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)$_2$](NO$_3$) (complex 1).
Fig. S2 The IR spectrum of [Fe(tsc-acpy)_2](NO_3) (complex 2).
**Fig. S3** The IR spectrum of \([\text{Fe(tsc-\text{VB}_6)}_2](\text{NO}_3)\) (complex 3).
Fig. S4 The ESI-MS spectrum of $[\text{Fe(tsc-py)}_2](\text{NO}_3)$ (complex 1) in 10% aqueous methanol showing the $[\text{M}-(\text{NO}_3)]^{+}$ peak.
Fig. S5 The isotopic distribution pattern for the $[\text{M}-(\text{NO}_3^-)]^+$ peak of $[\text{Fe(tsc-py)}_2](\text{NO}_3)$ (complex 1) in the ESI-MS spectrum shown in Fig. S4.
Fig. S6 The ESI-MS spectrum of [Fe(tsc-acpy)$_2$](NO$_3$) (complex 2) in 10% aqueous methanol showing the [M-(NO$_3$)]$^+$ peak.

Fig S7 The isotopic distribution pattern for the [M-(NO$_3$)]$^+$ peak of [Fe(tsc-acpy)$_2$](NO$_3$) (complex 2) in the ESI-MS spectrum shown in Fig. S6.
Fig. S8 The ESI-MS spectrum of \([\text{Fe(tsc-VB}_6\text{)}_2](\text{NO}_3)\) (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.

<table>
<thead>
<tr>
<th>Complex</th>
<th>$E_{pc1}$</th>
<th>$E_{pc2}$</th>
<th>$E_{pa1}$</th>
<th>$E_{pa2}$</th>
<th>$E_{pa3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-1.51</td>
<td>-0.66</td>
<td>-1.01</td>
<td>-0.27</td>
<td>0.13</td>
</tr>
<tr>
<td>2</td>
<td>-0.74</td>
<td>-0.14</td>
<td>-1.14</td>
<td>-0.23</td>
<td>0.19</td>
</tr>
<tr>
<td>3</td>
<td>-0.89</td>
<td>0.49</td>
<td>-1.27</td>
<td>0.21</td>
<td>-0.52</td>
</tr>
</tbody>
</table>

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.