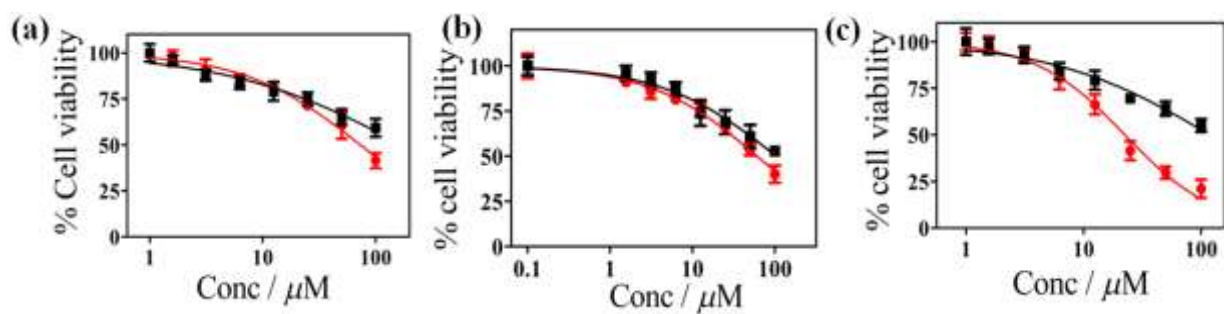


Fig. S11 Cell viability plots showing the photocytotoxicity of the complexes **1** (in a), **2** (in b) and **3** (in c) in visible light (red circles) and dark (black squares) in HeLa cells on 4 h incubation in dark followed by exposure to visible light (400-700 nm, 10 J cm^{-2}) for 1 h, as determined from the MTT assay.