

## Electronic Supporting Information (ESI†)

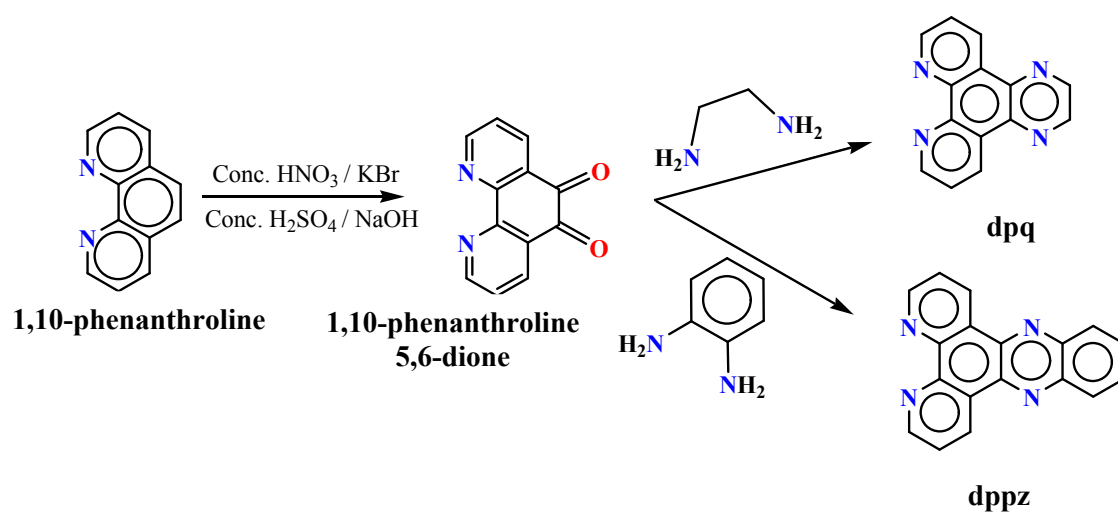
for

### **Remarkable visible light-triggered cytotoxicity of mitochondria targeting mixed-ligand cobalt(III) complexes of curcumin and phenanthroline bases binding to human serum albumin**

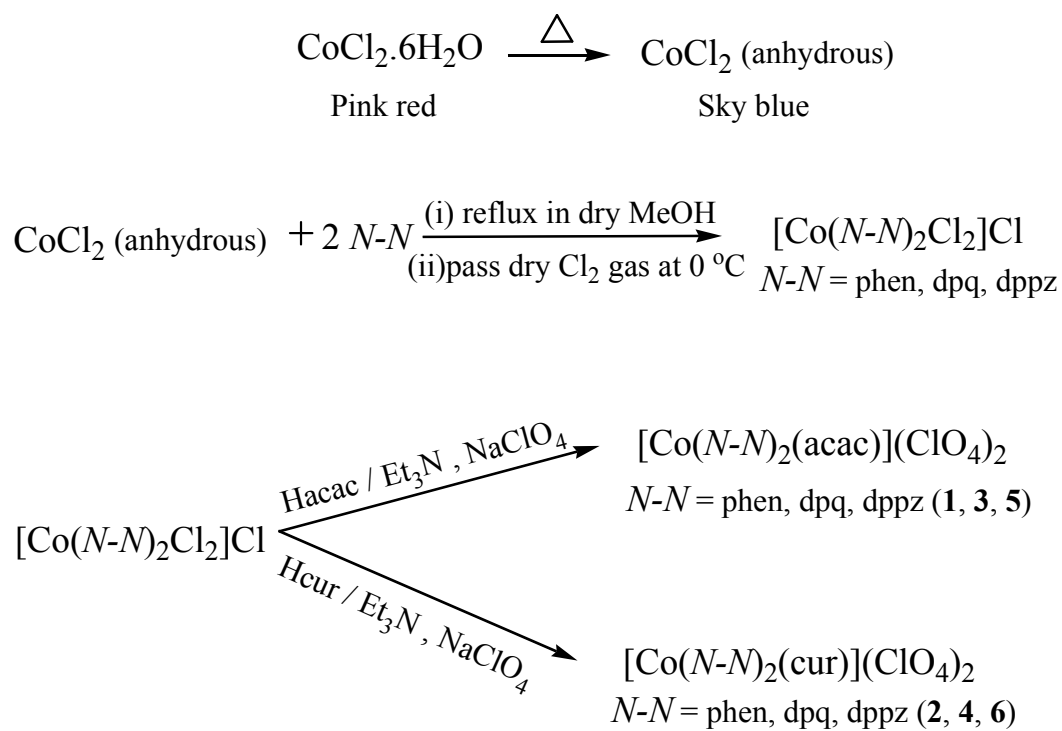
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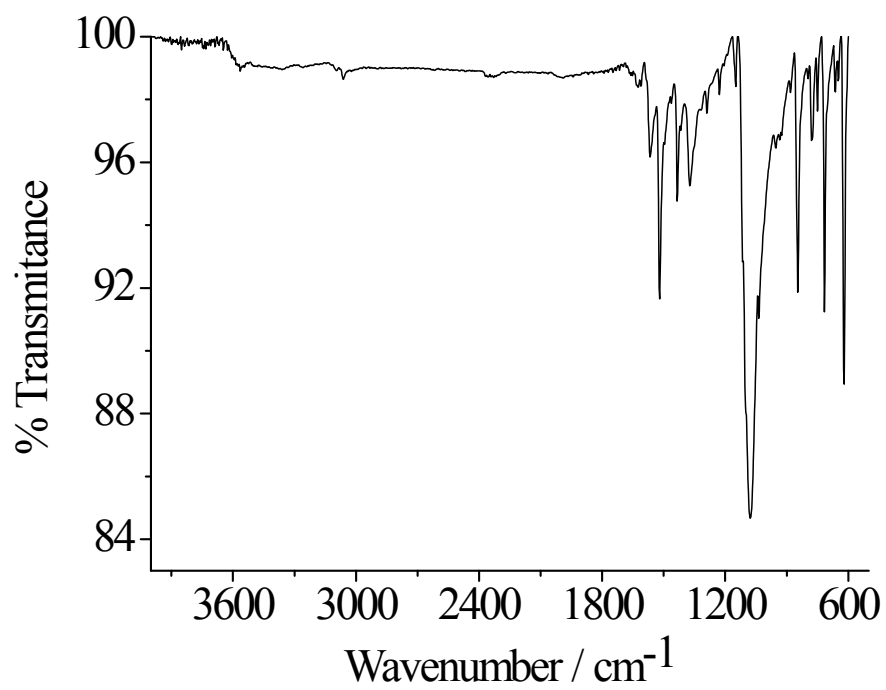
<sup>b</sup> Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore-560 012, India. [E-mail: [samya@ipc.iisc.ernet.in](mailto:samya@ipc.iisc.ernet.in); Tel: +91-80-22932240].



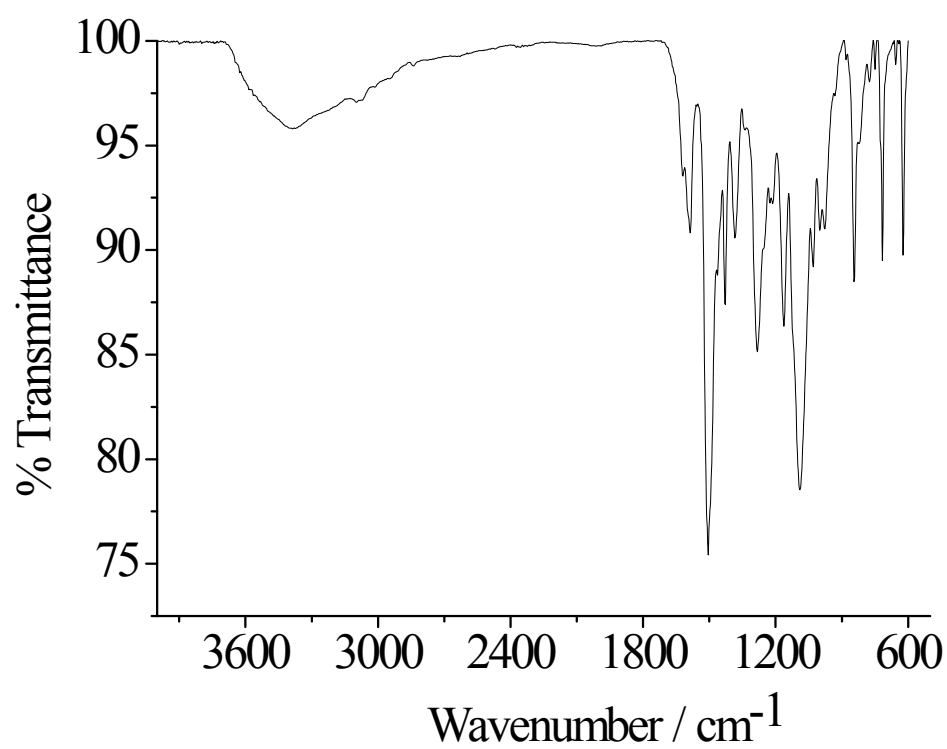
**Figure S1.** Schematic representation showing the synthetic route to dpq and dppz ligands.



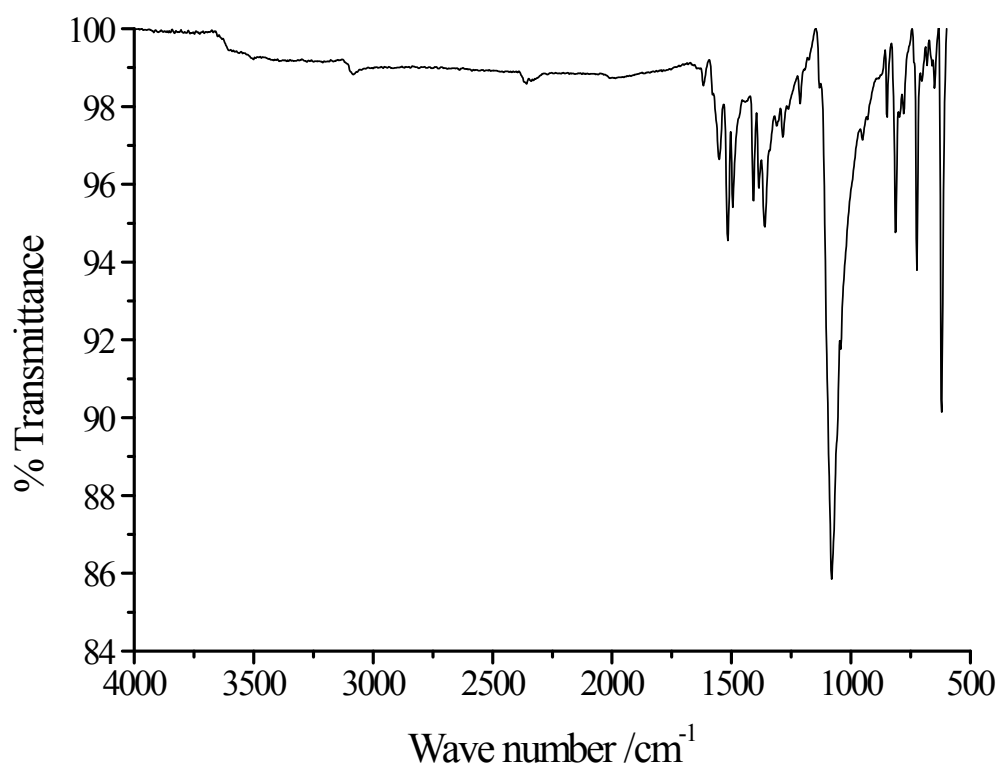
**Figure S2.** A generalized reaction scheme showing the syntheses of complexes **1–6**.



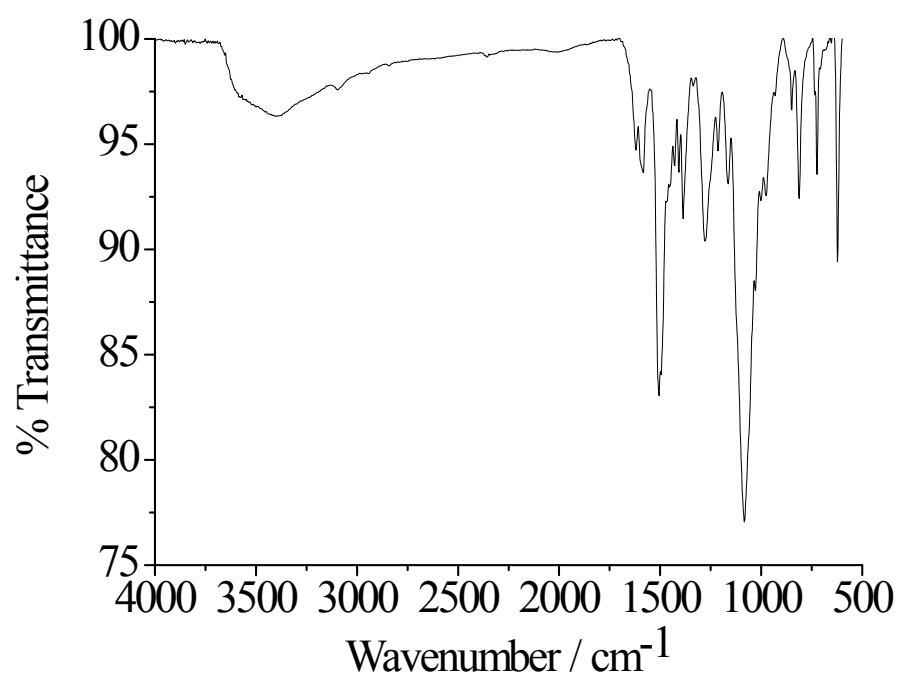
**Figure S3.** The IR spectrum of  $[\text{Co}(\text{phen})_2(\text{acac})](\text{ClO}_4)_2$  (**1**).



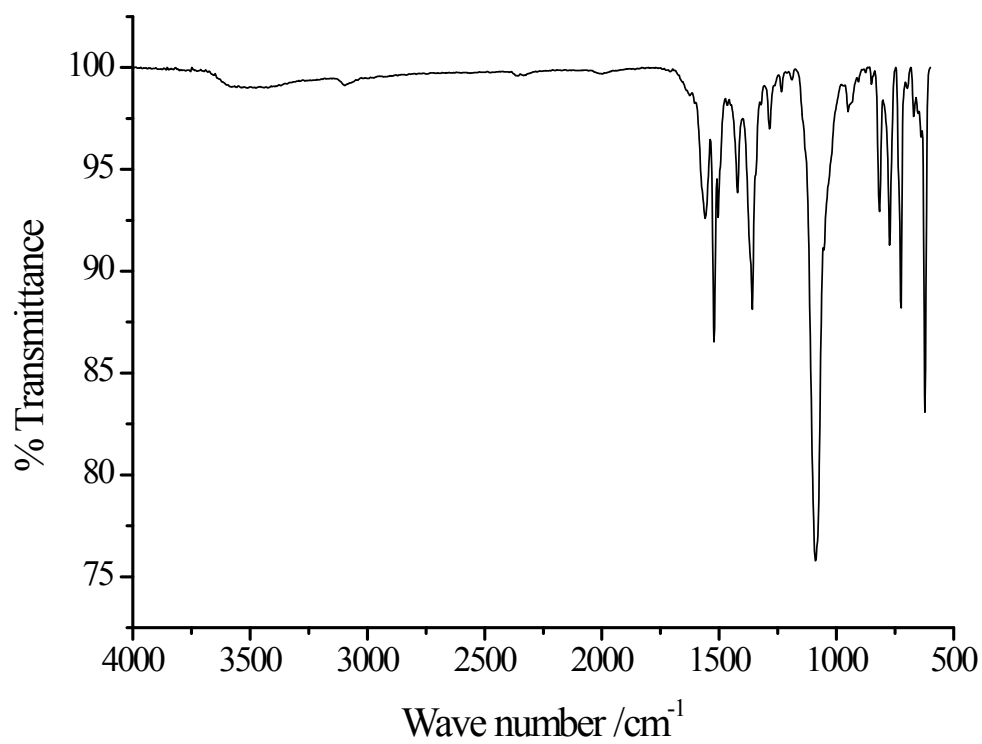
**Figure S4.** The IR spectrum of  $[\text{Co}(\text{phen})_2(\text{cur})](\text{ClO}_4)_2$  (**2**).



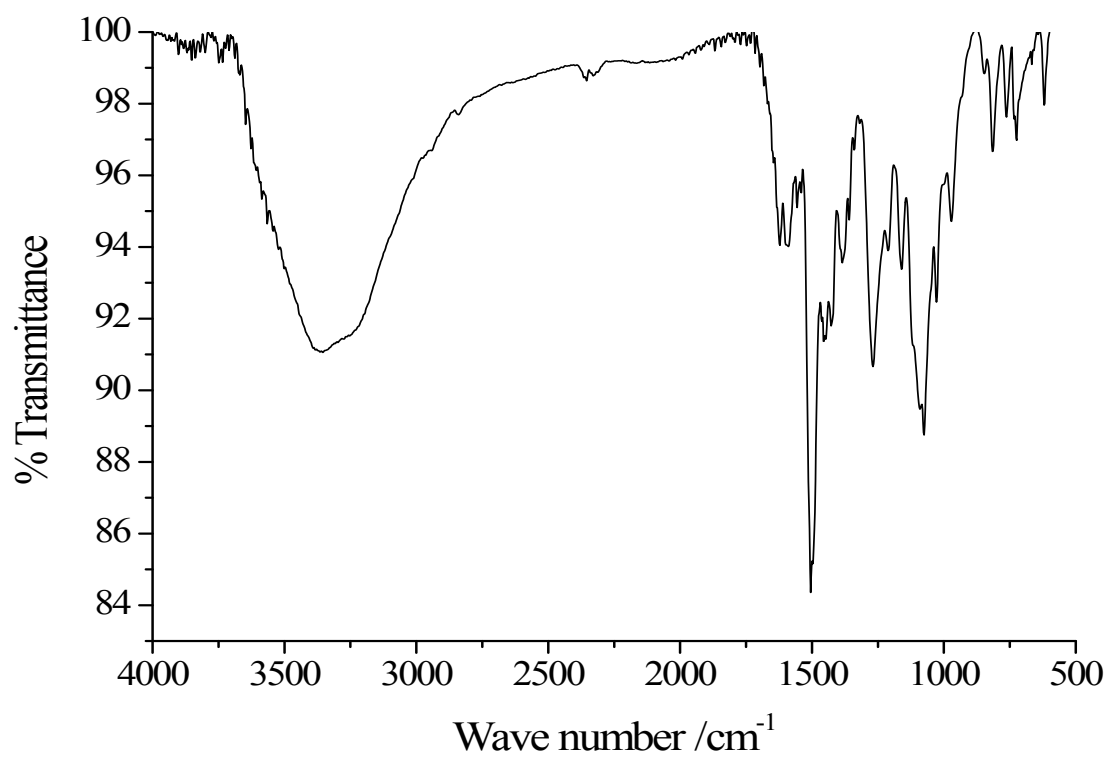
**Figure S5.** The IR spectrum of  $[\text{Co}(\text{dpq})_2(\text{acac})](\text{ClO}_4)_2$  (**3**).



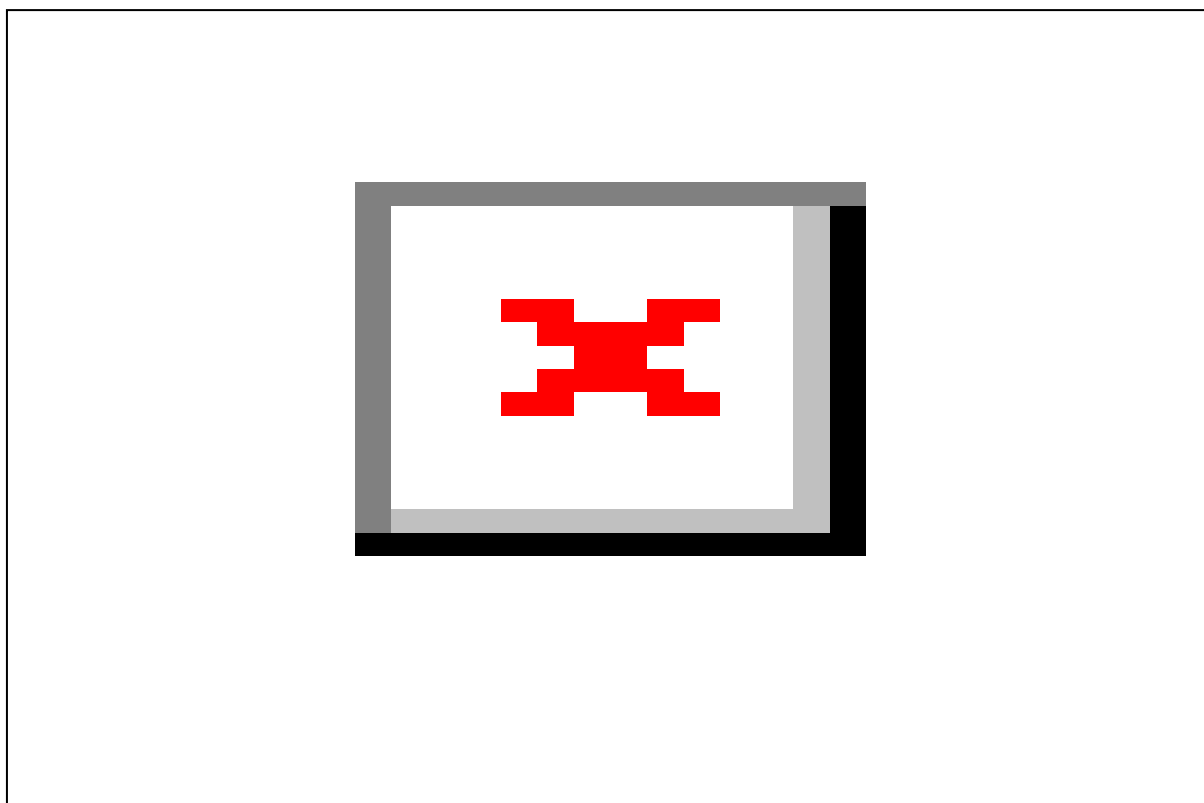
**Figure S6.** The IR spectrum of  $[\text{Co}(\text{dpq})_2(\text{cur})](\text{ClO}_4)_2$  (**4**)



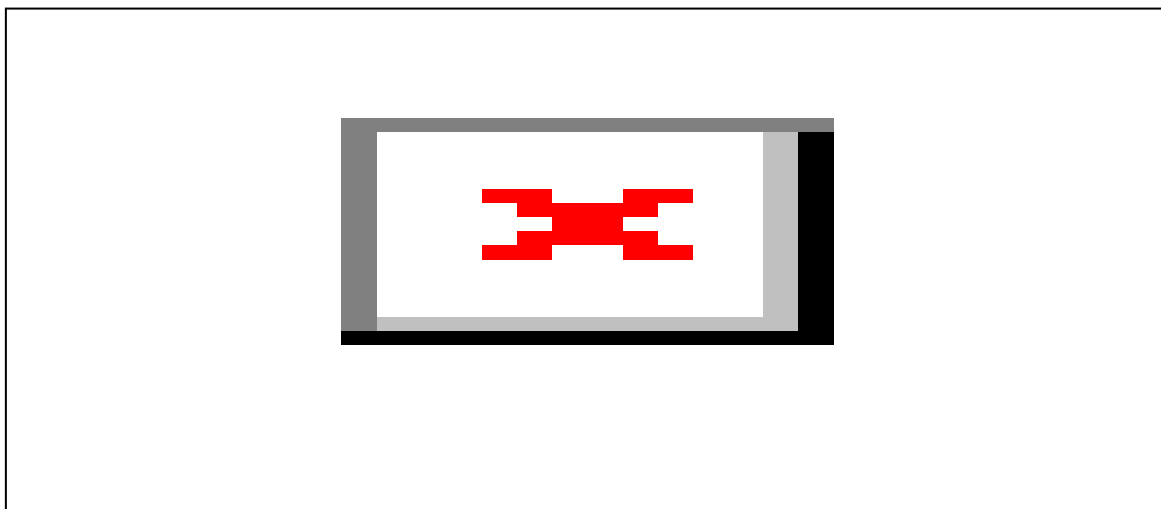
**Figure S7.** The IR spectrum of  $[\text{Co}(\text{dppz})_2(\text{acac})](\text{ClO}_4)_2$  (**5**).



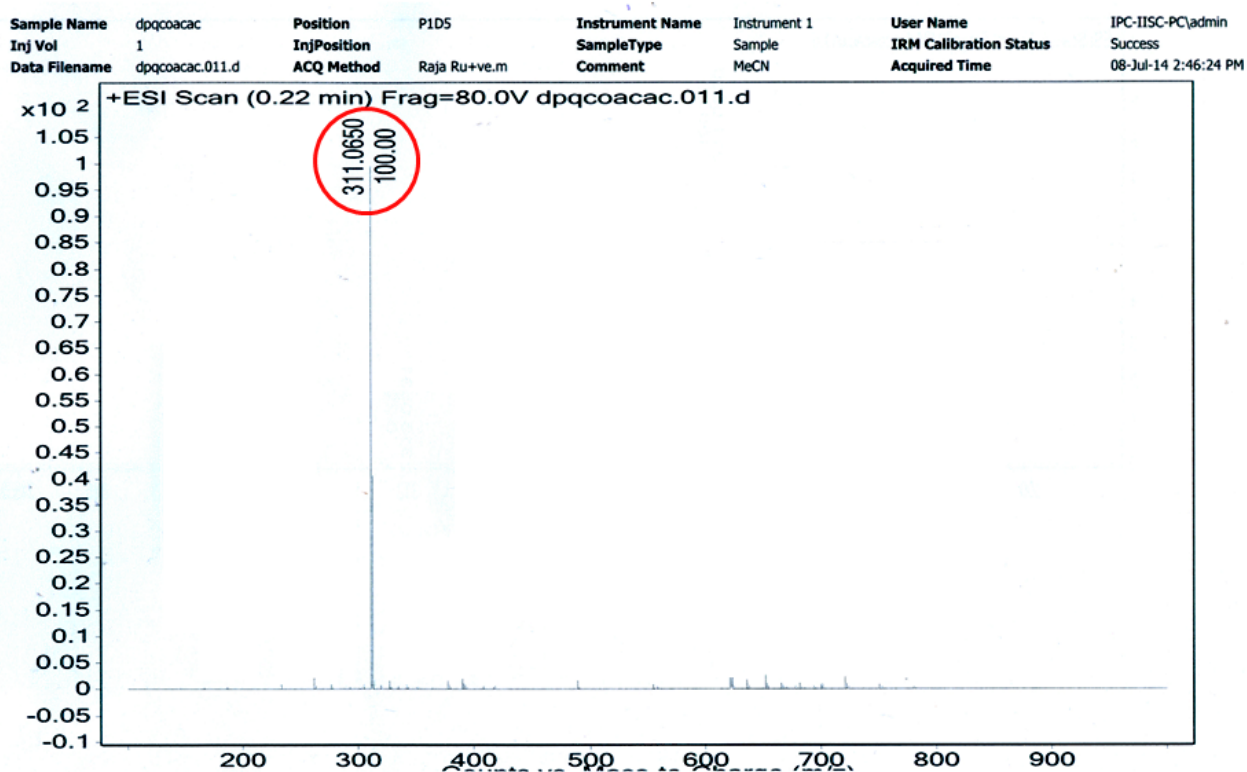
**Figure S8.** The IR spectrum of  $[\text{Co}(\text{dppz})_2(\text{cur})](\text{ClO}_4)_2$  (**6**).



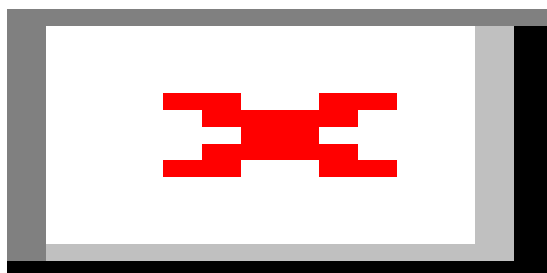
**Figure S9.** The ESI-MS spectrum of  $[\text{Co}(\text{phen})_2(\text{cur})](\text{ClO}_4)_2$  (**2**) in 5% aqueous acetonitrile showing the  $[\text{M}-2\text{ClO}_4^-]^{2+}$  peak.



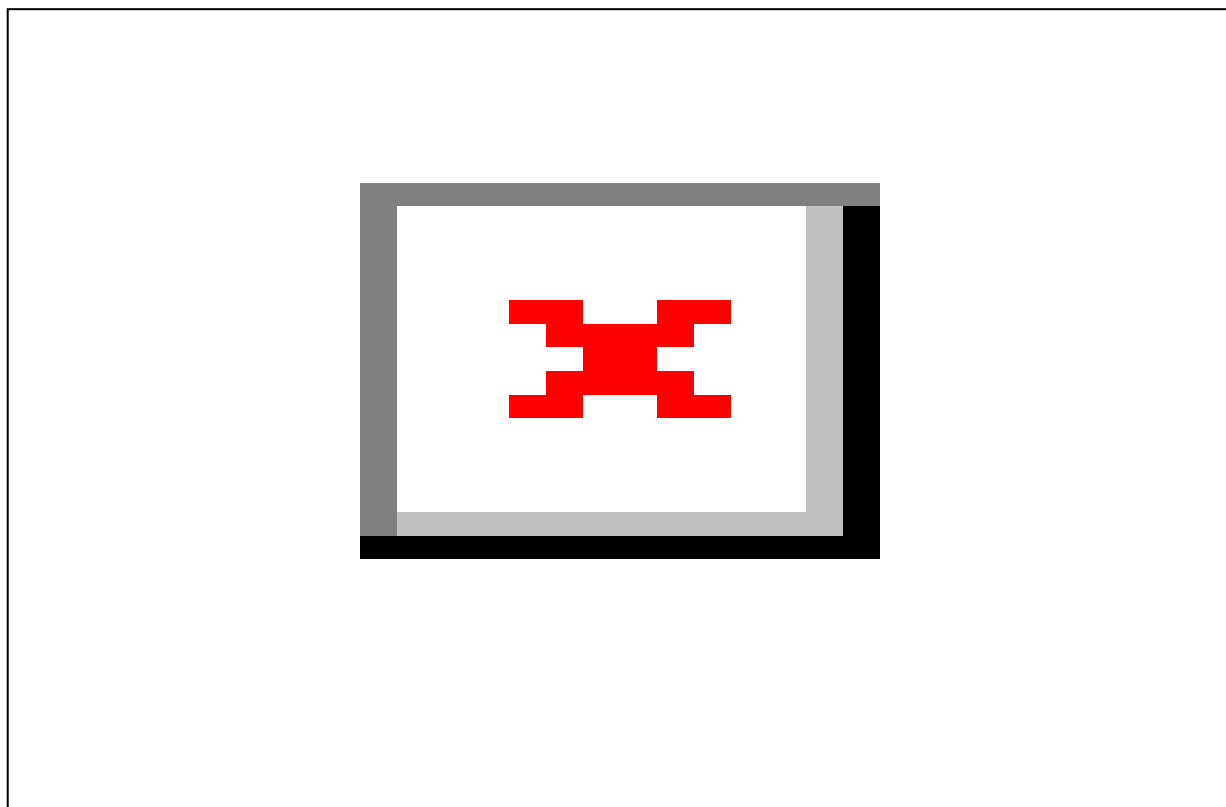
**Figure S10.** The isotopic distribution pattern for the  $[M-2ClO_4]^{2+}$  peak of  $[Co(phen)_2(cur)](ClO_4)_2$  (**2**) in the ESI-MS spectrum shown in Figure S9.



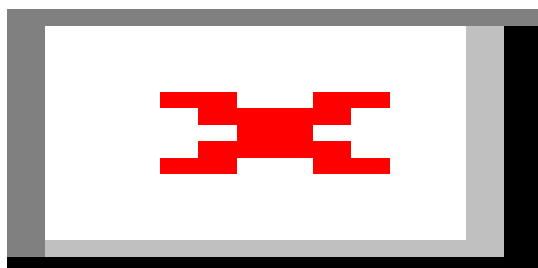
**Figure S11.** The ESI-MS spectrum of  $[\text{Co}(\text{dpq})_2(\text{acac})](\text{ClO}_4)_2$  (**3**) in 5% aqueous acetonitrile showing the  $[\text{M}-2\text{ClO}_4]^{2+}$  peak.



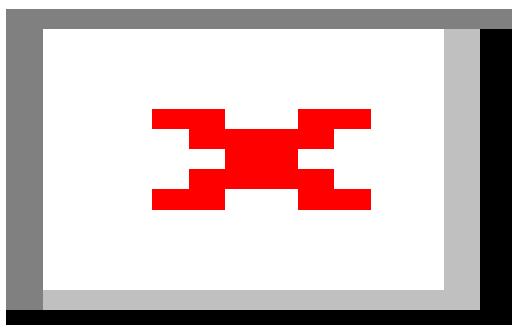
**Figure S12.** The isotopic distribution pattern for the  $[M-2\text{ClO}_4]^{2+}$  peak of  $[\text{Co}(\text{dpq})_2(\text{acac})](\text{ClO}_4)_2$  (**3**) in the ESI-MS spectrum shown in Figure S11.



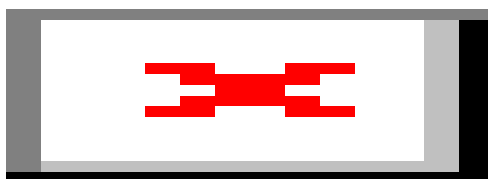
**Figure S13.** The ESI-MS spectrum of  $[\text{Co}(\text{dpq})_2(\text{cur})](\text{ClO}_4)_2$  (**4**) in 5% aqueous acetonitrile showing the  $[\text{M}-2\text{ClO}_4^-]^{2+}$  peak.



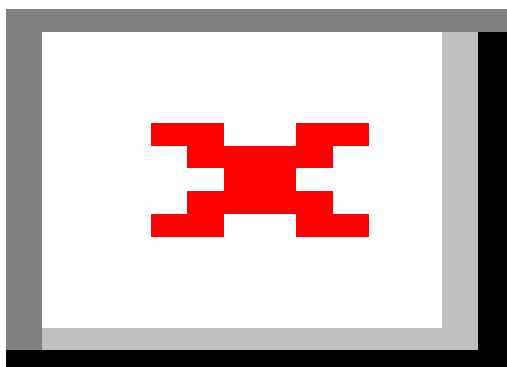
**Figure S14.** The isotopic distribution pattern for the  $[M-2\text{ClO}_4]^{2+}$  peak of  $[\text{Co}(\text{dpq})_2(\text{cur})](\text{ClO}_4)_2$  (**4**) in the ESI-MS spectrum shown in Figure S13.



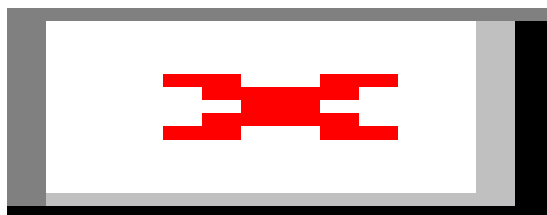
**Figure S15.** The ESI-MS spectrum of  $[\text{Co}(\text{dppz})_2(\text{acac})](\text{ClO}_4)_2$  (**5**) in 5% aqueous acetonitrile showing the  $[\text{M}-2\text{ClO}_4]^{2+}$  peak.



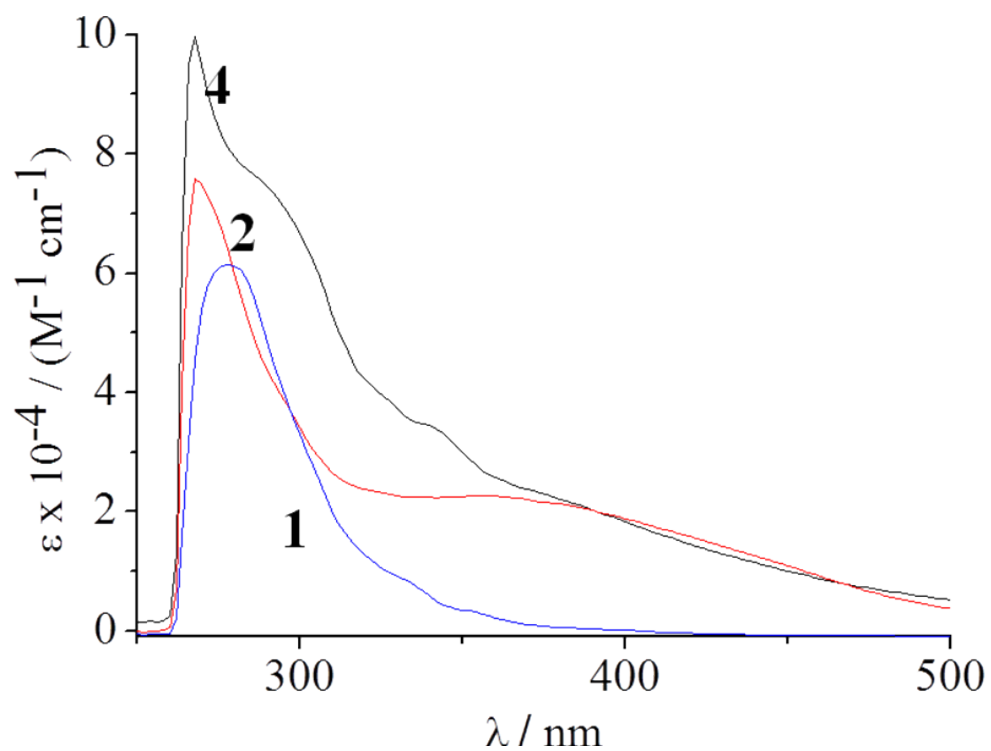
**Figure S16.** The isotopic distribution pattern for the  $[M-2\text{ClO}_4^-]^{2+}$  peak of  $[\text{Co}(\text{dppz})_2(\text{acac})](\text{ClO}_4)_2$  (**5**) in the ESI-MS spectrum shown in Figure S15.



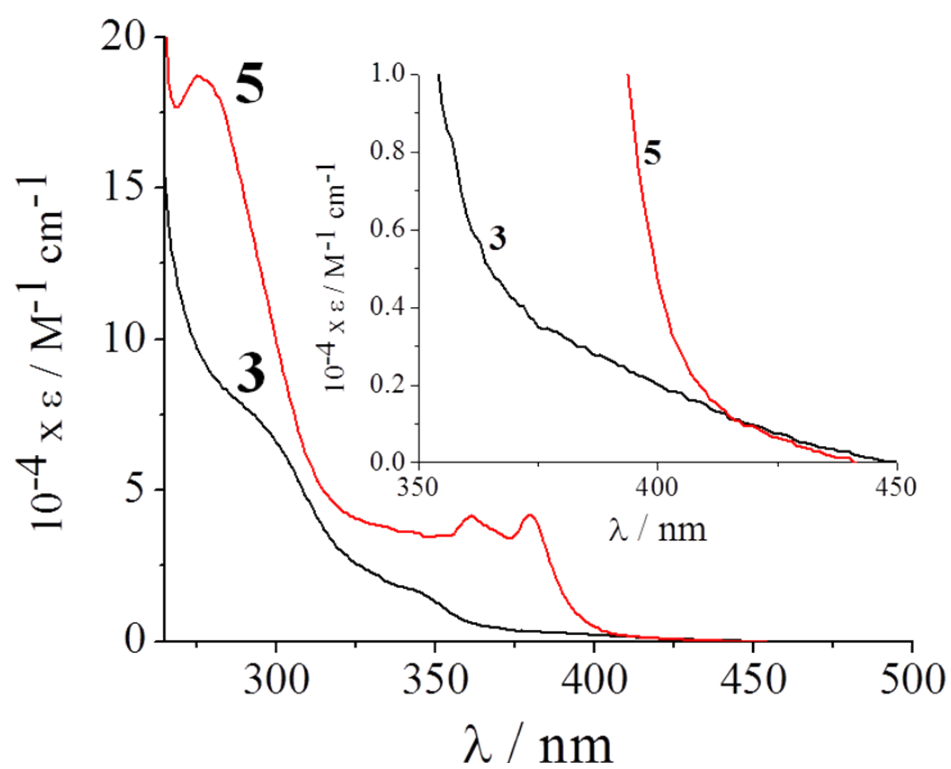
**Figure S17.** The ESI-MS spectrum of  $[\text{Co}(\text{dppz})_2(\text{cur})](\text{ClO}_4)_2$  (**6**) in 5% aqueous acetonitrile showing the  $[\text{M}-2\text{ClO}_4]^{2+}$  peak.



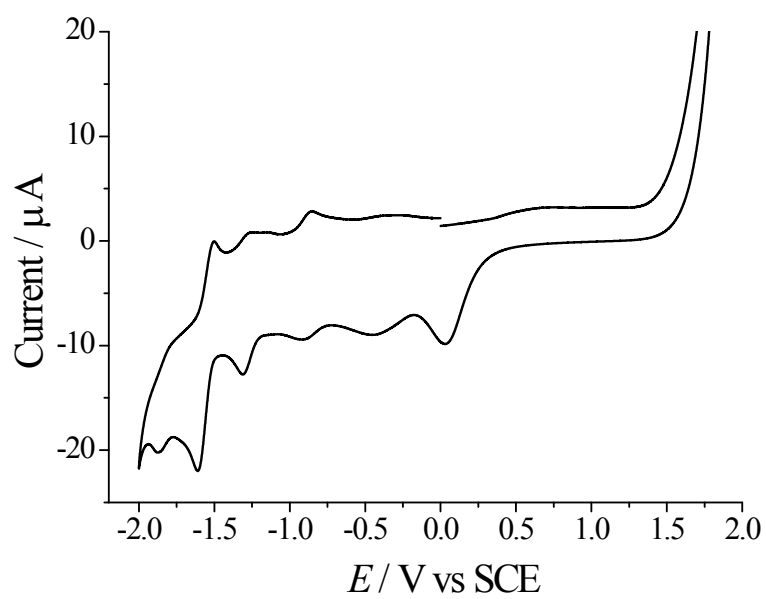
**Figure S18.** The isotopic distribution pattern for the  $[M-2\text{ClO}_4]^{2+}$  peak of  $[\text{Co}(\text{dppz})_2(\text{cur})](\text{ClO}_4)_2$  (**6**) in the ESI-MS spectrum shown in Figure S17.



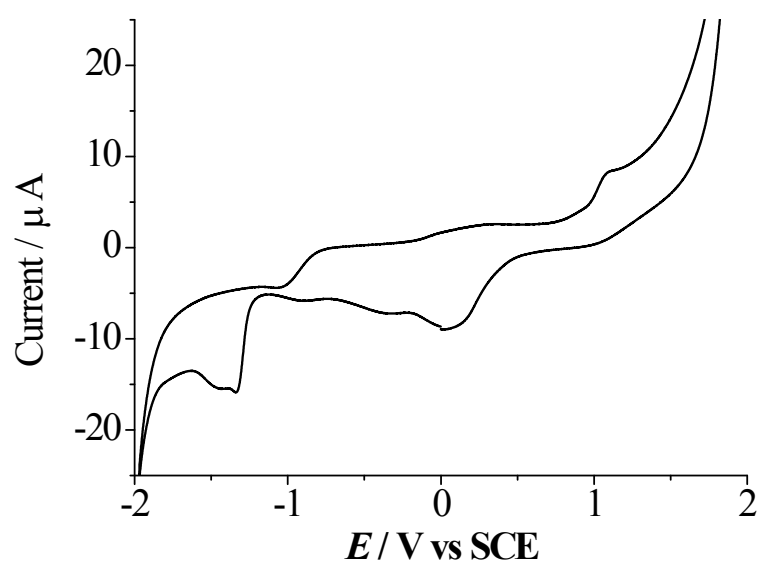
**Figure S19.** The absorption spectra of complexes **1**, **2**, and **4** in 5% aqueous DMF. Note that the absorption spectra of complexes **2** and **4** extend up to 500 nm.



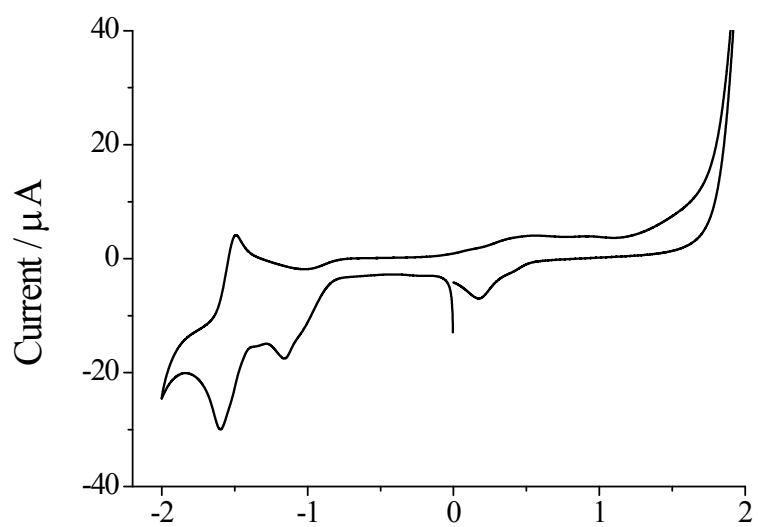
**Figure S20.** The electronic absorption spectra of complexes **3** and **5**. The inset depicts magnified portions of their spectra indicating that the spectral tails enter into the visible region.



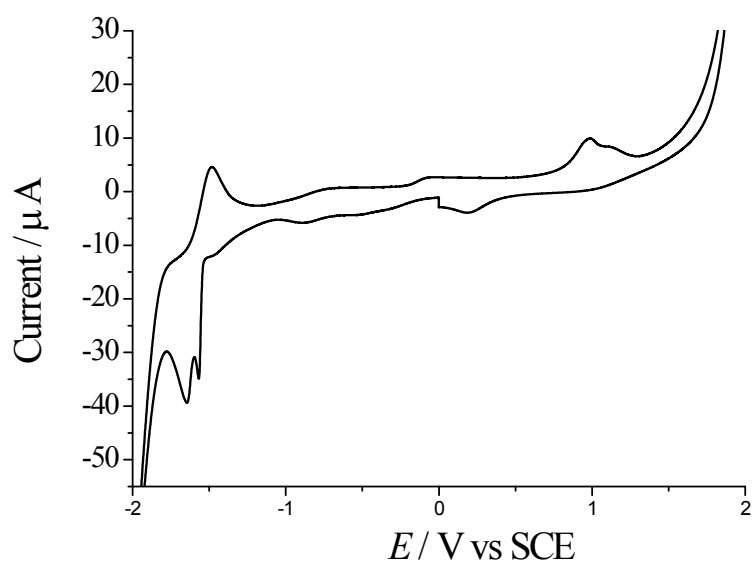
**Figure S21.** The cyclic voltammogram of **1** in DMF (0.1 M TBAP) showing the cathodic and anodic peaks.



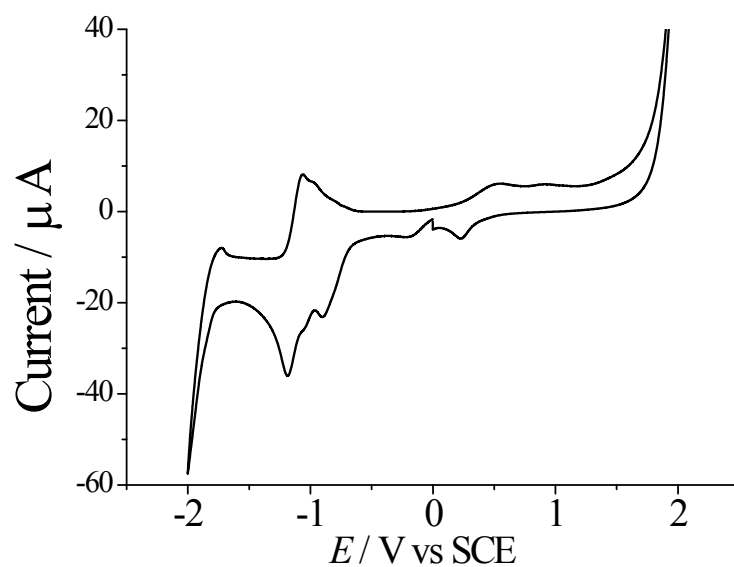
**Figure S22.** The cyclic voltammogram of **2** in DMF (0.1 M TBAP) showing the cathodic and anodic peaks.



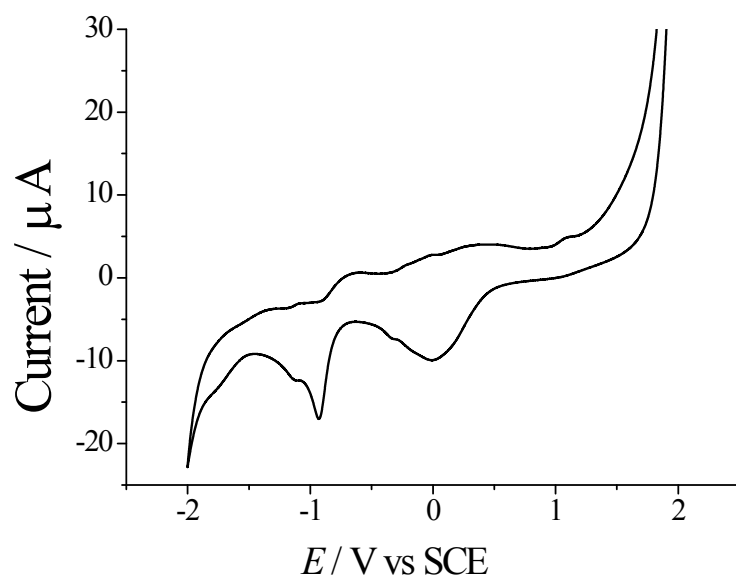
**Figure S23.** The cyclic voltammogram of **3** in DMF (0.1 M TBAP) showing the cathodic and anodic peaks.



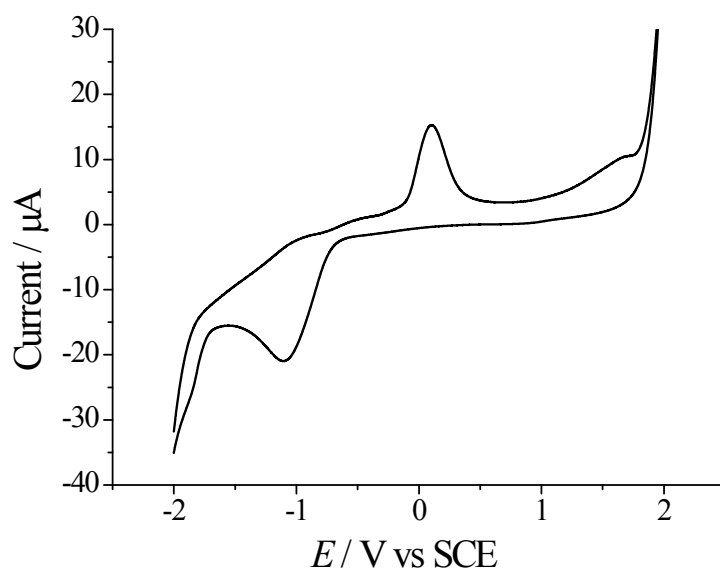
**Figure S24.** The cyclic voltammogram of **4** in DMF (0.1 M TBAP) showing the cathodic and anodic peaks.



**Figure S25.** The cyclic voltammogram of **5** in DMF (0.1 M TBAP) showing the cathodic and anodic peaks.



**Figure S26.** The cyclic voltammogram of **6** in DMF (0.1 M TBAP) showing the cathodic and anodic peaks.



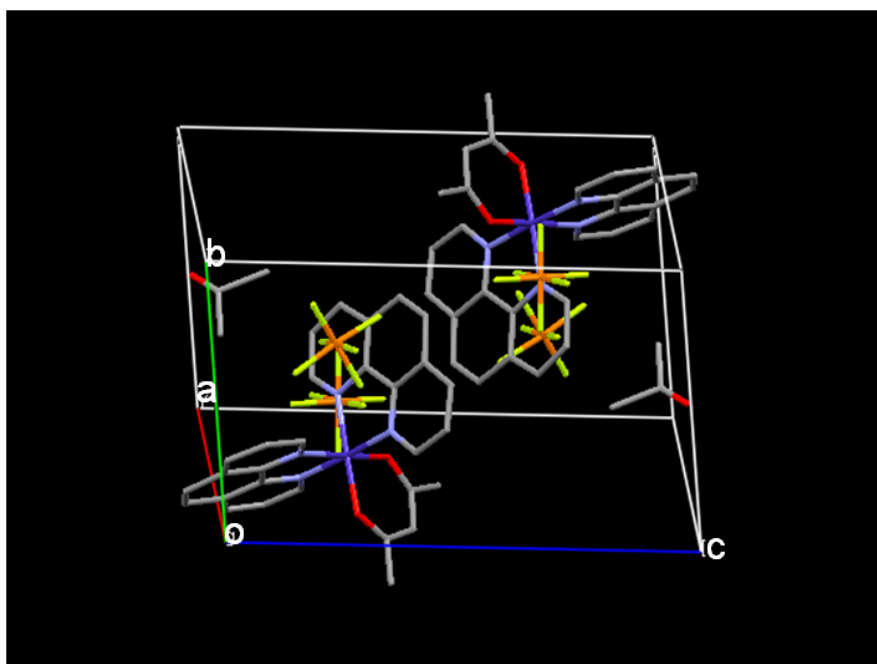
**Figure S27.** The cyclic voltammogram of curcumin in DMF (0.1 M TBAP) showing the cathodic and anodic peaks.

**Table S1** Cathodic and anodic peak potentials (Volt vs SCE) for complexes **1-6** and the curcumin ligand.

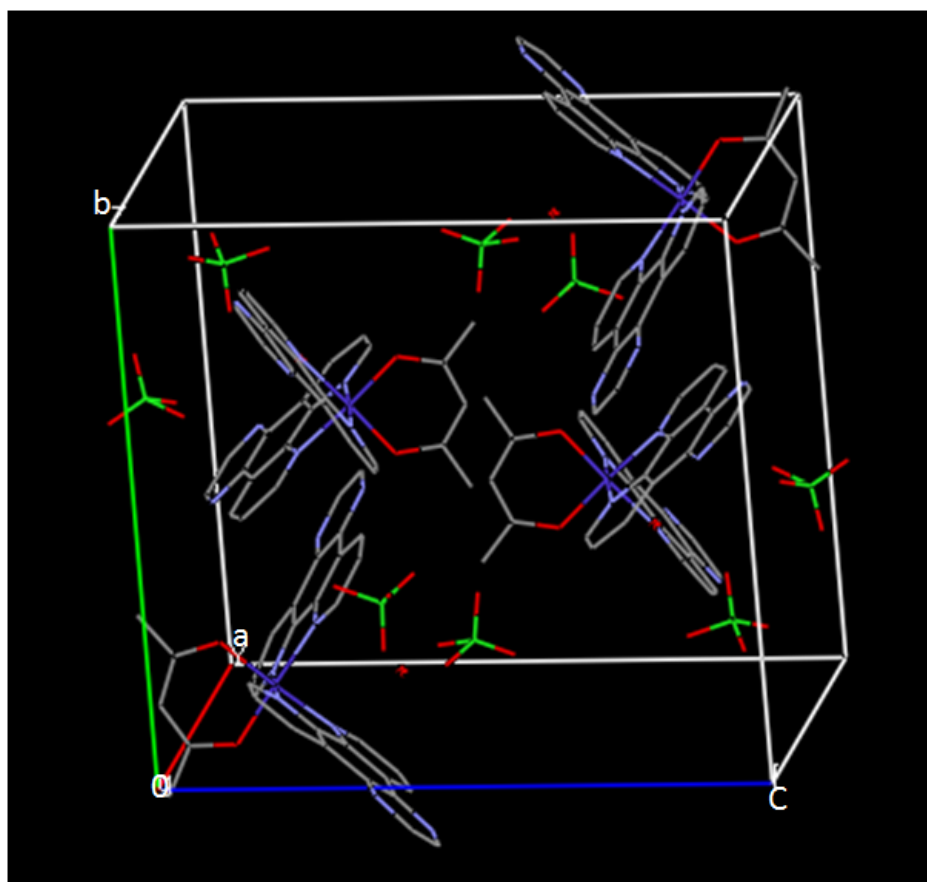
| Complex  | $E_{pc1}$ | $E_{pc2}$ | $E_{pc3}$ | $E_{pa1}$ | $E_{pa2}$ | $E_{pa3}$ | $E_{pa4}$ | $E_{pa5}$ | $E_{pa6}$ |
|----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| <b>1</b> | -1.50     | -1.25     | -0.86     | -1.87     | -1.61     | -1.30     | -0.90     | -0.43     | 0.03      |
| <b>2</b> | -0.80     | 1.08      | -         | -1.33     | 0.06      | -         | -         |           |           |
| <b>3</b> | -1.50     | -         | -         | -1.60     | -1.15     | 0.18      | -         | -         | -         |
| <b>4</b> | -1.50     | 0.98      | -         | 1.64      | 0.20      | -         | -         | -         | -         |
| <b>5</b> | -1.06     | 0.51      | -         | -1.18     | -0.90     | 0.24      | -         | -         | -         |
| <b>6</b> | -0.65     | 1.10      | -         | -0.93     | 0.00      | -         | -         | -         | -         |
| Curcumin | 0.11      | -         | -         | -1.11     | -         | -         | -         | -         | -         |

**Notes:**

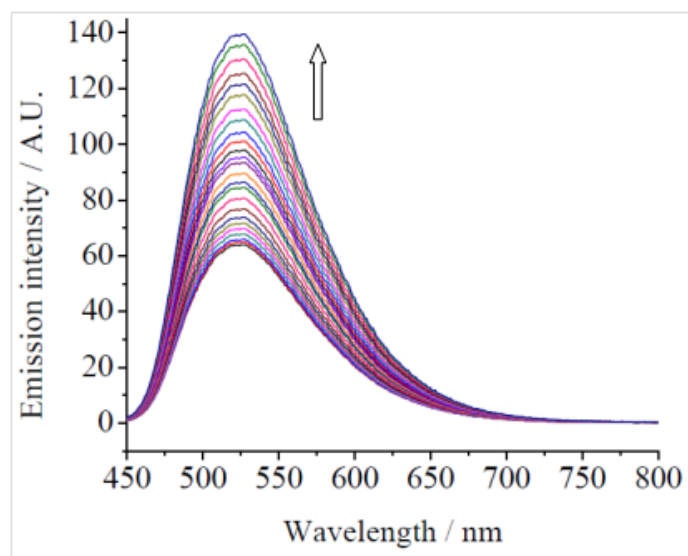
1.  $E_{pc}$  and  $E_{pa}$  are the cathodic and anodic peak potentials, respectively.
2. The cyclic voltammograms of the dpq and dppz ligands in DMF (0.1 M TBAP) were previously reported in the literature.<sup>39(c)</sup>



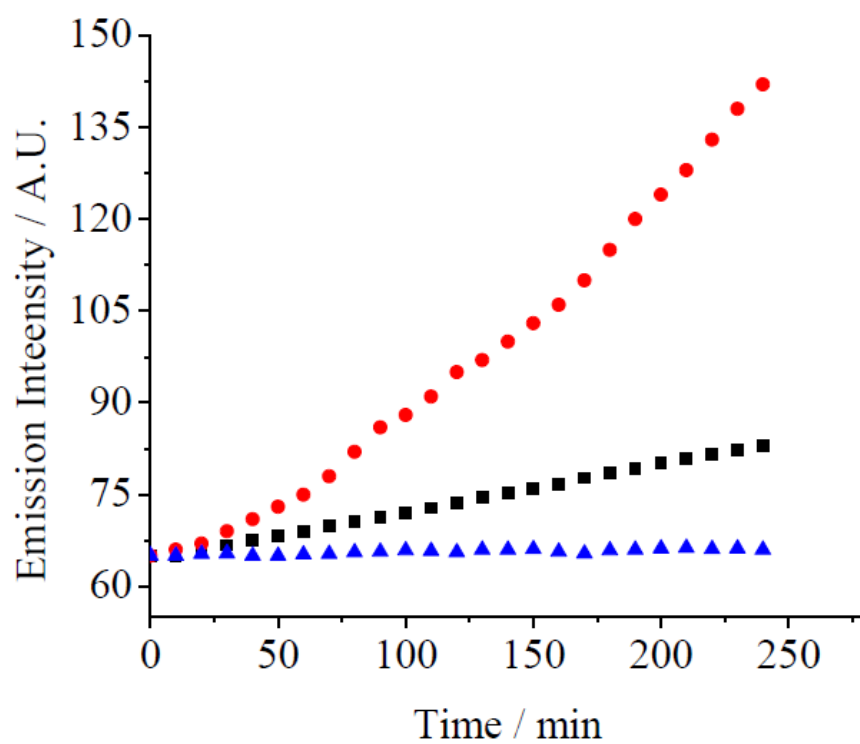
**Figure S28.** The unit cell packing diagram of  $[\text{Co}(\text{phen})_2(\text{acac})](\text{PF}_6)_2 \cdot \text{acetone}$  (**1a.acetone**). The complex crystallized in the Triclinic  $P\bar{1}$  space group with  $Z = 2$ .



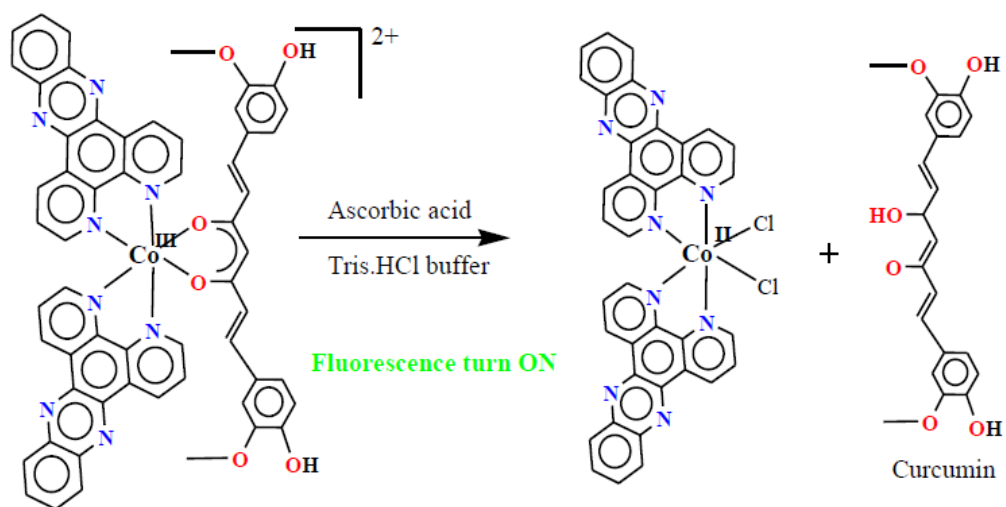
**Figure S29.** The unit cell packing diagram of  $[\text{Co}(\text{dpq})_2(\text{acac})](\text{ClO}_4)_2 \cdot \text{H}_2\text{O}$  (**3**· $\text{H}_2\text{O}$ ). The complex crystallized in the monoclinic  $P2_1/n$  space group with  $Z = 4$ .



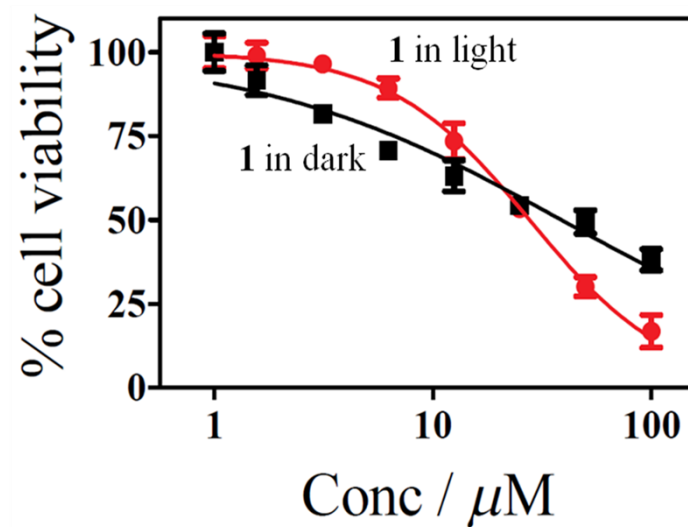
**Figure S30.** Emission spectral traces of **6** in a properly deaerated 5% aqueous DMF solution in the presence of ascorbic acid monitored up to 4 hours.



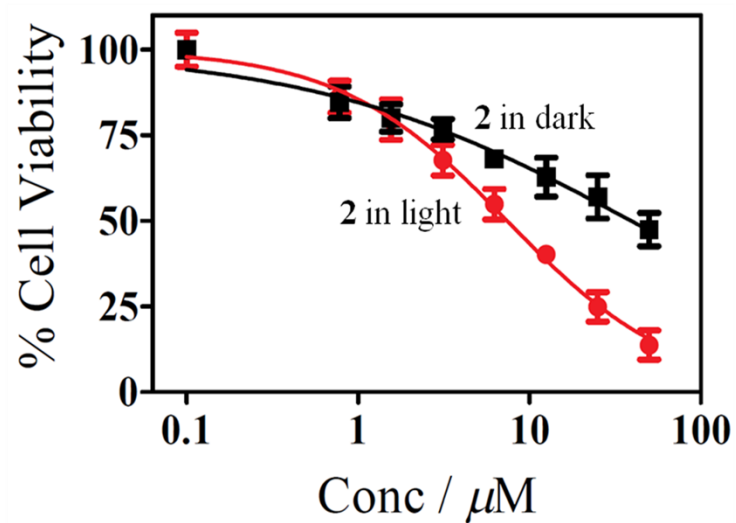
**Figure S31.** Time dependence of spectral emission intensity of **6** in 5% aqueous DMF in the presence of oxygen but no ascorbate (▲), in the presence of oxygen and ascorbate (■), and in the absence of oxygen but presence of ascorbate (●).



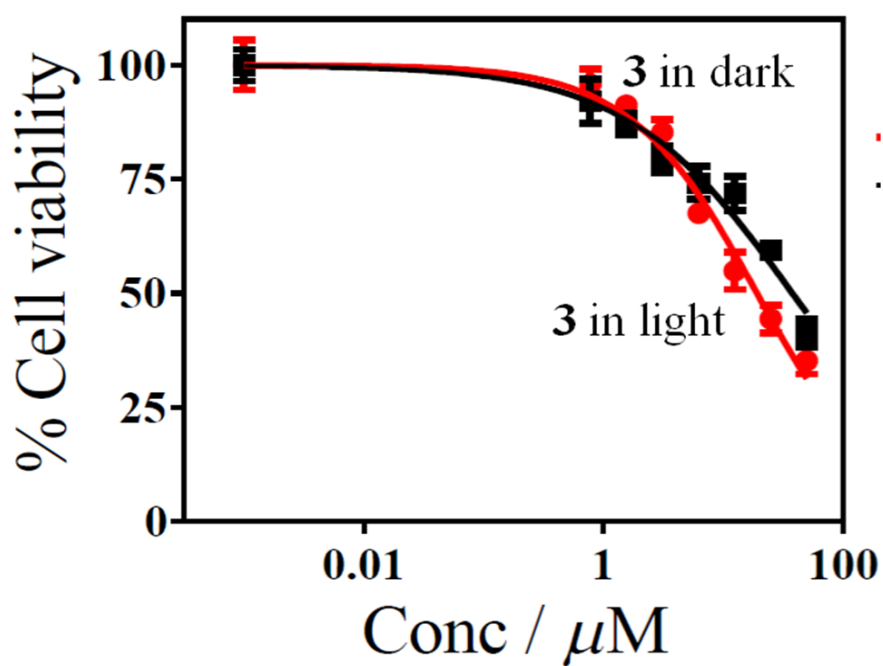
**Figure S32.** Reduction of Co(III) to Co(II) in  $[\text{Co}(\text{dppz})_2(\text{cur})]^{2+}$  by ascorbic acid in the absence of oxygen and subsequent turn-on of curcumin fluorescence resulting from the release of the curcumin ligand from the complex.



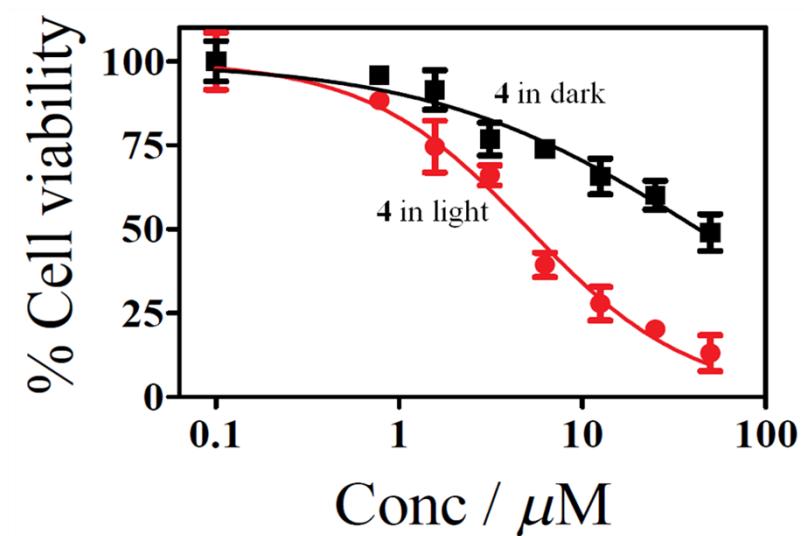
**Figure S33.** Cell viability plot showing the photocytotoxicity of **1** in light (red circles) and dark (black squares) in HeLa cells on 4 h incubation in dark followed by exposure to visible light (400-700 nm,  $10 \text{ J cm}^{-2}$ ) for 1 h, as determined from the MTT assay.



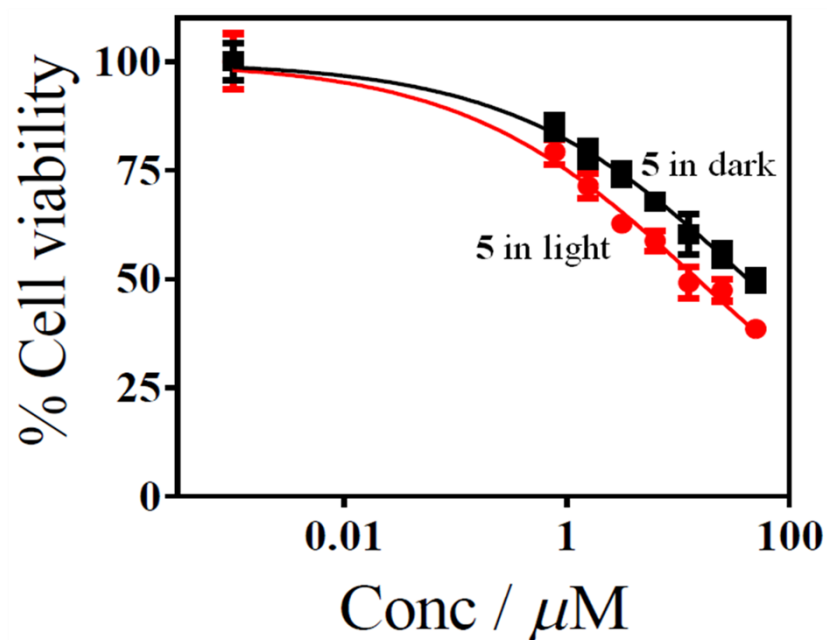
**Figure S34.** Cell viability plot showing the photocytotoxicity of **2** in light (red circles) and dark (black squares) in HeLa cells on 4 h incubation in dark followed by exposure to visible light (400-700 nm,  $10 \text{ J cm}^{-2}$ ) for 1 h, as determined from the MTT assay.



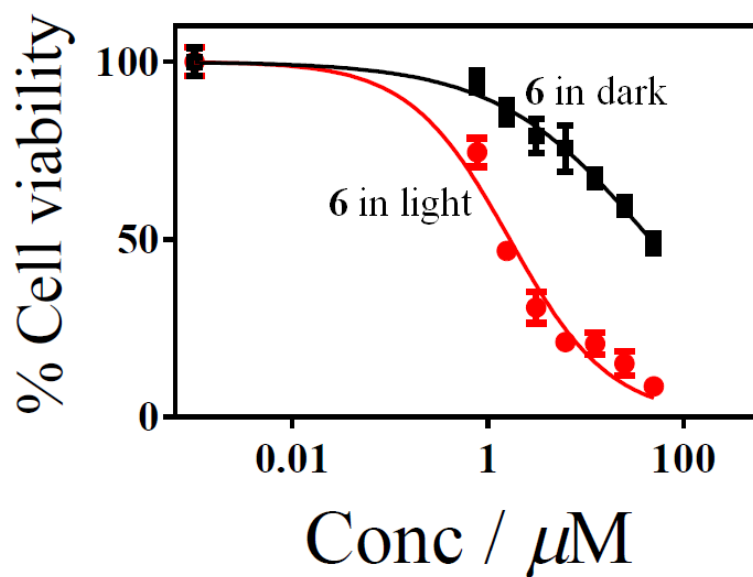
**Figure S35.** Cell viability plot showing the photocytotoxicity of **3** in light (red circles) and dark (black squares) in HeLa cells on 4 h incubation in dark followed by exposure to visible light (400-700 nm, 10 J cm<sup>-2</sup>) for 1 h, as determined from the MTT assay.



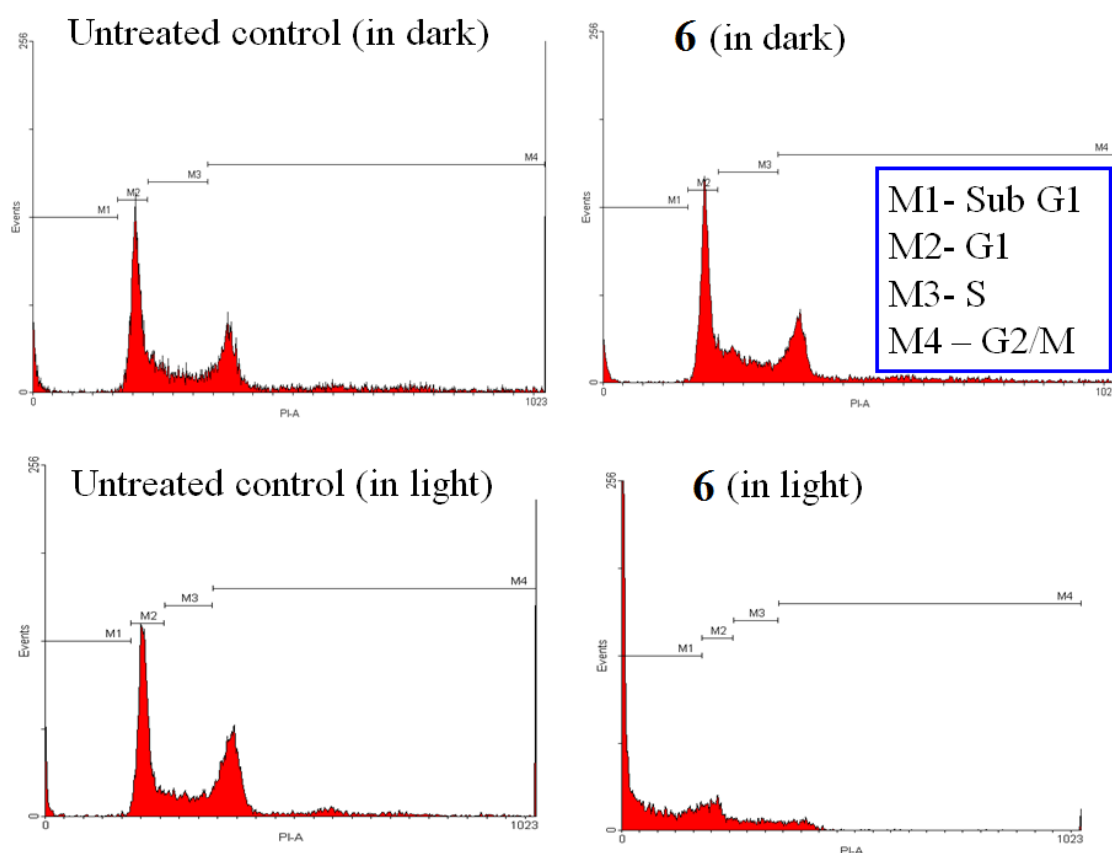
**Figure S36.** Cell viability plot showing the photocytotoxicity of **4** in light (red circles) and dark (black squares) in HeLa cells on 4 h incubation in dark followed by exposure to visible light (400-700 nm,  $10 \text{ J cm}^{-2}$ ) for 1 h, as determined from the MTT assay.



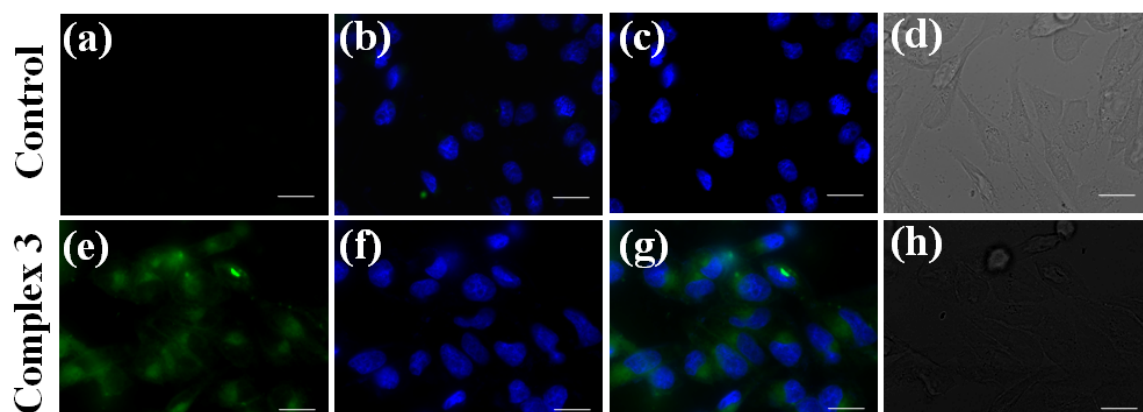
**Figure S37.** Cell viability plot showing the photocytotoxicity of **5** in light (red circles) and dark (black squares) in HeLa cells on 4 h incubation in dark followed by exposure to visible light (400-700 nm,  $10 \text{ J cm}^{-2}$ ) for 1 h, as determined from the MTT assay.



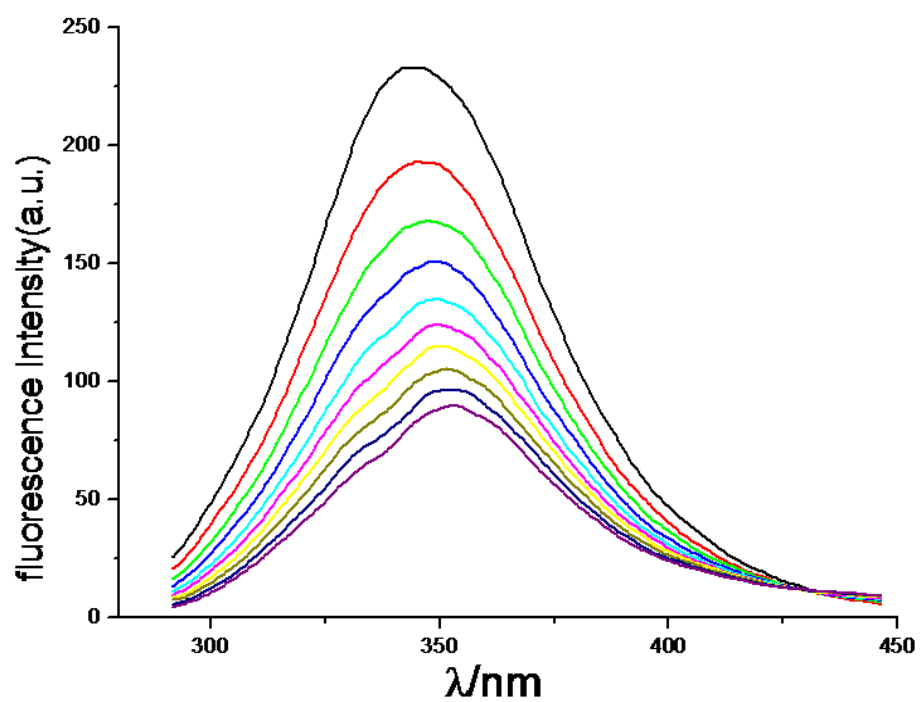
**Figure S38.** Cell viability plot showing the photocytotoxicity of **6** in light (red circles) and dark (black squares) in HeLa cells on 4 h incubation in dark followed by exposure to visible light (400-700 nm,  $10 \text{ J cm}^{-2}$ ) for 1 h, as determined from the MTT assay.



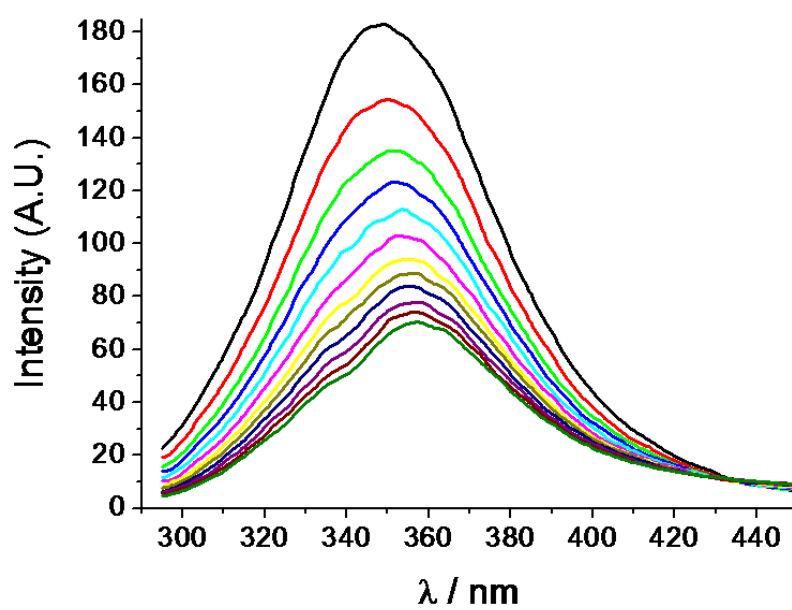
**Figure S39.** Flow cytometric analysis showing apoptotic cell death induced by **6**. Photo-exposure time = 1 h, light source = 400-700 nm visible light ( $10 \text{ J cm}^{-2}$ ), fluence rate of  $2.4 \text{ mW cm}^{-2}$ .



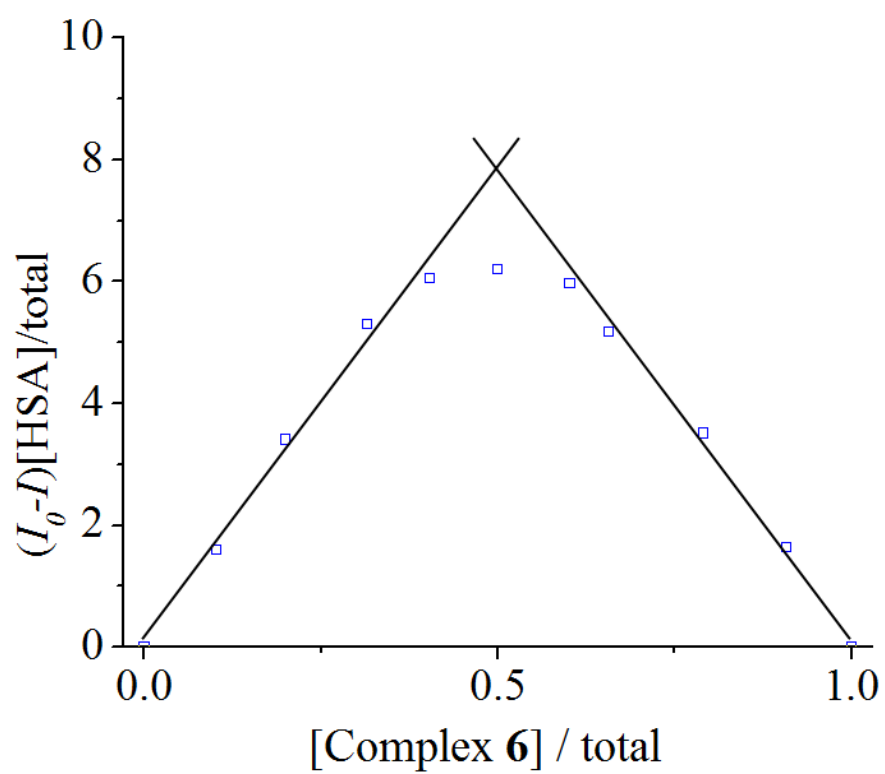
**Figure S40.** Fluorescence microscopic images of HeLa cells [control and treated with **6** (10  $\mu\text{mol}$ )] on 2 h incubation and Hoechst 33342 dye (5  $\mu\text{g m}^{-1}$ ). Panel (b) is of the control. Panel (e) shows the green emission of **6**. Panels (b, f) show the blue emission of Hoechst 33342 dye which stains the nucleus. Panels (c, g) correspond to the merged images showing cytosolic localization of the complex. Panels (d, h) show the control and complex treated bright field images. Scale bar = 20  $\mu\text{m}$ .



**Figure S41.** Emission spectral traces of human serum albumin (2  $\mu\text{M}$ ) in the presence of complex **3**.



**Figure S42.** Emission spectral traces of human serum albumin (2 μM) in the presence of complex 5.



**Figure S43.** Job plot showing 1:1 binding stoichiometry of interaction between HSA and complex 6.

**Table S2.** Computational data for the complex in **2**

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 27               | 0              | 0.000042                | -1.500024 | -0.000065 |
| 2                | 8                | 0              | -1.396327               | -0.244396 | -0.213053 |
| 3                | 8                | 0              | 1.396455                | -0.244317 | 0.212175  |
| 4                | 7                | 0              | 1.423518                | -2.887357 | 0.072275  |
| 5                | 7                | 0              | -1.423497               | -2.887307 | -0.071720 |
| 6                | 7                | 0              | 0.373536                | -1.505936 | -1.923666 |
| 7                | 7                | 0              | -0.373439               | -1.504971 | 1.923557  |
| 8                | 6                | 0              | 1.448818                | -2.300017 | -2.235243 |
| 9                | 6                | 0              | 1.909971                | -3.569945 | 1.121677  |
| 10               | 1                | 0              | 1.436037                | -3.418158 | 2.083387  |
| 11               | 6                | 0              | 2.011092                | -3.050954 | -1.158364 |
| 12               | 6                | 0              | -0.208562               | -0.768073 | -2.884773 |
| 13               | 1                | 0              | -1.055121               | -0.159740 | -2.591837 |
| 14               | 6                | 0              | 1.988595                | -2.389366 | -3.542789 |
| 15               | 6                | 0              | -3.118623               | -3.907839 | 1.384274  |
| 16               | 6                | 0              | 1.251491                | 1.089543  | 0.133027  |
| 17               | 6                | 0              | 3.118550                | -3.908728 | -1.383240 |
| 18               | 6                | 0              | -3.617855               | -4.625748 | 0.260041  |
| 19               | 1                | 0              | -4.463945               | -5.297711 | 0.374681  |
| 20               | 6                | 0              | -1.448793               | -2.298819 | 2.235506  |
| 21               | 6                | 0              | 0.271369                | -0.798150 | -4.219949 |
| 22               | 1                | 0              | -0.222177               | -0.186841 | -4.967397 |
| 23               | 6                | 0              | -0.000037               | 1.729553  | -0.000125 |
| 24               | 1                | 0              | -0.000093               | 2.813661  | 0.000046  |
| 25               | 6                | 0              | 0.208717                | -0.766721 | 2.884334  |
| 26               | 1                | 0              | 1.055383                | -0.158652 | 2.591171  |
| 27               | 6                | 0              | 3.010100                | -4.455192 | 0.986130  |
| 28               | 1                | 0              | 3.366939                | -4.987337 | 1.861119  |
| 29               | 6                | 0              | -1.909994               | -3.570368 | -1.120794 |
| 30               | 1                | 0              | -1.436038               | -3.419083 | -2.082571 |
| 31               | 6                | 0              | -1.251516               | 1.089475  | -0.133537 |
| 32               | 6                | 0              | -2.011102               | -3.050253 | 1.158992  |
| 33               | 6                | 0              | -1.988590               | -2.387501 | 3.543090  |
| 34               | 6                | 0              | 3.617741                | -4.626124 | -0.258662 |
| 35               | 1                | 0              | 4.463780                | -5.298206 | -0.372981 |
| 36               | 6                | 0              | 3.120771                | -3.263083 | -3.757649 |
| 37               | 1                | 0              | 3.541239                | -3.336249 | -4.756855 |
| 38               | 6                | 0              | 1.364566                | -1.600413 | -4.552588 |
| 39               | 1                | 0              | 1.740447                | -1.625269 | -5.571762 |
| 40               | 6                | 0              | -3.661838               | -3.991844 | 2.722177  |
| 41               | 1                | 0              | -4.511321               | -4.645801 | 2.899255  |
| 42               | 6                | 0              | -1.364525               | -1.598101 | 4.552517  |
| 43               | 1                | 0              | -1.740437               | -1.622426 | 5.571694  |
| 44               | 6                | 0              | -3.010190               | -4.455465 | -0.984828 |
| 45               | 1                | 0              | -3.367061               | -4.988008 | -1.859562 |
| 46               | 6                | 0              | -0.271250               | -0.796101 | 4.219513  |
| 47               | 1                | 0              | 0.222337                | -0.184470 | 4.966671  |
| 48               | 6                | 0              | 3.661744                | -3.993421 | -2.721109 |
| 49               | 1                | 0              | 4.511183                | -4.647519 | -2.897878 |
| 50               | 6                | 0              | -3.120826               | -3.261037 | 3.758365  |
| 51               | 1                | 0              | -3.541303               | -3.333694 | 4.757605  |
| 52               | 1                | 0              | -2.296324               | 2.971927  | -0.173564 |
| 53               | 1                | 0              | -3.801430               | 0.292082  | -0.406164 |
| 54               | 1                | 0              | 2.296133                | 2.972096  | 0.173415  |
| 55               | 1                | 0              | 3.801457                | 0.292313  | 0.405494  |
| 56               | 6                | 0              | -2.452271               | 1.897846  | -0.224486 |
| 57               | 6                | 0              | -3.716343               | 1.378306  | -0.360065 |
| 58               | 6                | 0              | 2.452190                | 1.898020  | 0.224122  |
| 59               | 6                | 0              | 3.716302                | 1.378541  | 0.359599  |
| 60               | 6                | 0              | -4.961895               | 2.121677  | -0.446443 |
| 61               | 6                | 0              | -5.020597               | 3.539530  | -0.387524 |
| 62               | 6                | 0              | -6.179036               | 1.404983  | -0.597363 |
| 63               | 6                | 0              | -6.231734               | 4.237153  | -0.457868 |
| 64               | 1                | 0              | -4.125566               | 4.142855  | -0.276299 |
| 65               | 6                | 0              | -7.398795               | 2.084096  | -0.670283 |
| 66               | 1                | 0              | -6.164335               | 0.319165  | -0.653543 |
| 67               | 6                | 0              | -7.443348               | 3.491212  | -0.587260 |
| 68               | 1                | 0              | -8.328362               | 1.527738  | -0.776838 |

|    |   |   |           |          |           |
|----|---|---|-----------|----------|-----------|
| 69 | 6 | 0 | 4.961835  | 2.121949 | 0.446059  |
| 70 | 6 | 0 | 5.020496  | 3.539773 | 0.387236  |
| 71 | 6 | 0 | 6.178979  | 1.405257 | 0.597077  |
| 72 | 6 | 0 | 6.231631  | 4.237478 | 0.457646  |
| 73 | 1 | 0 | 4.125446  | 4.143093 | 0.276110  |
| 74 | 6 | 0 | 7.398702  | 2.084415 | 0.670024  |
| 75 | 1 | 0 | 6.164291  | 0.319444 | 0.653302  |
| 76 | 6 | 0 | 7.443214  | 3.491536 | 0.586977  |
| 77 | 1 | 0 | 8.328292  | 1.528103 | 0.776625  |
| 78 | 8 | 0 | 8.635555  | 4.198409 | 0.605323  |
| 79 | 1 | 0 | 9.427167  | 3.625067 | 0.673599  |
| 80 | 8 | 0 | 6.147424  | 5.609529 | 0.312607  |
| 81 | 8 | 0 | -8.635611 | 4.198113 | -0.605596 |
| 82 | 1 | 0 | -9.427271 | 3.624834 | -0.673721 |
| 83 | 8 | 0 | -6.147839 | 5.609229 | -0.312547 |
| 84 | 6 | 0 | -7.067338 | 6.532958 | -1.007804 |
| 85 | 1 | 0 | -8.066055 | 6.486763 | -0.572145 |
| 86 | 1 | 0 | -6.620814 | 7.517520 | -0.858107 |
| 87 | 1 | 0 | -7.111305 | 6.296229 | -2.077773 |
| 88 | 6 | 0 | 7.067974  | 6.533484 | 1.006093  |
| 89 | 1 | 0 | 8.065926  | 6.487482 | 0.568657  |
| 90 | 1 | 0 | 6.620957  | 7.517927 | 0.857109  |
| 91 | 1 | 0 | 7.113986  | 6.296876 | 2.075999  |

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**Table S3.** Computational data for the complex in **4**

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 27               | 0              | 0.000011                | -0.998711 | 0.000022  |
| 2                | 8                | 0              | -1.351279               | 0.257181  | -0.408879 |
| 3                | 8                | 0              | 1.351298                | 0.257200  | 0.408863  |
| 4                | 7                | 0              | 1.401029                | -2.382413 | 0.273333  |
| 5                | 7                | 0              | -1.401011               | -2.382426 | -0.273198 |
| 6                | 7                | 0              | 0.639490                | -1.010196 | -1.851232 |
| 7                | 7                | 0              | -0.639480               | -1.010068 | 1.851279  |
| 8                | 6                | 0              | 1.745964                | -1.800462 | -2.013716 |
| 9                | 6                | 0              | 1.734020                | -3.057918 | 1.389844  |
| 10               | 1                | 0              | 1.126709                | -2.898317 | 2.271789  |
| 11               | 6                | 0              | 2.157152                | -2.553024 | -0.856432 |
| 12               | 6                | 0              | 0.188244                | -0.274073 | -2.886394 |
| 13               | 1                | 0              | -0.692073               | 0.330726  | -2.709583 |
| 14               | 6                | 0              | 2.445474                | -1.887278 | -3.234308 |
| 15               | 6                | 0              | -3.276968               | -3.409617 | 0.907018  |
| 16               | 6                | 0              | 1.215976                | 1.591781  | 0.323705  |
| 17               | 6                | 0              | 3.276905                | -3.409780 | -0.906855 |
| 18               | 6                | 0              | -3.618362               | -4.120094 | -0.271104 |
| 19               | 1                | 0              | -4.475158               | -4.785518 | -0.256507 |
| 20               | 6                | 0              | -1.745995               | -1.800270 | 2.013792  |
| 21               | 6                | 0              | 0.840944                | -0.306273 | -4.141687 |
| 22               | 1                | 0              | 0.452302                | 0.301319  | -4.951399 |
| 23               | 6                | 0              | 0.000043                | 2.231822  | -0.000146 |
| 24               | 1                | 0              | 0.000054                | 3.315948  | -0.000211 |
| 25               | 6                | 0              | -0.188254               | -0.273854 | 2.886384  |
| 26               | 1                | 0              | 0.692095                | 0.330893  | 2.709547  |
| 27               | 6                | 0              | 2.839320                | -3.940051 | 1.418981  |
| 28               | 1                | 0              | 3.069917                | -4.465819 | 2.338993  |
| 29               | 6                | 0              | -1.733995               | -3.058016 | -1.389660 |
| 30               | 1                | 0              | -1.126648               | -2.898525 | -2.271599 |
| 31               | 6                | 0              | -1.215921               | 1.591777  | -0.323874 |
| 32               | 6                | 0              | -2.157179               | -2.552910 | 0.856560  |
| 33               | 6                | 0              | -2.445553               | -1.886946 | 3.234366  |
| 34               | 6                | 0              | 3.618307                | -4.120169 | 0.271319  |
| 35               | 1                | 0              | 4.475075                | -4.785631 | 0.256753  |
| 36               | 6                | 0              | 1.972340                | -1.109374 | -4.322164 |
| 37               | 1                | 0              | 2.498109                | -1.154507 | -5.270169 |
| 38               | 6                | 0              | -1.972436               | -1.108950 | 4.322166  |
| 39               | 1                | 0              | -2.498243               | -1.153973 | 5.270154  |
| 40               | 6                | 0              | -2.839330               | -3.940108 | -1.418756 |
| 41               | 1                | 0              | -3.069914               | -4.465949 | -2.338729 |
| 42               | 6                | 0              | -0.841006               | -0.305905 | 4.141654  |
| 43               | 1                | 0              | -0.452380               | 0.301760  | 4.951319  |
| 44               | 1                | 0              | -2.237452               | 3.473684  | -0.556965 |
| 45               | 1                | 0              | -3.687256               | 0.787978  | -0.988695 |
| 46               | 1                | 0              | 2.237503                | 3.473701  | 0.556722  |
| 47               | 1                | 0              | 3.687310                | 0.788011  | 0.988521  |
| 48               | 6                | 0              | -2.384765               | 2.398905  | -0.617192 |
| 49               | 6                | 0              | -3.609986               | 1.875125  | -0.950264 |
| 50               | 6                | 0              | 2.384821                | 2.398924  | 0.616996  |
| 51               | 6                | 0              | 3.610027                | 1.875158  | 0.950112  |
| 52               | 6                | 0              | -4.823042               | 2.613610  | -1.257065 |
| 53               | 6                | 0              | -4.885275               | 4.032511  | -1.254525 |
| 54               | 6                | 0              | -6.002815               | 1.890211  | -1.577776 |
| 55               | 6                | 0              | -6.067156               | 4.725329  | -1.540366 |
| 56               | 1                | 0              | -4.016651               | 4.640702  | -1.024001 |
| 57               | 6                | 0              | -7.193274               | 2.564443  | -1.864852 |
| 58               | 1                | 0              | -5.982958               | 0.803186  | -1.596743 |
| 59               | 6                | 0              | -7.245605               | 3.973425  | -1.835458 |
| 60               | 1                | 0              | -8.096141               | 2.003266  | -2.099236 |
| 61               | 6                | 0              | 4.823073                | 2.613646  | 1.256944  |
| 62               | 6                | 0              | 4.885286                | 4.032537  | 1.254438  |
| 63               | 6                | 0              | 6.002837                | 1.890243  | 1.577692  |
| 64               | 6                | 0              | 6.067155                | 4.725380  | 1.540339  |
| 65               | 1                | 0              | 4.016652                | 4.640723  | 1.023935  |
| 66               | 6                | 0              | 7.193275                | 2.564491  | 1.864816  |
| 67               | 1                | 0              | 5.982986                | 0.803219  | 1.596655  |
| 68               | 6                | 0              | 7.245595                | 3.973470  | 1.835437  |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 69 | 1 | 0 | 8.096138  | 2.003323  | 2.099235  |
| 70 | 8 | 0 | 8.417407  | 4.677313  | 2.066389  |
| 71 | 1 | 0 | 9.190496  | 4.100241  | 2.237670  |
| 72 | 8 | 0 | 6.001996  | 6.101749  | 1.431674  |
| 73 | 8 | 0 | -8.417425 | 4.677258  | -2.066288 |
| 74 | 1 | 0 | -9.190513 | 4.100183  | -2.237554 |
| 75 | 8 | 0 | -6.002172 | 6.101718  | -1.431510 |
| 76 | 6 | 0 | -6.797597 | 6.998340  | -2.294829 |
| 77 | 1 | 0 | -7.851264 | 6.971818  | -2.014554 |
| 78 | 1 | 0 | -6.371001 | 7.987293  | -2.118293 |
| 79 | 1 | 0 | -6.680849 | 6.718405  | -3.348745 |
| 80 | 6 | 0 | 6.798412  | 6.998504  | 2.293912  |
| 81 | 1 | 0 | 7.851560  | 6.972872  | 2.011585  |
| 82 | 1 | 0 | 6.370771  | 7.987236  | 2.118657  |
| 83 | 1 | 0 | 6.683968  | 6.717993  | 3.347916  |
| 84 | 6 | 0 | -3.610479 | -2.766449 | 3.306361  |
| 85 | 6 | 0 | -4.018937 | -3.514364 | 2.162365  |
| 86 | 6 | 0 | -5.360329 | -3.673592 | 4.524443  |
| 87 | 6 | 0 | -5.769978 | -4.419721 | 3.380521  |
| 88 | 1 | 0 | -5.901941 | -3.745285 | 5.461837  |
| 89 | 1 | 0 | -6.633070 | -5.075934 | 3.421153  |
| 90 | 6 | 0 | 4.018836  | -3.514657 | -2.162212 |
| 91 | 6 | 0 | 3.610361  | -2.766837 | -3.306265 |
| 92 | 6 | 0 | 5.769786  | -4.420207 | -3.380356 |
| 93 | 6 | 0 | 5.360139  | -3.674148 | -4.524325 |
| 94 | 1 | 0 | 6.632854  | -5.076453 | -3.420959 |
| 95 | 1 | 0 | 5.901717  | -3.745943 | -5.461730 |
| 96 | 7 | 0 | -4.293697 | -2.857174 | 4.488096  |
| 97 | 7 | 0 | -5.107497 | -4.341577 | 2.214041  |
| 98 | 7 | 0 | 5.107351  | -4.341931 | -2.213860 |
| 99 | 7 | 0 | 4.293539  | -2.857686 | -4.488013 |

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**Table S4.** Computational data for the complex in **6**

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 27               | 0              | 0.000050                | -0.519657 | -0.000022 |
| 2                | 8                | 0              | 1.222663                | 0.739603  | 0.708130  |
| 3                | 8                | 0              | -1.222604               | 0.739472  | -0.708344 |
| 4                | 7                | 0              | -1.292684               | -1.900343 | -0.595105 |
| 5                | 7                | 0              | 1.292826                | -1.900235 | 0.595222  |
| 6                | 7                | 0              | -1.059469               | -0.530202 | 1.646194  |
| 7                | 7                | 0              | 1.059569                | -0.530361 | -1.646235 |
| 8                | 6                | 0              | -2.175237               | -1.315429 | 1.542110  |
| 9                | 6                | 0              | -1.342779               | -2.575788 | -1.760378 |
| 10               | 1                | 0              | -0.538970               | -2.415534 | -2.467403 |
| 11               | 6                | 0              | -2.299096               | -2.069587 | 0.317403  |
| 12               | 6                | 0              | -0.860633               | 0.206384  | 2.758485  |
| 13               | 1                | 0              | 0.039907                | 0.806027  | 2.793833  |
| 14               | 6                | 0              | -3.145724               | -1.397754 | 2.559850  |
| 15               | 6                | 0              | 3.398542                | -2.923827 | -0.095803 |
| 16               | 6                | 0              | -1.113534               | 2.071631  | -0.585826 |
| 17               | 6                | 0              | -3.398385               | -2.923895 | 0.096025  |
| 18               | 6                | 0              | 3.442809                | -3.632338 | 1.129843  |
| 19               | 1                | 0              | 4.278441                | -4.296358 | 1.323168  |
| 20               | 6                | 0              | 2.175355                | -1.315552 | -1.542066 |
| 21               | 6                | 0              | -1.792588               | 0.179121  | 3.820964  |
| 22               | 1                | 0              | -1.605775               | 0.786036  | 4.700006  |
| 23               | 6                | 0              | -0.000077               | 2.712205  | -0.000104 |
| 24               | 1                | 0              | -0.000134               | 3.796299  | -0.000105 |
| 25               | 6                | 0              | 0.860721                | 0.206108  | -2.758601 |
| 26               | 1                | 0              | -0.039830               | 0.805732  | -2.794006 |
| 27               | 6                | 0              | -2.407961               | -3.455924 | -2.055231 |
| 28               | 1                | 0              | -2.409736               | -3.983263 | -3.002847 |
| 29               | 6                | 0              | 1.342941                | -2.575544 | 1.760573  |
| 30               | 1                | 0              | 0.539133                | -2.415222 | 2.467584  |
| 31               | 6                | 0              | 1.113453                | 2.071750  | 0.585609  |
| 32               | 6                | 0              | 2.299235                | -2.069567 | -0.317274 |
| 33               | 6                | 0              | 3.145843                | -1.397965 | -2.559797 |
| 34               | 6                | 0              | -3.442631               | -3.632547 | -1.129540 |
| 35               | 1                | 0              | -4.278250               | -4.296605 | -1.322793 |
| 36               | 6                | 0              | -2.938852               | -0.619246 | 3.726409  |
| 37               | 1                | 0              | -3.675106               | -0.659789 | 4.522022  |
| 38               | 6                | 0              | 2.938956                | -0.619583 | -3.726438 |
| 39               | 1                | 0              | 3.675211                | -0.660194 | -4.522047 |
| 40               | 6                | 0              | 2.408141                | -3.455627 | 2.055521  |
| 41               | 1                | 0              | 2.409932                | -3.982856 | 3.003198  |
| 42               | 6                | 0              | 1.792678                | 0.178753  | -3.821075 |
| 43               | 1                | 0              | 1.605855                | 0.785575  | -4.700180 |
| 44               | 1                | 0              | 2.063991                | 3.956144  | 1.020389  |
| 45               | 1                | 0              | 3.382325                | 1.274652  | 1.774993  |
| 46               | 1                | 0              | -2.064247               | 3.955928  | -1.020639 |
| 47               | 1                | 0              | -3.382320               | 1.274304  | -1.775233 |
| 48               | 6                | 0              | 2.193232                | 2.881871  | 1.119497  |
| 49               | 6                | 0              | 3.317463                | 2.361202  | 1.710199  |
| 50               | 6                | 0              | -2.193387               | 2.881641  | -1.119733 |
| 51               | 6                | 0              | -3.317560               | 2.360862  | -1.710445 |
| 52               | 6                | 0              | 4.440115                | 3.103597  | 2.260094  |
| 53               | 6                | 0              | 4.509286                | 4.521918  | 2.245383  |
| 54               | 6                | 0              | 5.518659                | 2.385288  | 2.841055  |
| 55               | 6                | 0              | 5.605075                | 5.217906  | 2.767863  |
| 56               | 1                | 0              | 3.715479                | 5.126808  | 1.819379  |
| 57               | 6                | 0              | 6.622226                | 3.063241  | 3.368200  |
| 58               | 1                | 0              | 5.489463                | 1.298802  | 2.874109  |
| 59               | 6                | 0              | 6.686908                | 4.471094  | 3.325755  |
| 60               | 1                | 0              | 7.449378                | 2.504911  | 3.803168  |
| 61               | 6                | 0              | -4.440277               | 3.103149  | -2.260352 |
| 62               | 6                | 0              | -4.509579               | 4.521464  | -2.245648 |
| 63               | 6                | 0              | -5.518753               | 2.384738  | -2.841313 |
| 64               | 6                | 0              | -5.605431               | 5.217347  | -2.768135 |
| 65               | 1                | 0              | -3.715829               | 5.126429  | -1.819645 |
| 66               | 6                | 0              | -6.622381               | 3.062585  | -3.368465 |
| 67               | 1                | 0              | -5.489454               | 1.298255  | -2.874363 |
| 68               | 6                | 0              | -6.687194               | 4.470433  | -3.326025 |

|     |   |   |           |           |           |
|-----|---|---|-----------|-----------|-----------|
| 69  | 1 | 0 | -7.449480 | 2.504177  | -3.803434 |
| 70  | 8 | 0 | -7.784967 | 5.178107  | -3.792946 |
| 71  | 1 | 0 | -8.499188 | 4.602853  | -4.137735 |
| 72  | 8 | 0 | -5.577928 | 6.592373  | -2.619621 |
| 73  | 8 | 0 | 7.784618  | 5.178871  | 3.792671  |
| 74  | 1 | 0 | 8.498885  | 4.603683  | 4.137478  |
| 75  | 8 | 0 | 5.577432  | 6.592928  | 2.619348  |
| 76  | 6 | 0 | 6.137117  | 7.500738  | 3.640971  |
| 77  | 1 | 0 | 7.226766  | 7.454303  | 3.646128  |
| 78  | 1 | 0 | 5.789582  | 8.490508  | 3.339656  |
| 79  | 1 | 0 | 5.743883  | 7.248325  | 4.633472  |
| 80  | 6 | 0 | -6.137608 | 7.500117  | -3.641306 |
| 81  | 1 | 0 | -7.227251 | 7.453543  | -3.646594 |
| 82  | 1 | 0 | -5.790236 | 8.489930  | -3.339947 |
| 83  | 1 | 0 | -5.744220 | 7.247757  | -4.633761 |
| 84  | 6 | 0 | 4.305325  | -2.272837 | -2.359102 |
| 85  | 6 | 0 | 4.430512  | -3.032357 | -1.132574 |
| 86  | 6 | 0 | 6.309998  | -3.173905 | -3.126392 |
| 87  | 6 | 0 | 6.436171  | -3.937305 | -1.893012 |
| 88  | 6 | 0 | 7.318860  | -3.287497 | -4.128648 |
| 89  | 6 | 0 | 7.566204  | -4.787561 | -1.705970 |
| 90  | 6 | 0 | 8.405484  | -4.123060 | -3.915740 |
| 91  | 1 | 0 | 7.207395  | -2.710325 | -5.040689 |
| 92  | 6 | 0 | 8.529579  | -4.875895 | -2.700159 |
| 93  | 1 | 0 | 7.641886  | -5.349444 | -0.780782 |
| 94  | 1 | 0 | 9.177205  | -4.214635 | -4.674610 |
| 95  | 1 | 0 | 9.392323  | -5.521807 | -2.565014 |
| 96  | 6 | 0 | -4.305188 | -2.272671 | 2.359248  |
| 97  | 6 | 0 | -4.430358 | -3.032327 | 1.132803  |
| 98  | 6 | 0 | -6.309847 | -3.173691 | 3.126630  |
| 99  | 6 | 0 | -6.436004 | -3.937227 | 1.893333  |
| 100 | 6 | 0 | -7.318711 | -3.287191 | 4.128896  |
| 101 | 6 | 0 | -7.566022 | -4.787521 | 1.706379  |
| 102 | 6 | 0 | -8.405321 | -4.122794 | 3.916074  |
| 103 | 1 | 0 | -7.207258 | -2.709919 | 5.040875  |
| 104 | 6 | 0 | -8.529399 | -4.875763 | 2.700574  |
| 105 | 1 | 0 | -7.641693 | -5.349505 | 0.781252  |
| 106 | 1 | 0 | -9.177043 | -4.214300 | 4.674952  |
| 107 | 1 | 0 | -9.392133 | -5.521704 | 2.565497  |
| 108 | 7 | 0 | -5.233573 | -2.351555 | 3.329474  |
| 109 | 7 | 0 | -5.480319 | -3.845027 | 0.916755  |
| 110 | 7 | 0 | 5.233709  | -2.351811 | -3.329322 |
| 111 | 7 | 0 | 5.480488  | -3.845015 | -0.916441 |

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