

# Supplementary Material

## Syntheses and Photodynamic Activity of Pegylated Cationic Zn(II)-Phthalocyanines in HEp2 Cells

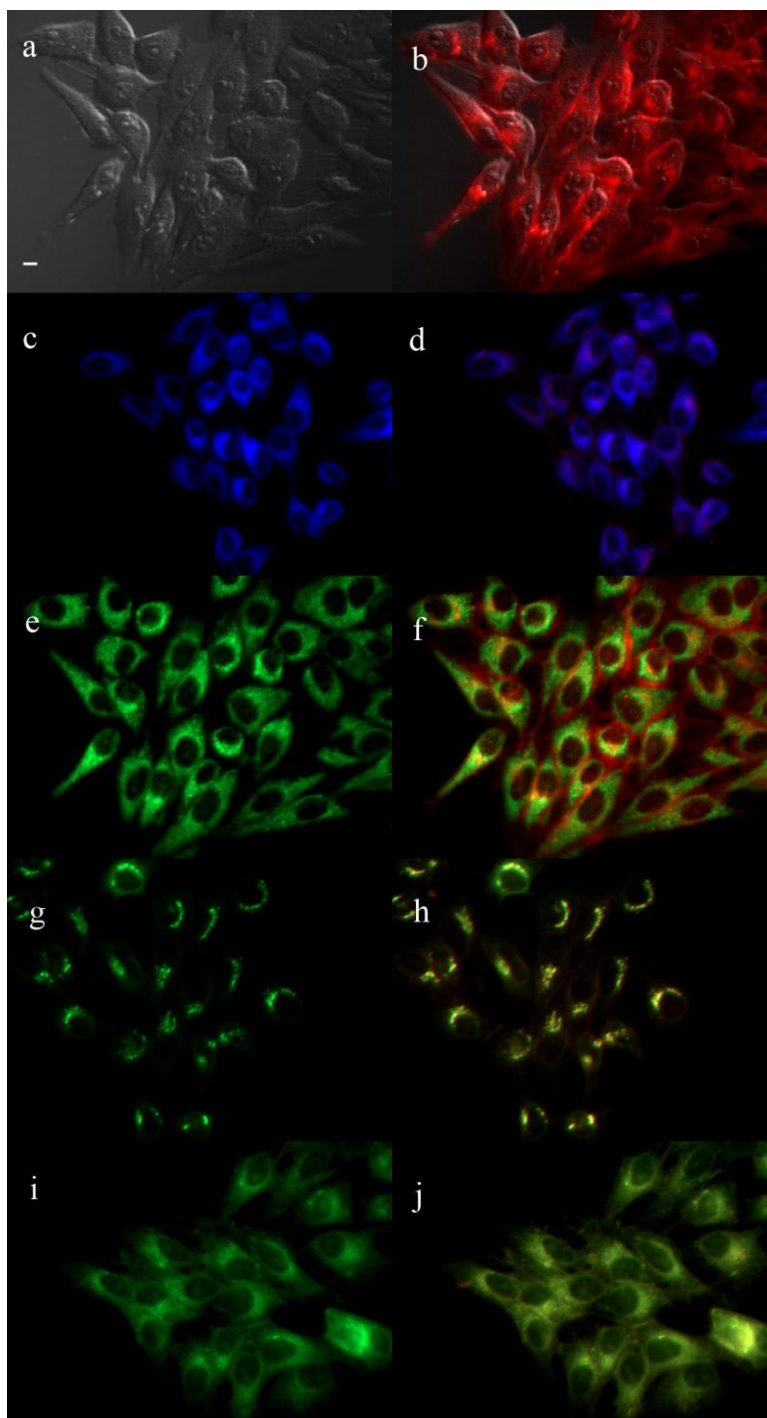
*Benson Ongarora, Xiaoke Hu, Susan Verberne-Sutton, Jayne Garno and M. Graça H. Vicente \**

*Department of Chemistry, Louisiana State University, Baton Rouge, LA 70803*

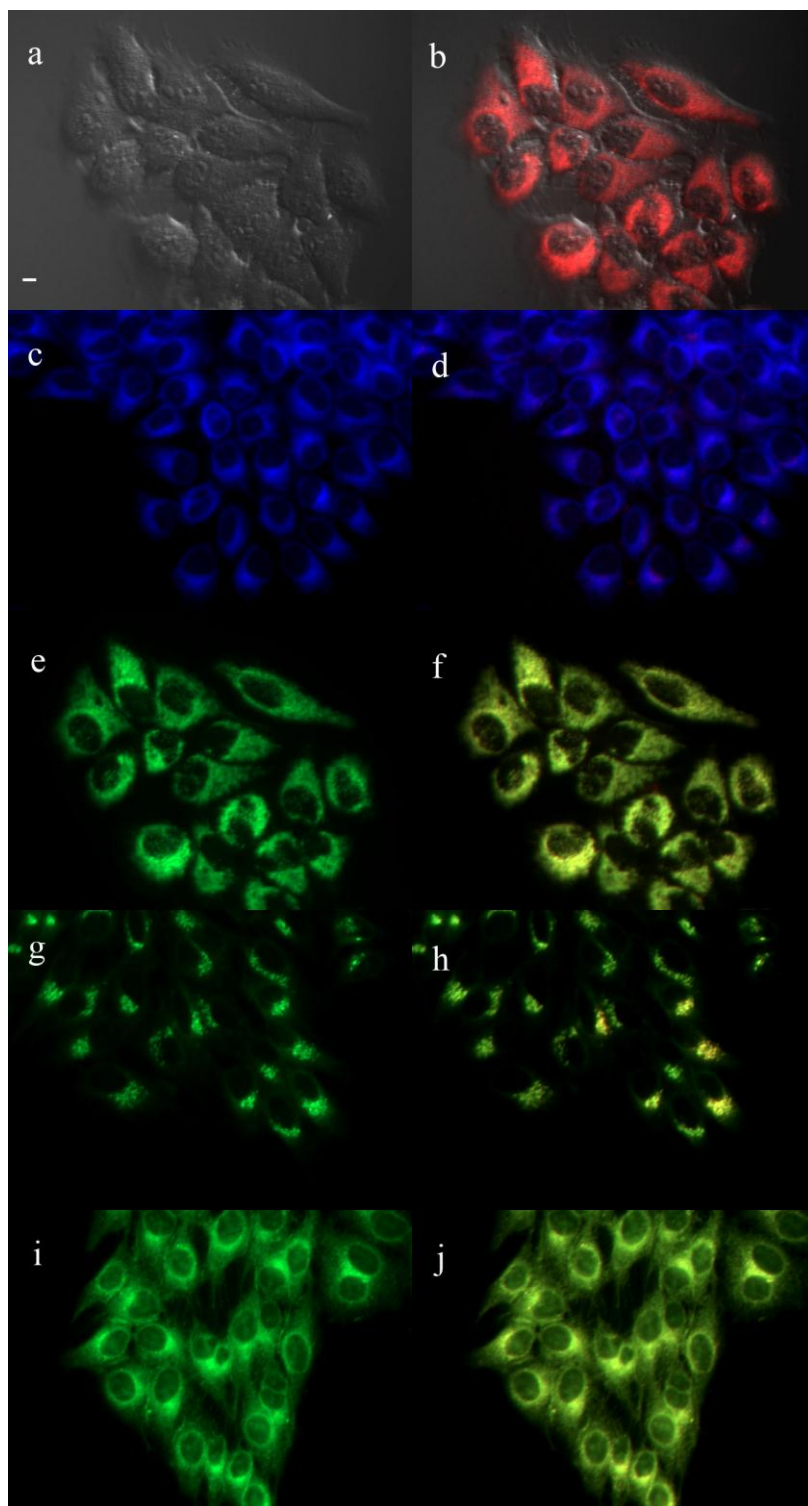
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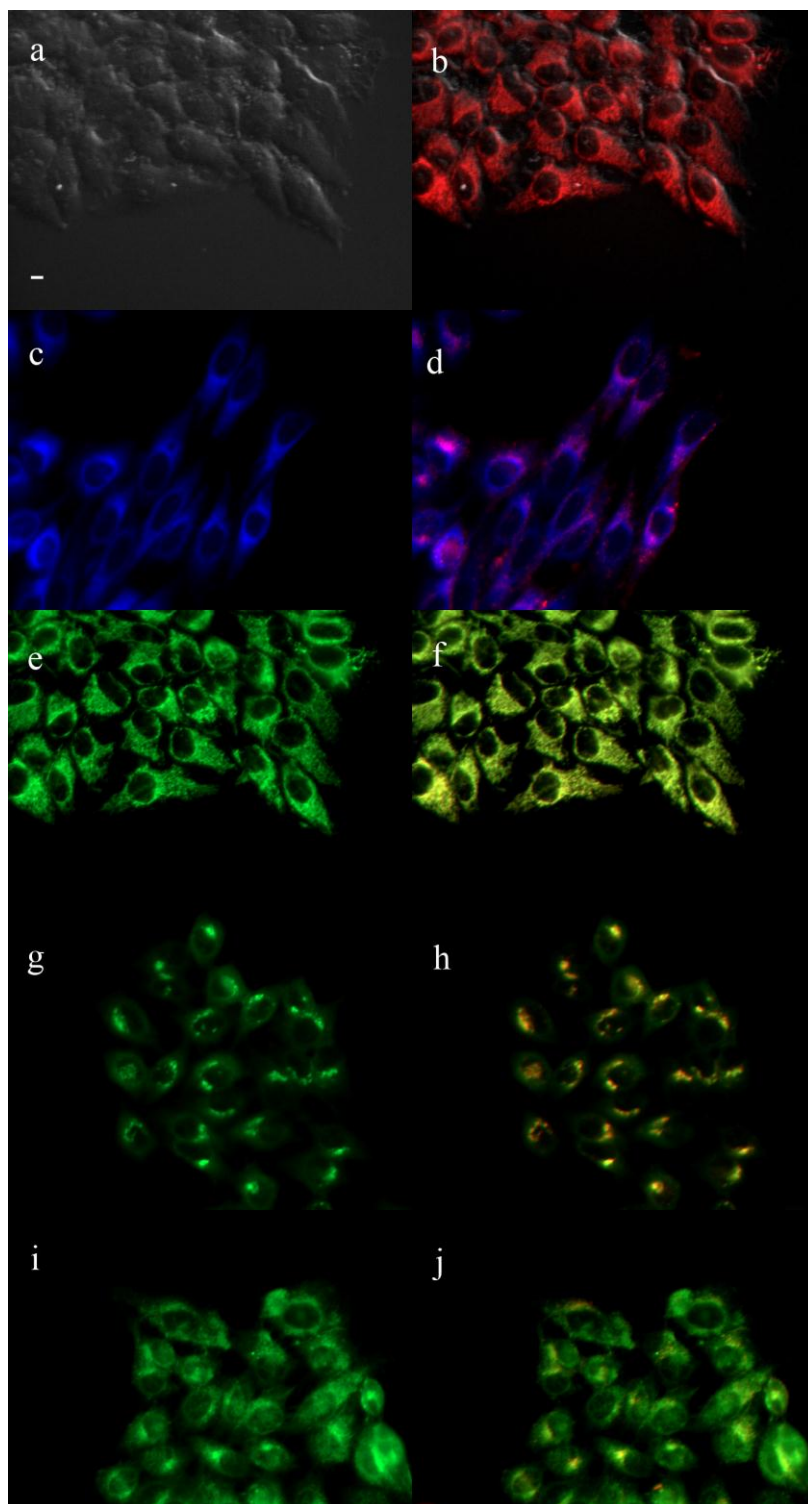
## Subcellular localization in HEP2 cells



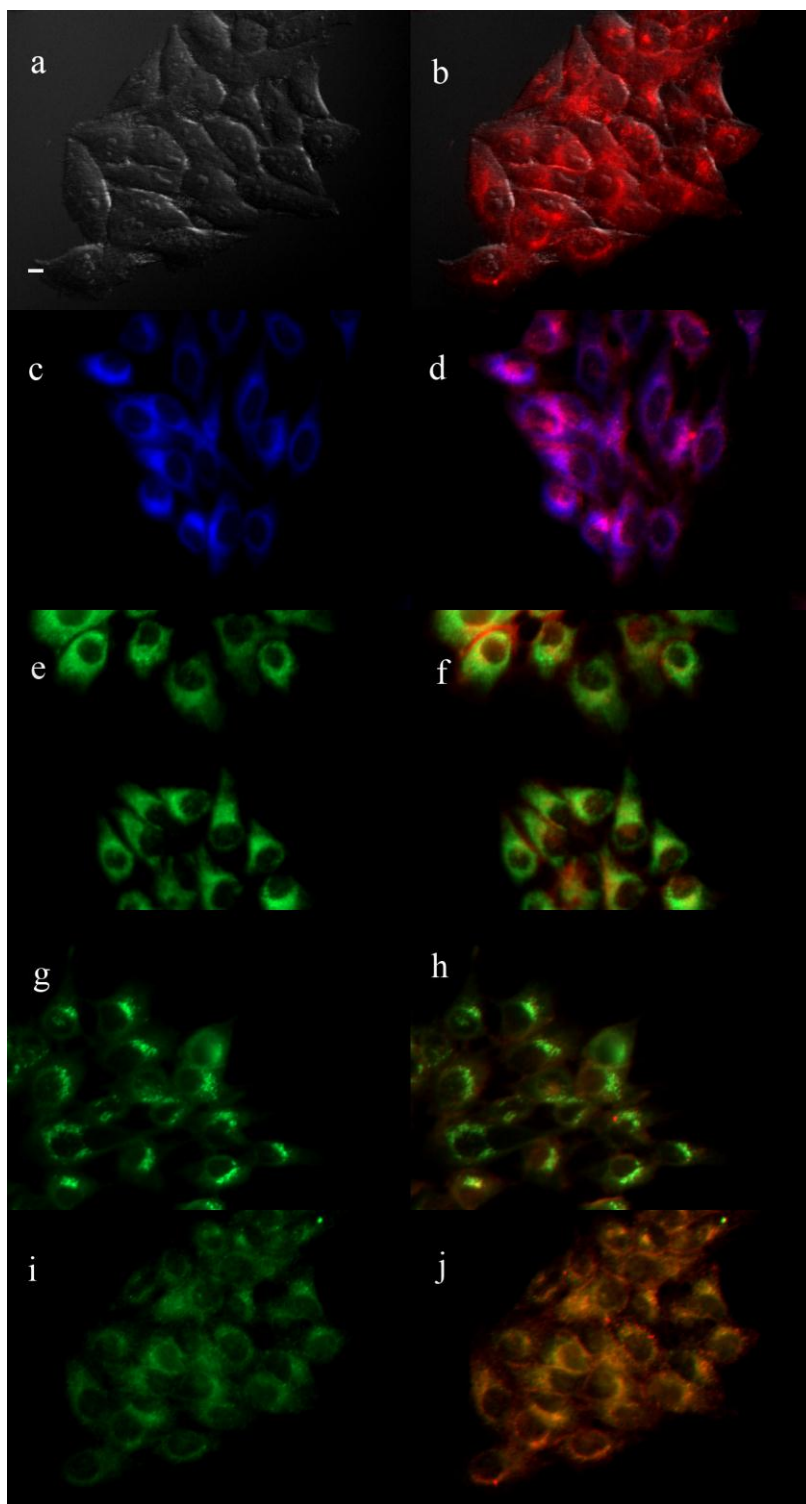
**Figure S1.** Subcellular localization of Pc **6a** in HEP2 cells at 10  $\mu$ M for 6 h. (a) Phase contrast, (b) Overlay of **6a** fluorescence and phase contrast, (c) ER Tracker Blue/White fluorescence, (e) MitoTrack green fluorescence, (g) BoDIPY Ceramide, (i) LysoSensor green fluorescence, and (d, f, h, j) overlays of organelle tracers with **6a** fluorescence. Scale bar: 10  $\mu$ m.



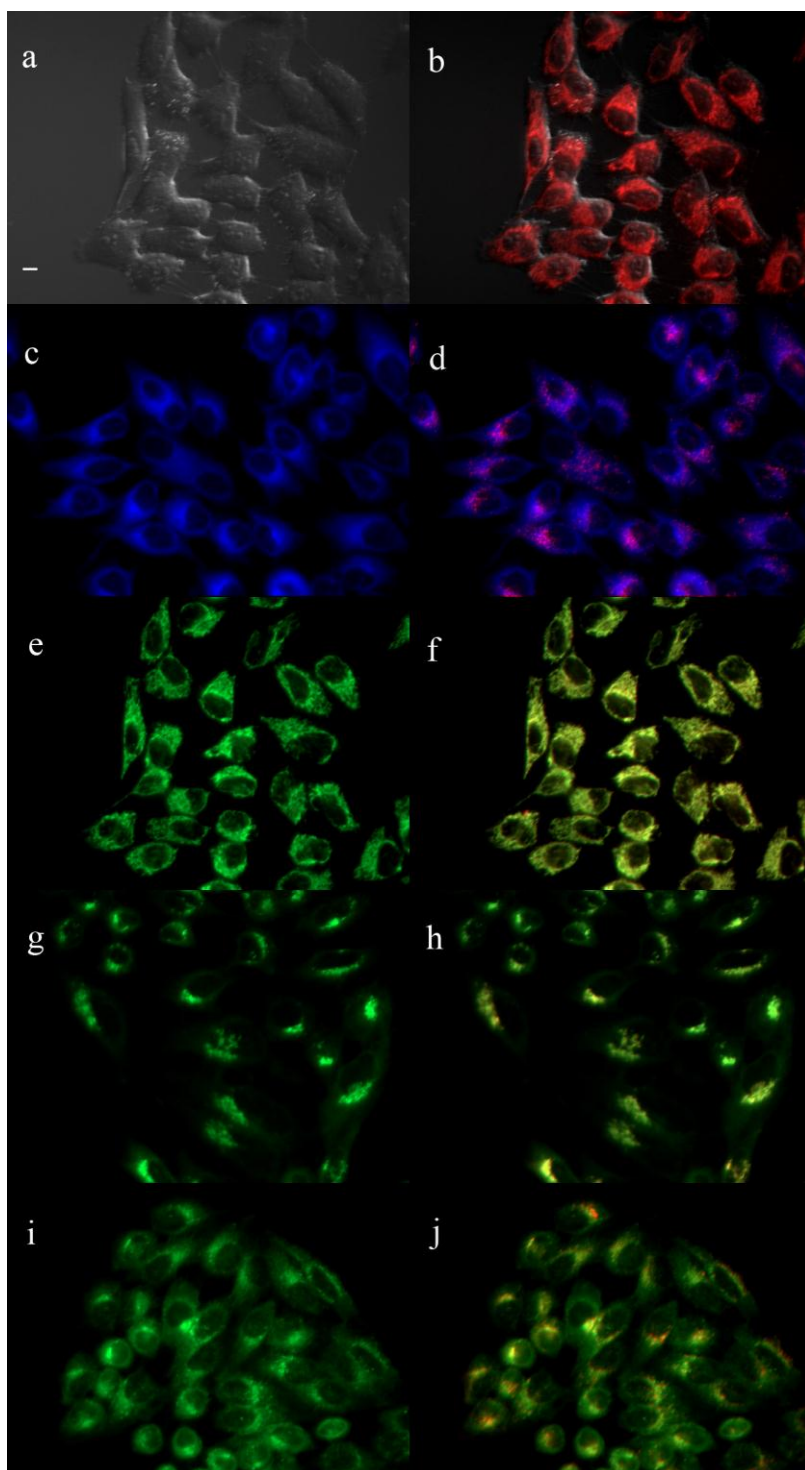
**Figure S2.** Subcellular localization of Pc **6b** in HEp2 cells at 10  $\mu$ M for 6 h. (a) Phase contrast, (b) Overlay of **6b** fluorescence and phase contrast, (c) ER Tracker Blue/White fluorescence, (e) MitoTrack green fluorescence, (g) BoDIPY Ceramide, (i) LysoSensor green fluorescence, and (d, f, h, j) overlays of organelle tracers with **6b** fluorescence. Scale bar: 10  $\mu$ m.



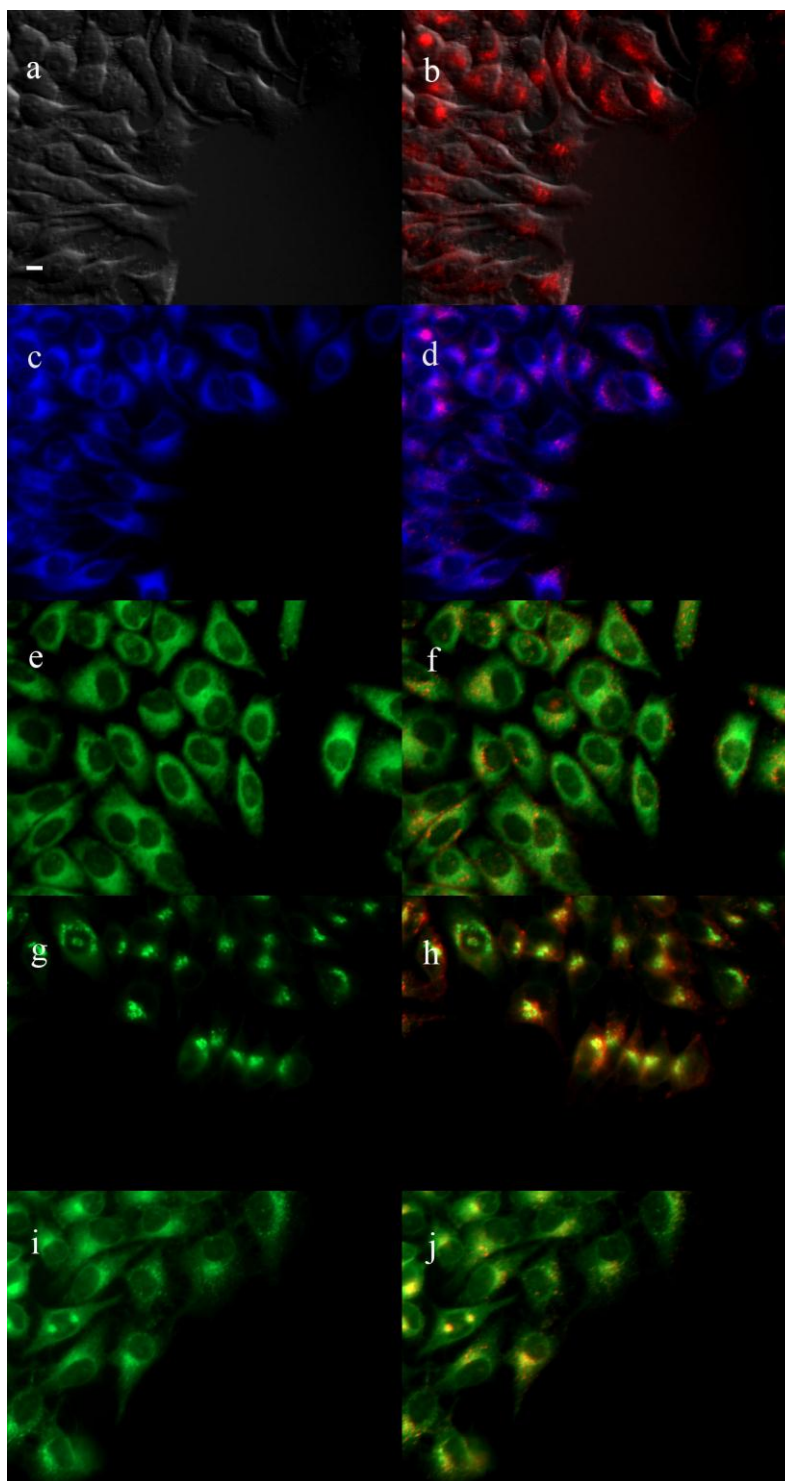
**Figure S3.** Subcellular localization of Pc **4b** in HEp2 cells at 10  $\mu$ M for 6 h. (a) Phase contrast, (b) Overlay of **4b** fluorescence and phase contrast, (c) ER Tracker Blue/White fluorescence, (e) MitoTrack green fluorescence, (g) BoDIPY Ceramide, (i) LysoSensor green fluorescence, and (d, f, h, j) overlays of organelle tracers with **4b** fluorescence. Scale bar: 10  $\mu$ m.



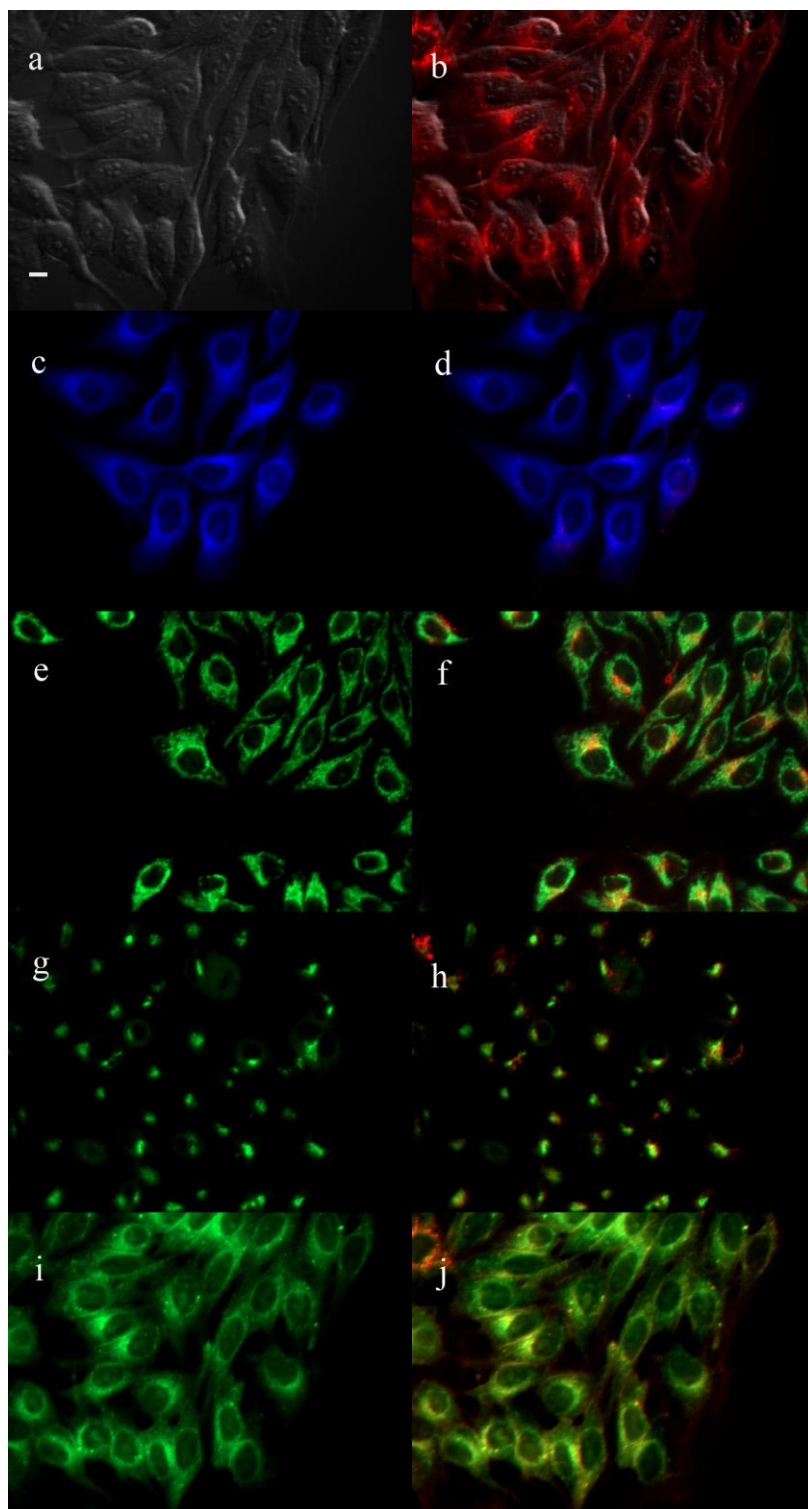
**Figure S4.** Subcellular localization of Pc **16b** in HEp2 cells at 10  $\mu\text{M}$  for 6 h. (a) Phase contrast, (b) Overlay of **16b** fluorescence and phase contrast, (c) ER Tracker Blue/White fluorescence, (e) MitoTrack green fluorescence, (g) BoDIPY Ceramide, (i) LysoSensor green fluorescence, and (d, f, h, j) overlays of organelle tracers with **16b** fluorescence. Scale bar: 10  $\mu\text{m}$ .



**Figure S5.** Subcellular localization of Pc **2b** in HEp2 cells at 10  $\mu$ M for 6 h. (a) Phase contrast, (b) Overlay of **2b** fluorescence and phase contrast, (c) ER Tracker Blue/White fluorescence, (e) MitoTrack green fluorescence, (g) BoDIPY Ceramide, (i) LysoSensor green fluorescence, and (d, f, h, j) overlays of organelle tracers with **2b** fluorescence. Scale bar: 10  $\mu$ m.

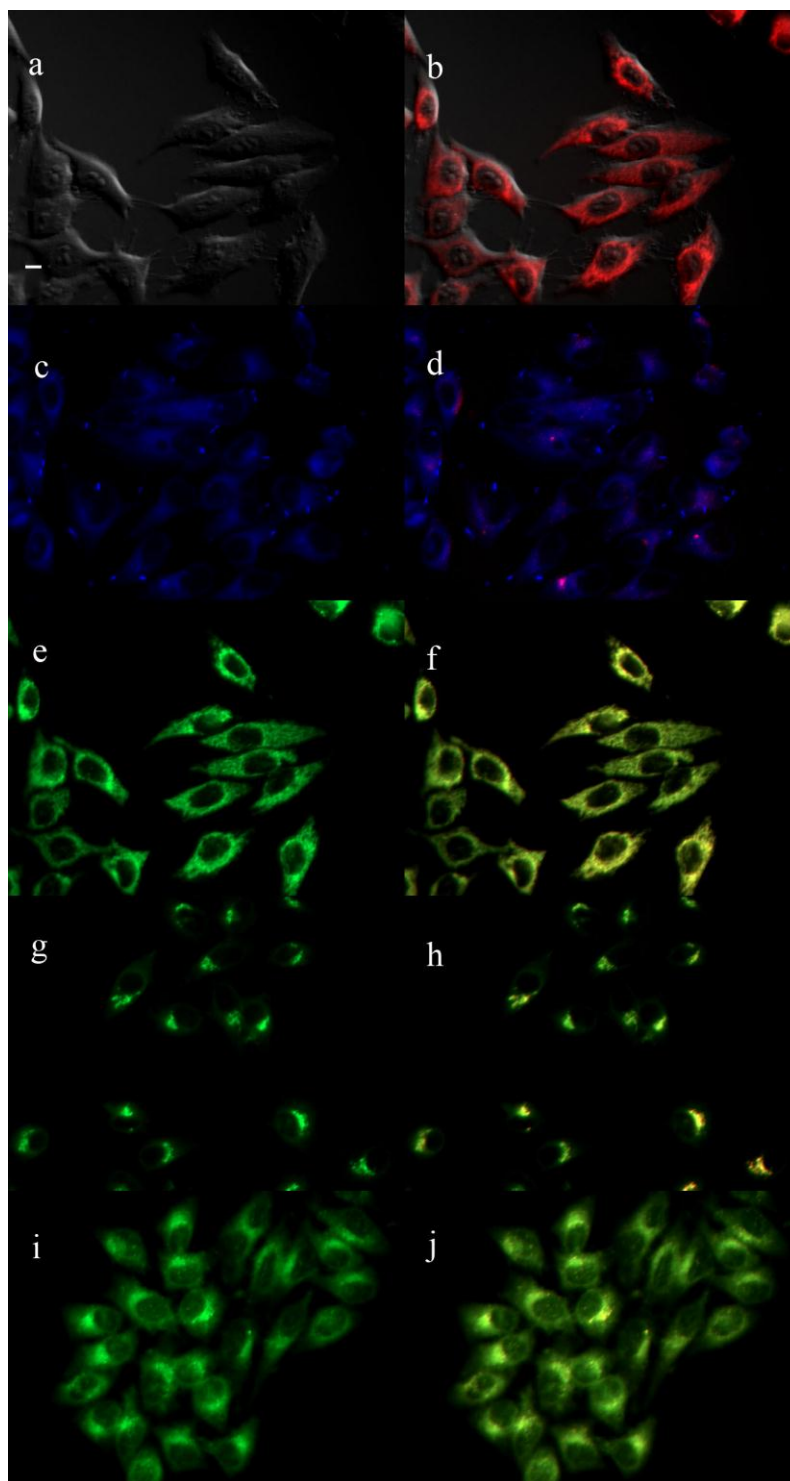


**Figure S6.** Subcellular localization of Pc **9a** in HEp2 cells at 10  $\mu$ M for 6 h. (a) Phase contrast, (b) Overlay of **9a** fluorescence and phase contrast, (c) ER Tracker Blue/White fluorescence, (e) MitoTrack green fluorescence, (g) BoDIPY Ceramide, (i) LysoSensor green fluorescence, and (d, f, h, j) overlays of organelle tracers with **9a** fluorescence. Scale bar: 10  $\mu$ m.



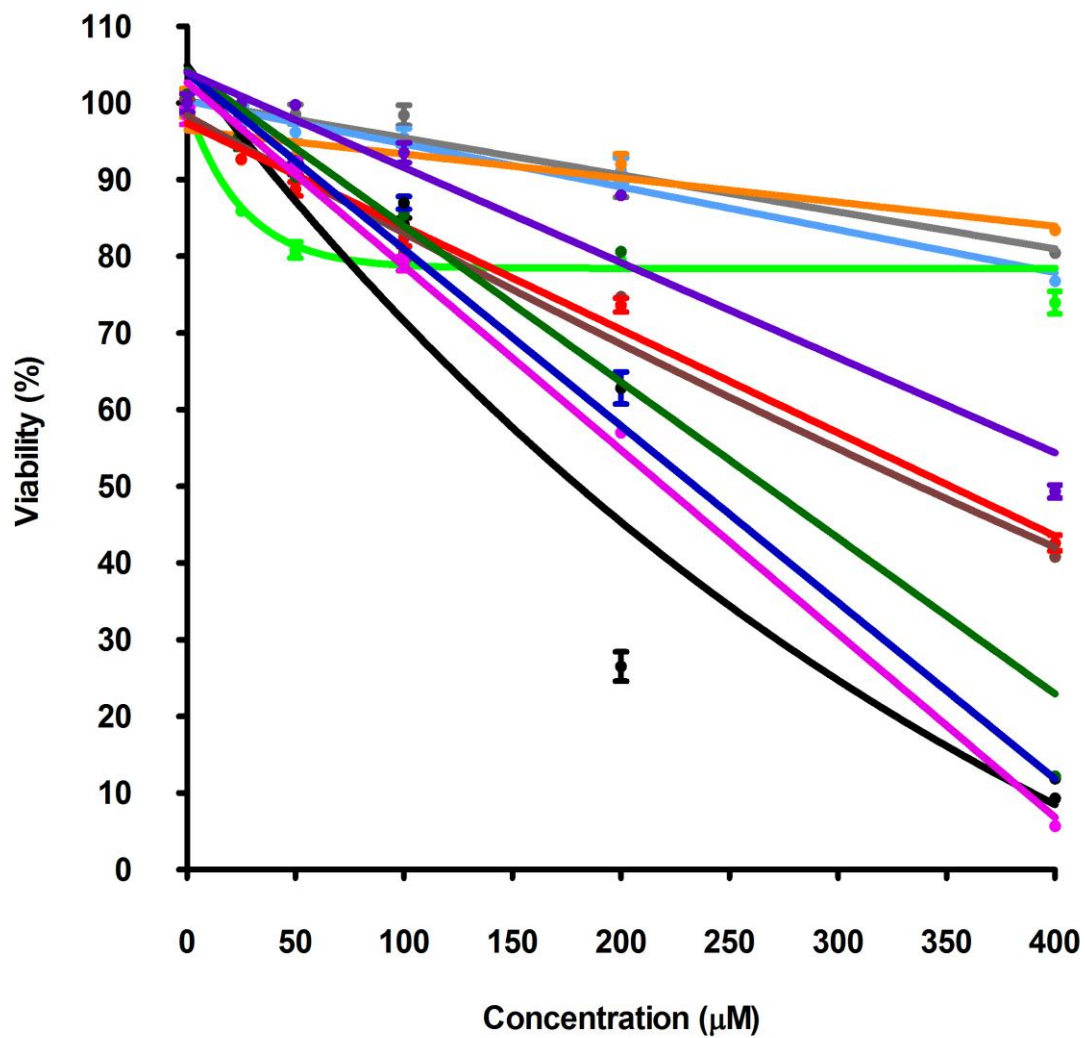
**Figure S7.** Subcellular localization of Pc **9b** in HEp2 cells at 10  $\mu$ M for 6 h. (a) Phase contrast, (b) Overlay of **9b** fluorescence and phase contrast, (c) ER Tracker Blue/White fluorescence, (e) MitoTrack green fluorescence, (g) BoDIPY Ceramide, (i) LysoSensor green fluorescence, and (d, f, h, j) overlays of organelle tracers with **9b** fluorescence. Scale bar: 10  $\mu$ m.



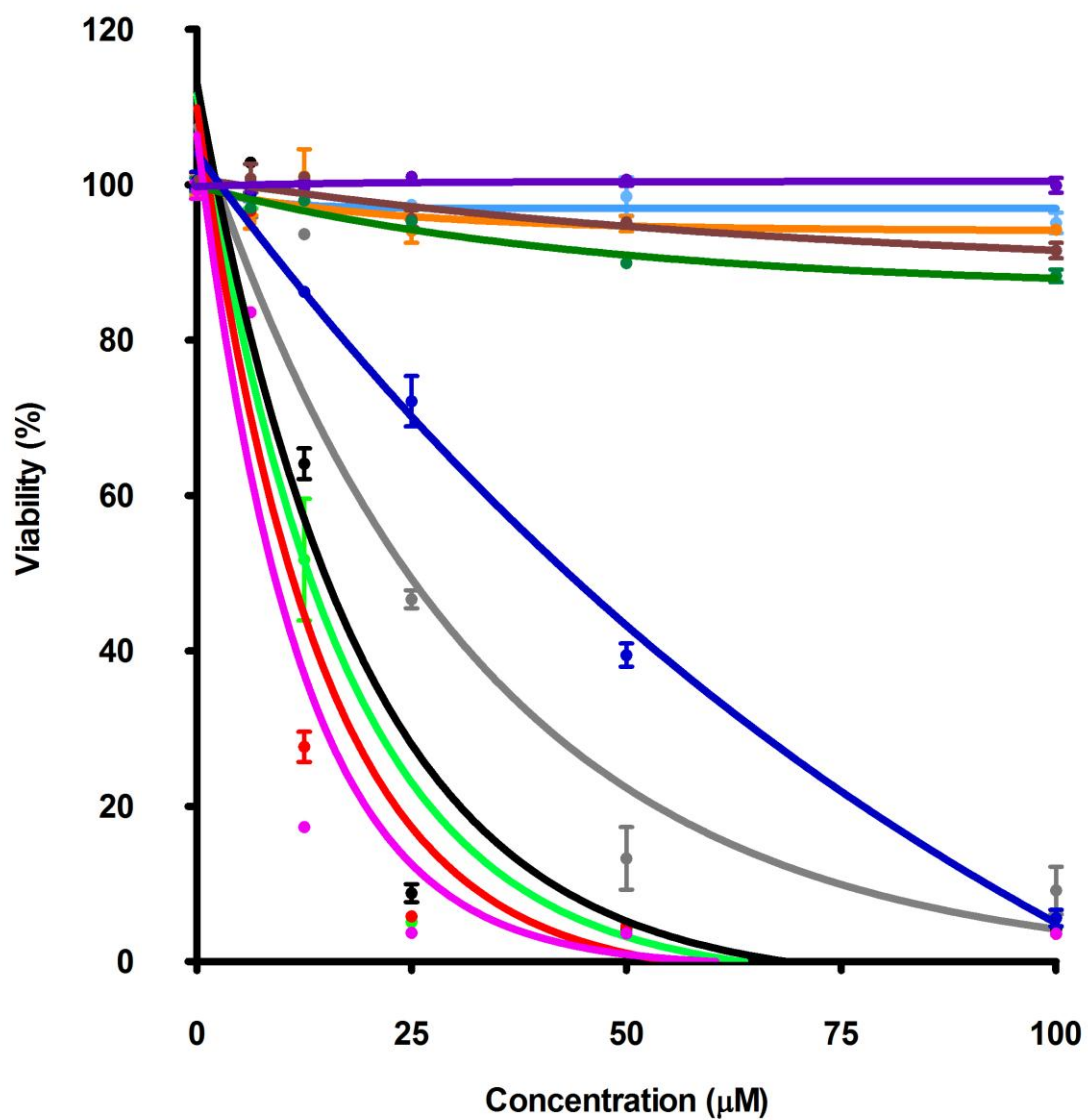


**Figure S8.** Subcellular localization of Pc **11b** in HEp2 cells at 10  $\mu$ M for 6 h. (a) Phase contrast, (b) Overlay of **11b** fluorescence and phase contrast, (c) ER Tracker Blue/White fluorescence, (e) MitoTrack green fluorescence, (g) BoDIPY Ceramide, (i) LysoSensor green fluorescence, and (d, f, h, j) overlays of organelle tracers with **11b** fluorescence. Scale bar: 10  $\mu$ m.

## Cytotoxicity in HEp2 cells

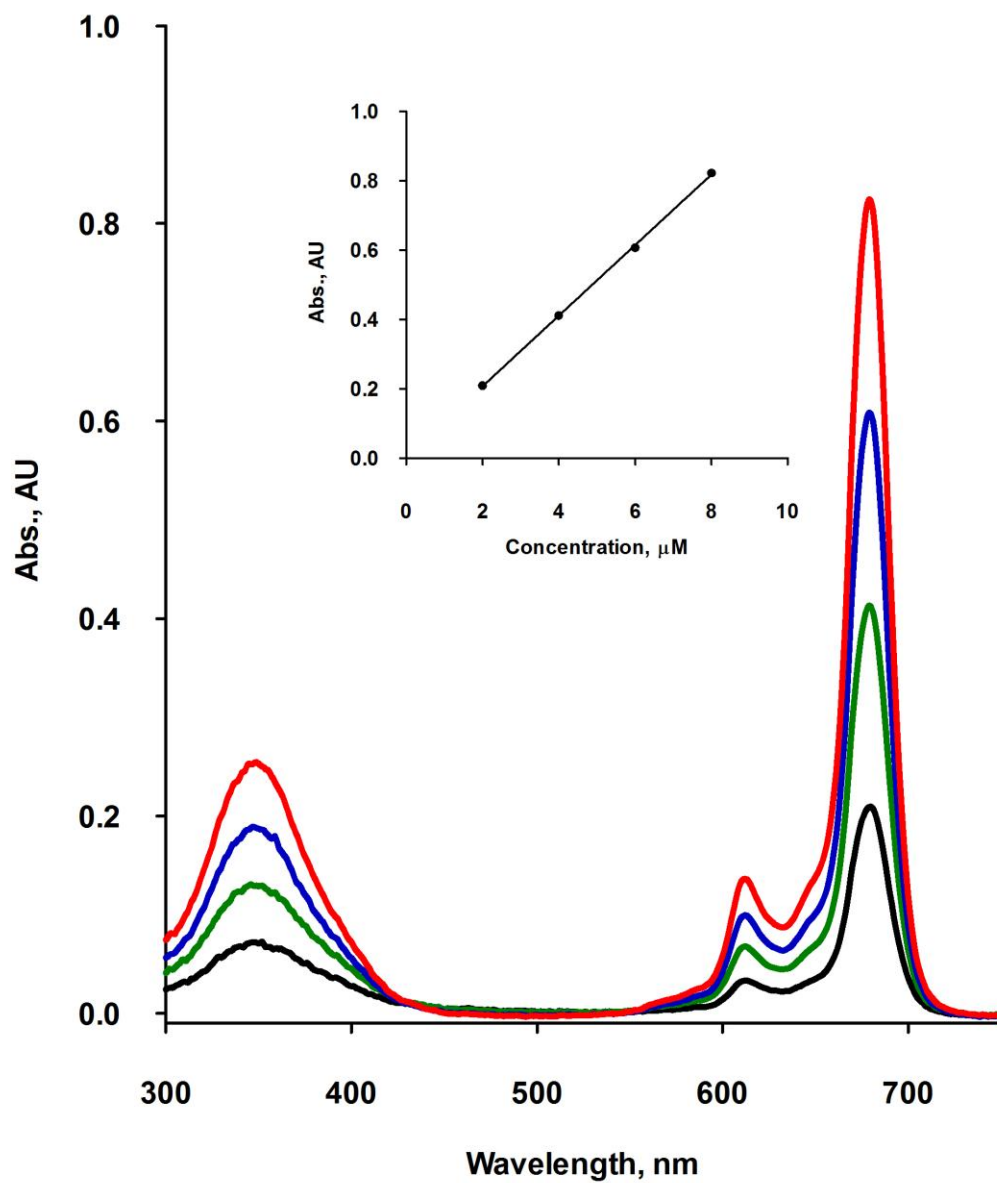


**Figure S9.** Dark toxicity of Pc **2b** (purple), **4a** (red), **4b** (green), **6a** (black), **6b** (brown square), **9a** (grey), **9b** (light-blue), **11a** (light green), **11b** (orange), **16b** (blue), **16a** (pink) at 10  $\mu\text{M}$  in HEp2 cells.

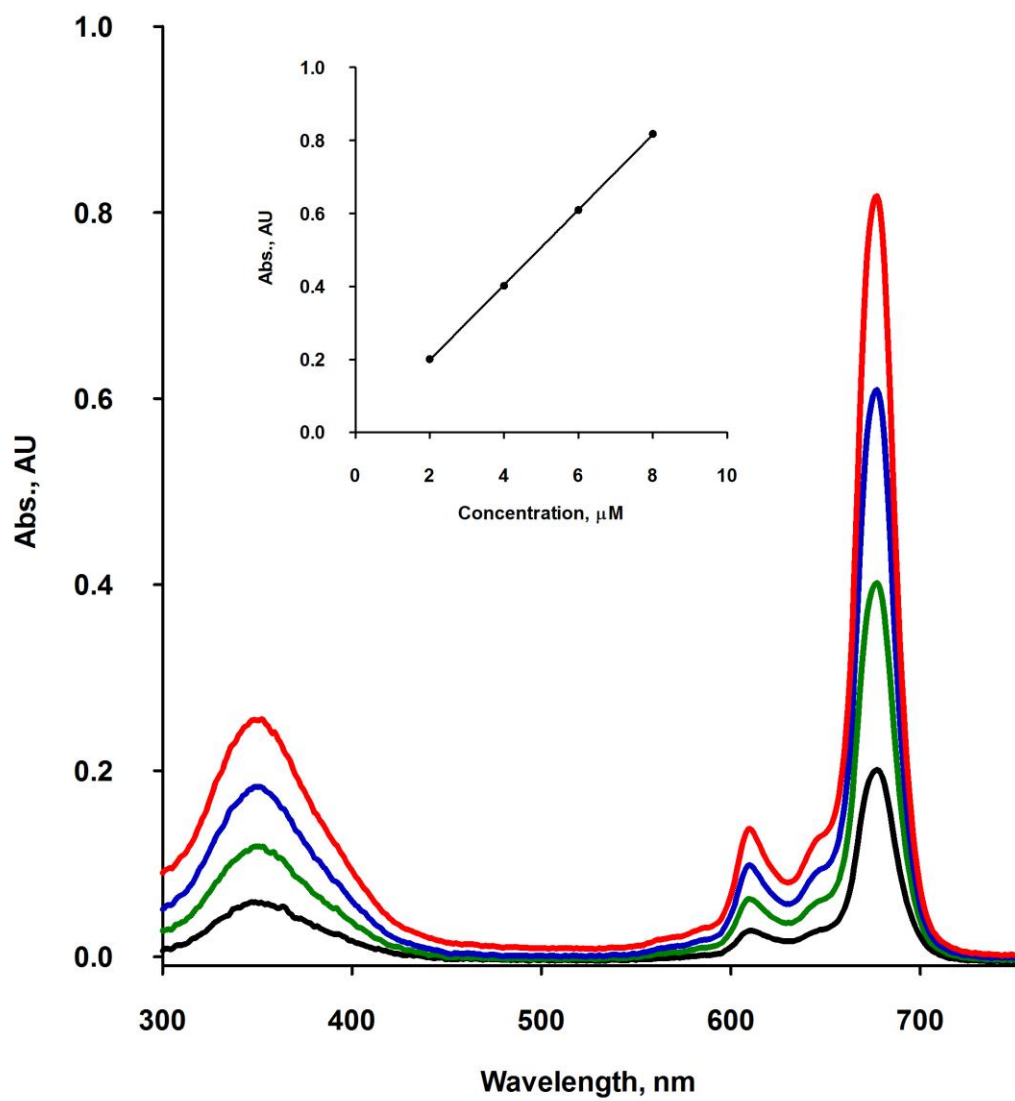


**Figure S10.** Phototoxicity of Pc **2b** (purple), **4a** (red), **4b** (green), **6a** (black), **6b** (brown square), **9a** (grey), **9b** (light-blue), **11a** (light green), **11b** (orange), **16b** (blue), **16a** (pink) at 10  $\mu\text{M}$  in HEp2 cells.

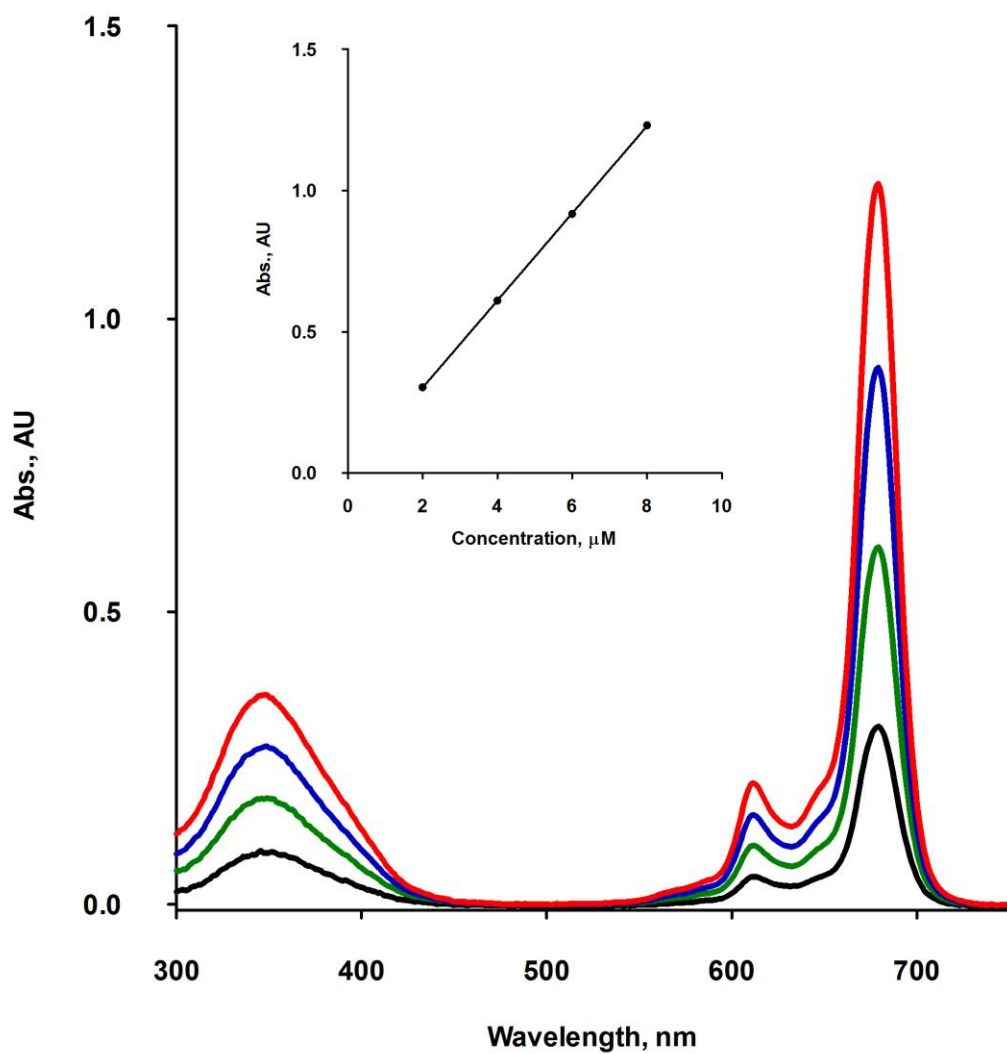
## UV-Vis Spectra for Cationic ZnPcS



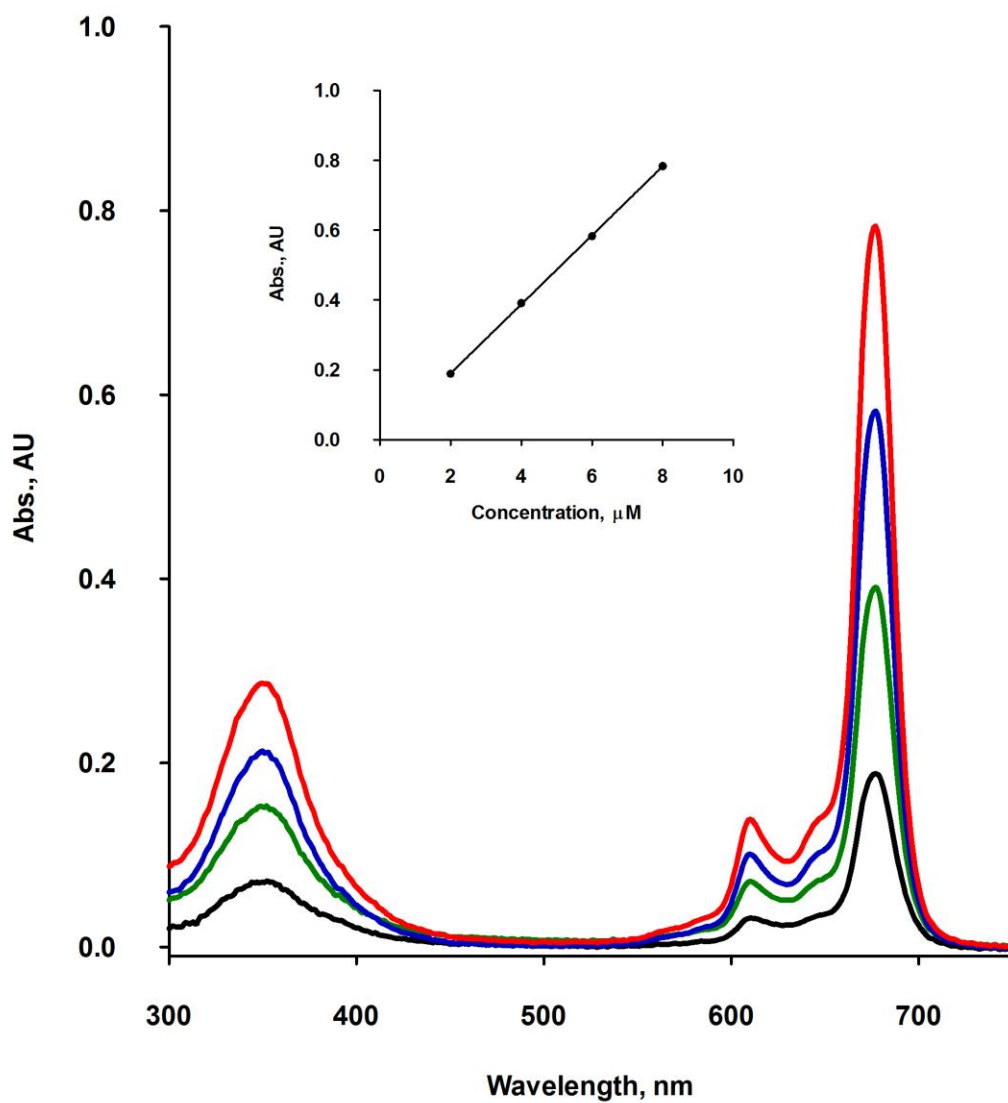
**Figure S11.** Absorption of Pc **9a** at 2.0 μM (black), 4.0 μM (green), 6.0 μM (blue), 8.0 μM (red) in DMF.



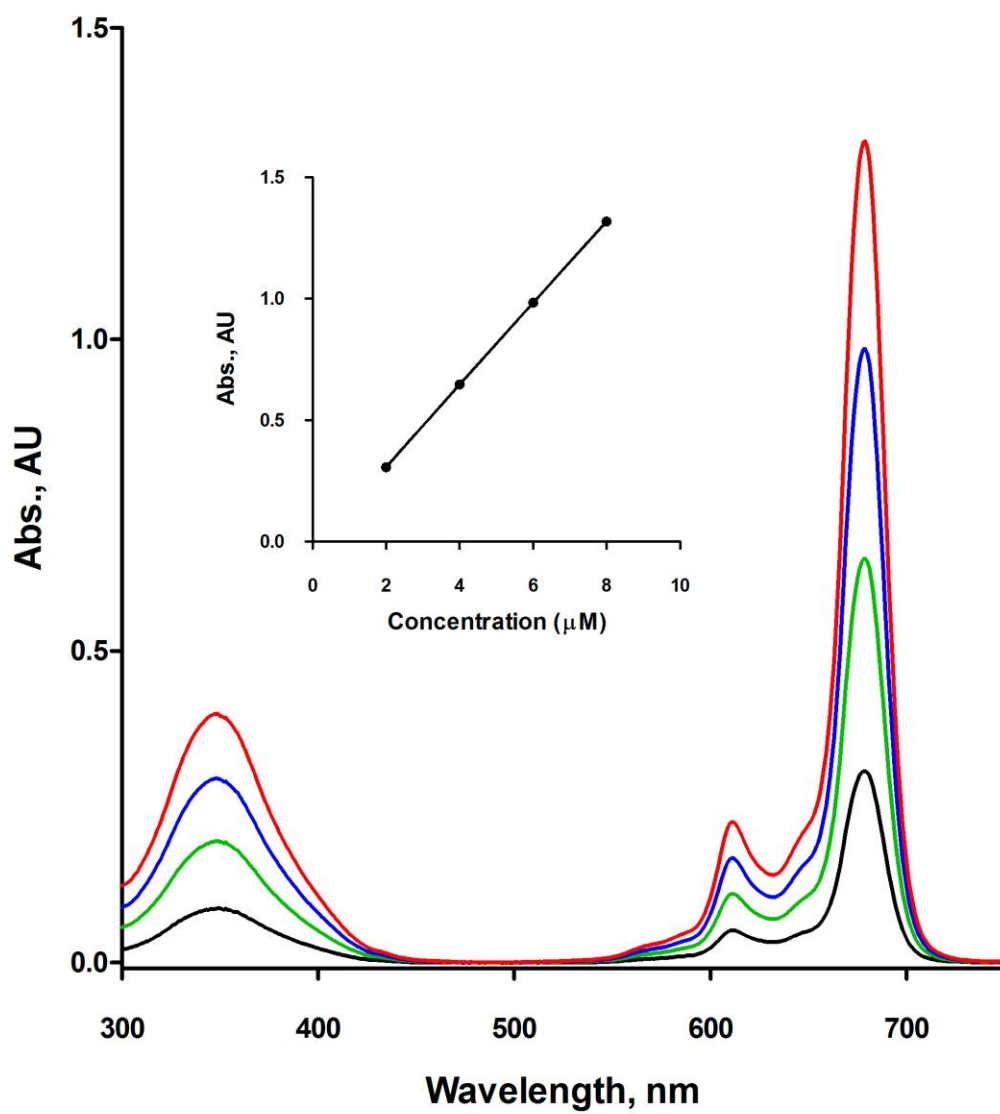
**Figure S12.** Absorption of Pc **9b** at 2.0  $\mu\text{M}$  (black), 4.0  $\mu\text{M}$  (green), 6.0  $\mu\text{M}$  (blue), 8.0  $\mu\text{M}$  (red) in DMF.



**Figure S13.** Absorption of Pc 11a at 2.0 μM (black), 4.0 μM (green), 6.0 μM (blue), 8.0 μM (red) in DMF.

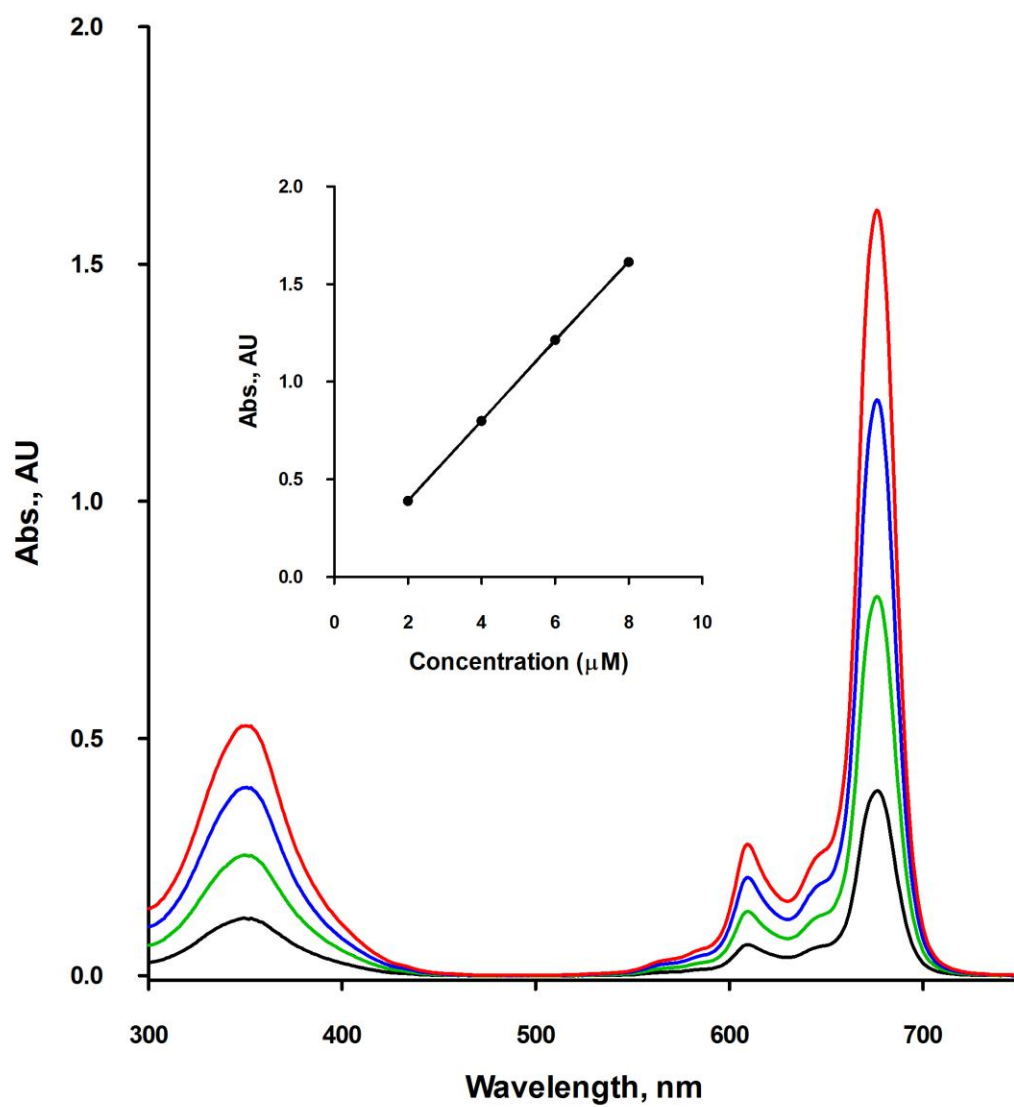


**Figure S14.** Absorption of Pc 11b at 2.0 μM (black), 4.0 μM (green), 6.0 μM (blue), 8.0 μM (red) in DMF.

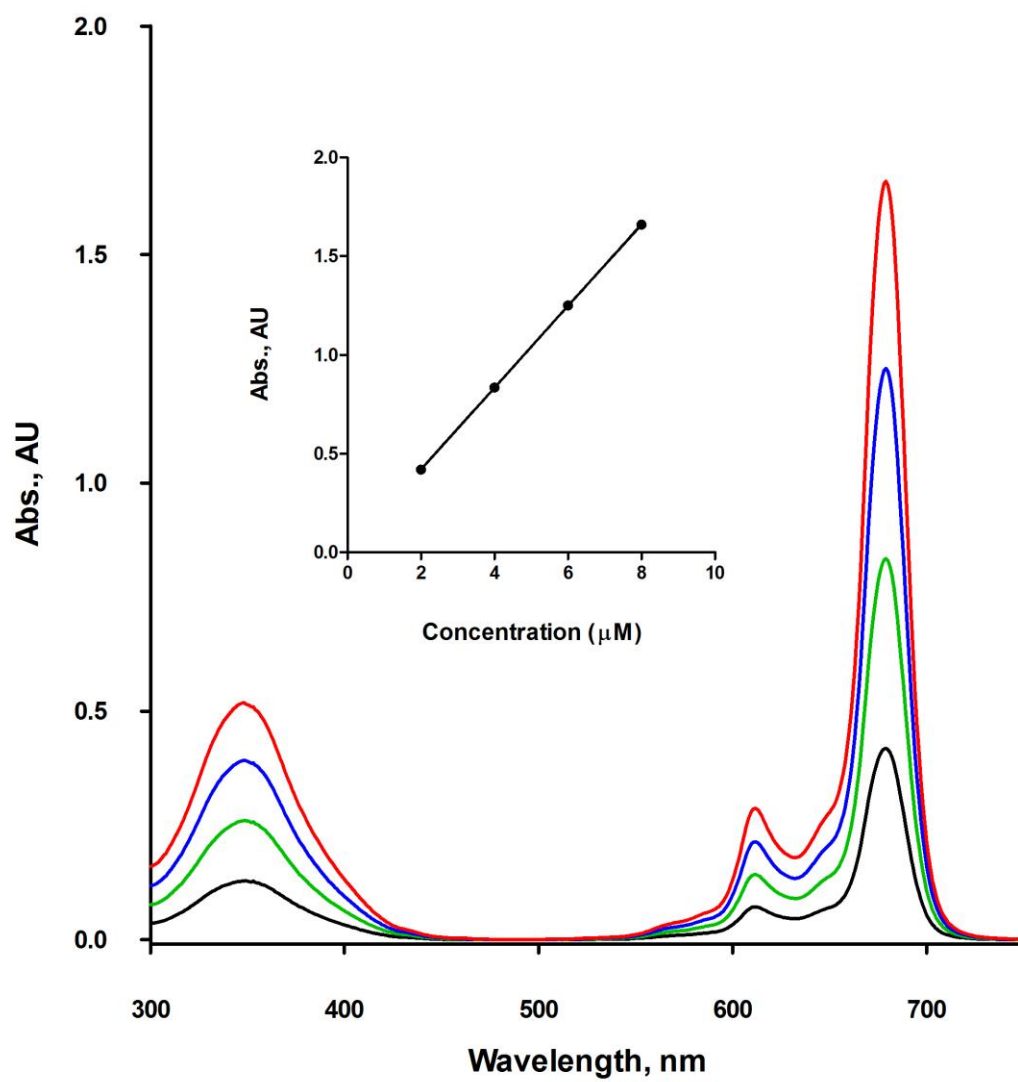


**Figure S15.** Absorption of Pc **6a** at 2.0 μM (black), 4.0 μM (green), 6.0 μM (blue), 8.0 μM (red) in DMF.

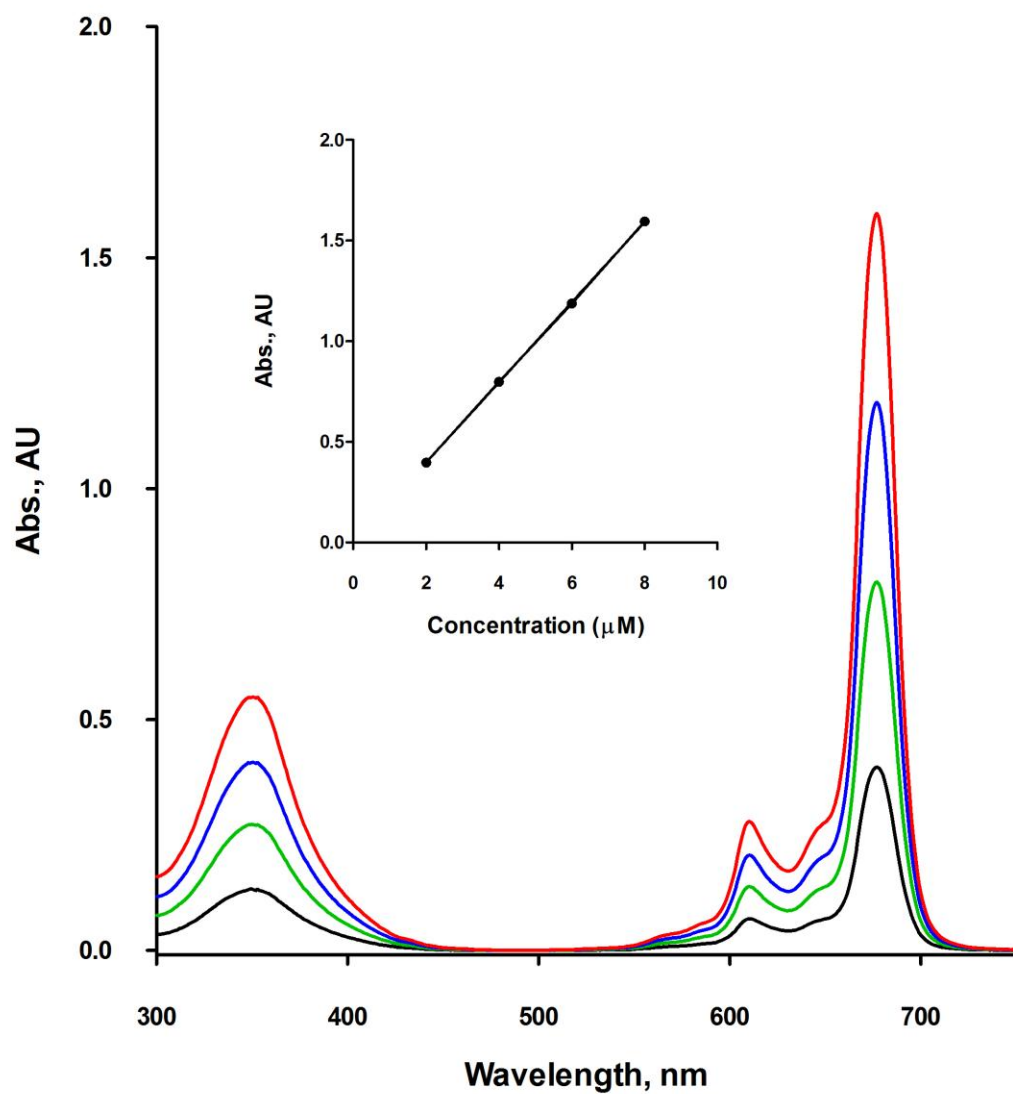




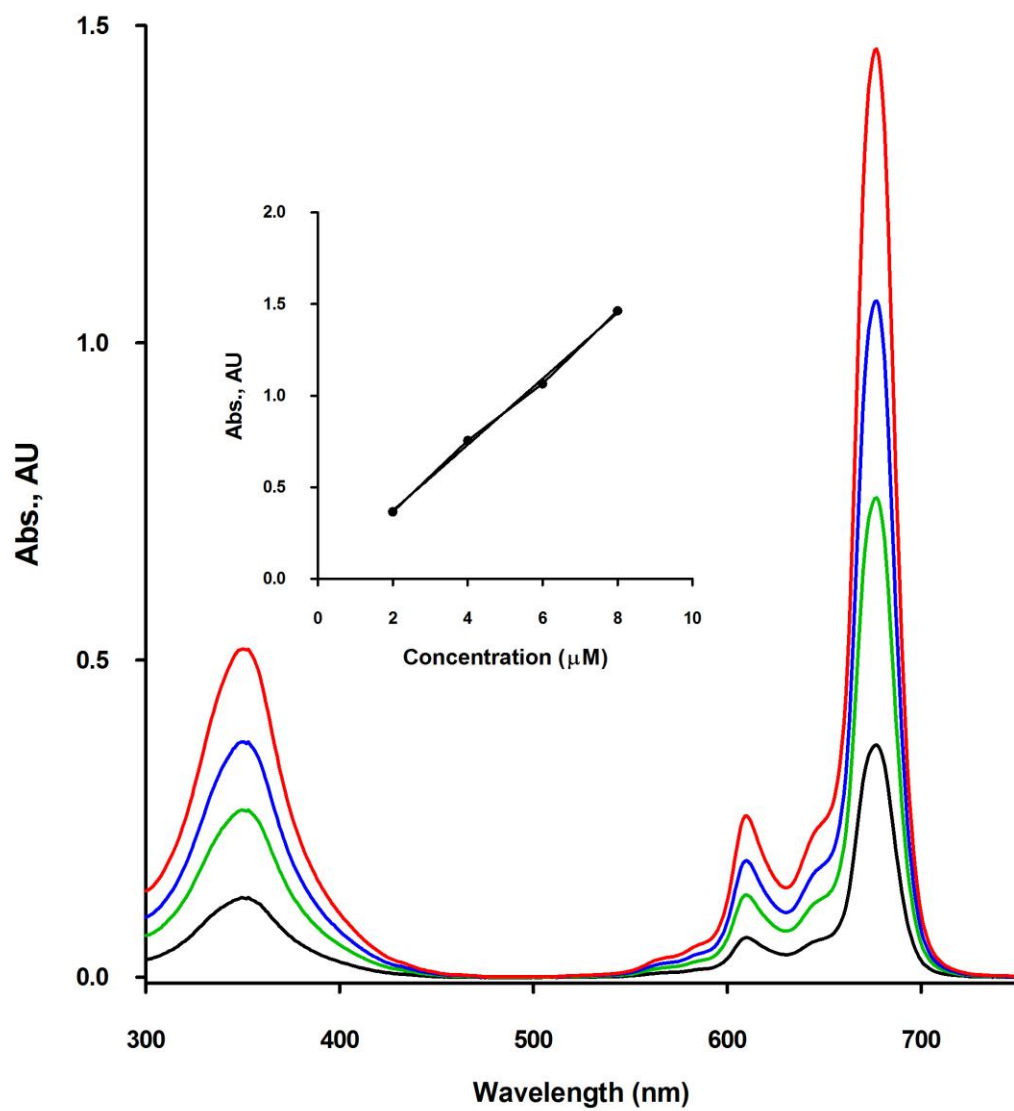
**Figure S16.** Absorption of Pc **6b** at 2.0  $\mu\text{M}$  (black), 4.0  $\mu\text{M}$  (green), 6.0  $\mu\text{M}$  (blue), 8.0  $\mu\text{M}$  (red) in DMF.



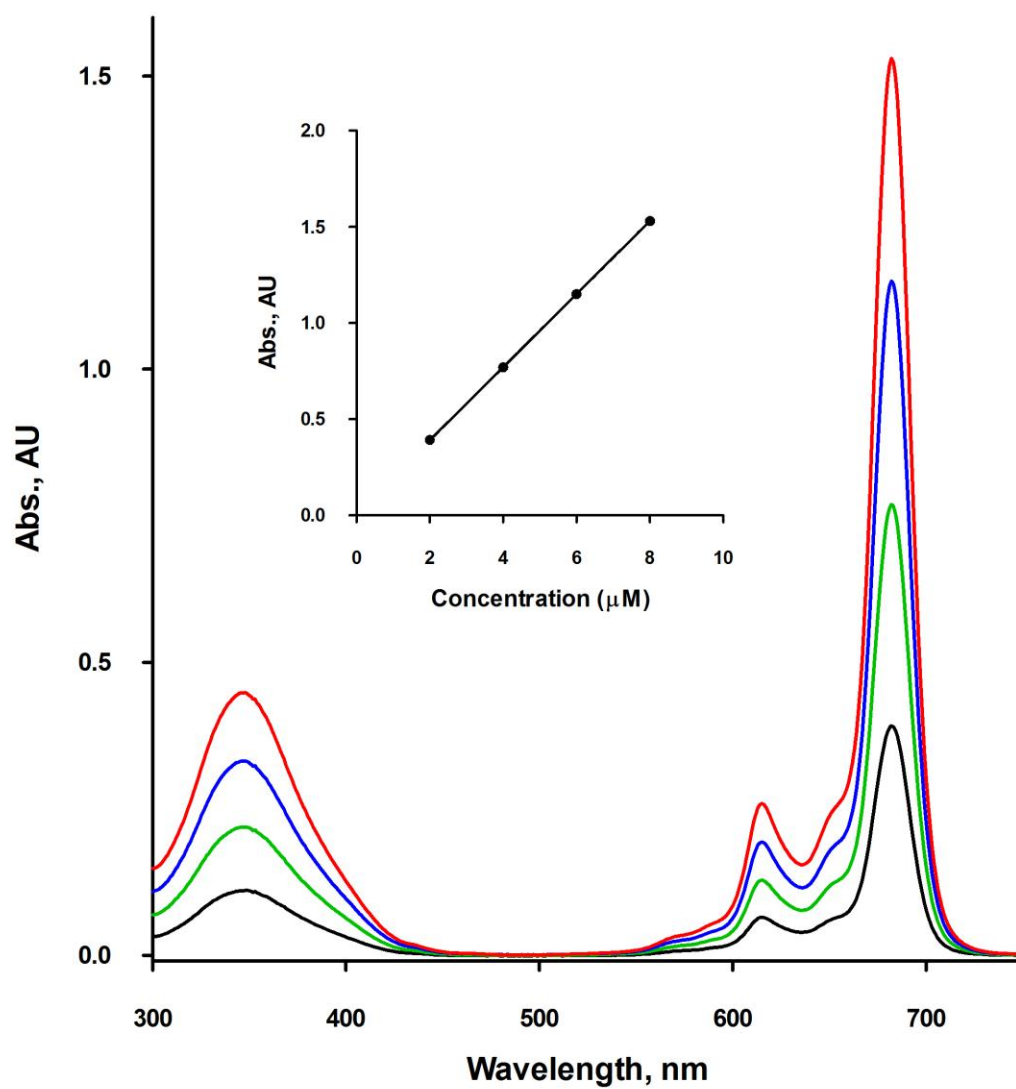
**Figure S17.** Absorption of Pc **4a** at 2.0 μM (black), 4.0 μM (green), 6.0 μM (blue), 8.0 μM (red) in DMF.



**Figure S18.** Absorption of Pc **4b** at 2.0 μM (black), 4.0 μM (green), 6.0 μM (blue), 8.0 μM (red) in DMF.

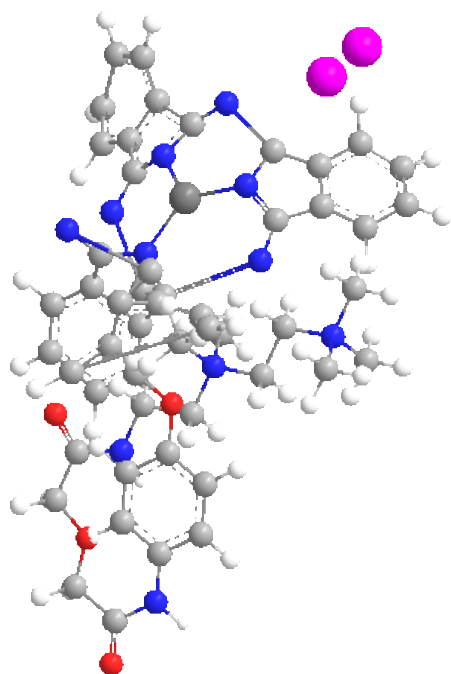


**Figure S19.** Absorption of Pc **16b** at 2.0 μM (black), 4.0 μM (green), 6.0 μM (blue), 8.0 μM (red) in DMF.

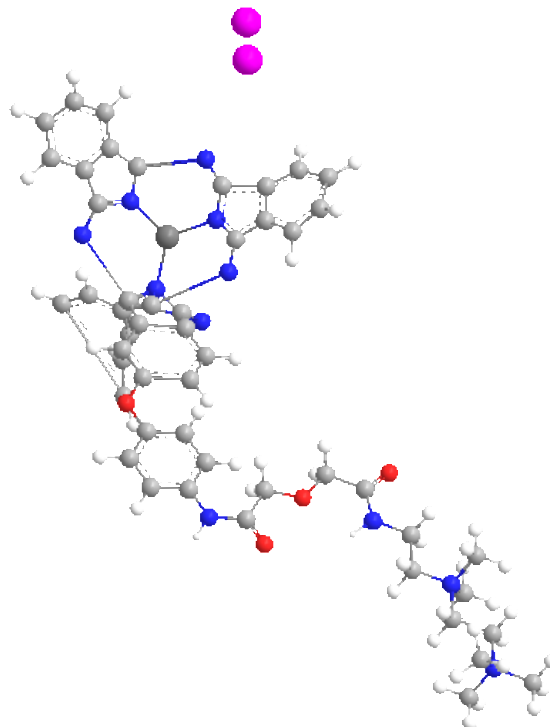


**Figure S20.** Absorption of Pc **16a** at 2.0 μM (black), 4.0 μM (green), 6.0 μM (blue), 8.0 μM (red) in DMF.

a)



b)



**Figure S21.** ChemBio3D HotLink Conformations of a) Pc **6a** and b) Pc **6b** without *tert*-butyl groups. Atoms: Carbon (grey), Hydrogen (white), Iodine (pink), Nitrogen (blue), Oxygen (red).