

Electronic Supplementary Information

Manuscript Title: Synthesis and *in vitro* photodynamic activity of new hexadeca-carboxy phthalocyanines

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Characterization Data for 3-5

3: ^1H NMR (CDCl_3 , 300 MHz) δ 8.55 (s, 2 H, ArH), 7.82 (s, 4 H, ArH), 7.32 (s, 2 H, ArH), 3.97 (s, 12 H, CH_3); $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 75.4 MHz) δ 164.9, 154.6, 150.8, 133.1, 127.6, 124.1, 124.0, 114.4, 112.3, 52.8; HRMS (LSI) m/z 545.1173 (calc. for MH^+ 545.1196); Anal. Calc. for $\text{C}_{28}\text{H}_{20}\text{N}_2\text{O}_{10}$: C, 61.77; H, 3.70; N, 5.14. Found: C, 61.56; H, 3.67; N, 5.07%.

4: ^1H NMR (DMSO-d_6 , 300 MHz) δ 8.70 (s, 8 H, Pc- H_α), 7.97 (s, 8 H, ArH), 7.86 (s, 16 H, ArH), -4.30 (s, 2 H, NH); $^{13}\text{C}\{^1\text{H}\}$ NMR (DMSO-d_6 , 75.4 MHz) δ 165.9, 156.8, 149.6, 147.4, 133.3, 132.3, 125.7, 122.1, 114.9; MS (MALDI-TOF) an isotopic cluster peaking at m/z 1955.18 (M^+); UV-Vis (THF) [$\lambda_{\text{max}}/\text{nm}$ ($\log \epsilon$)] 349 (4.77), 605 (4.37), 635 (4.55), 662 (4.95), 695 (4.97).

5: ^1H NMR (DMSO- d_6 , 300 MHz) δ 12.9 (br. s, 16 H, COOH), 8.71 (s, 8 H, Pc- H_α), 7.97 (s, 8 H, ArH), 7.80 (s, 16 H, ArH); $^{13}\text{C}\{^1\text{H}\}$ NMR (DMSO- d_6 , 75.4 MHz) δ 165.8, 157.3, 150.3, 148.1, 135.0, 133.0, 125.1, 121.5, 115.6; MS (MALDI-TOF) an isotopic cluster peaking at m/z 2018.25 (M^+); UV-Vis (THF) [$\lambda_{\text{max}}/\text{nm}$ ($\log \epsilon$)] 357 (4.95), 608 (4.57), 645 (4.55), 673 (5.36).

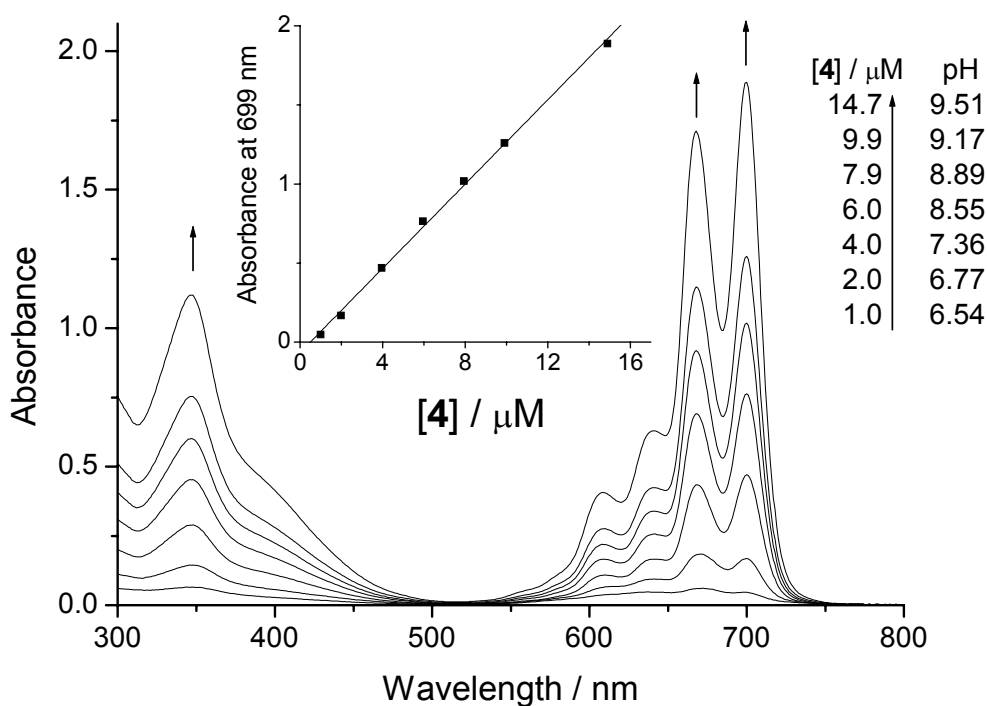


Fig. S1 UV-Vis spectra of **4** in the presence of NaOH (about 1.3 equiv. per COOH group) in water. The inset shows the plot of the absorbance of the longest-wavelength Q band vs. the concentration of **4**.

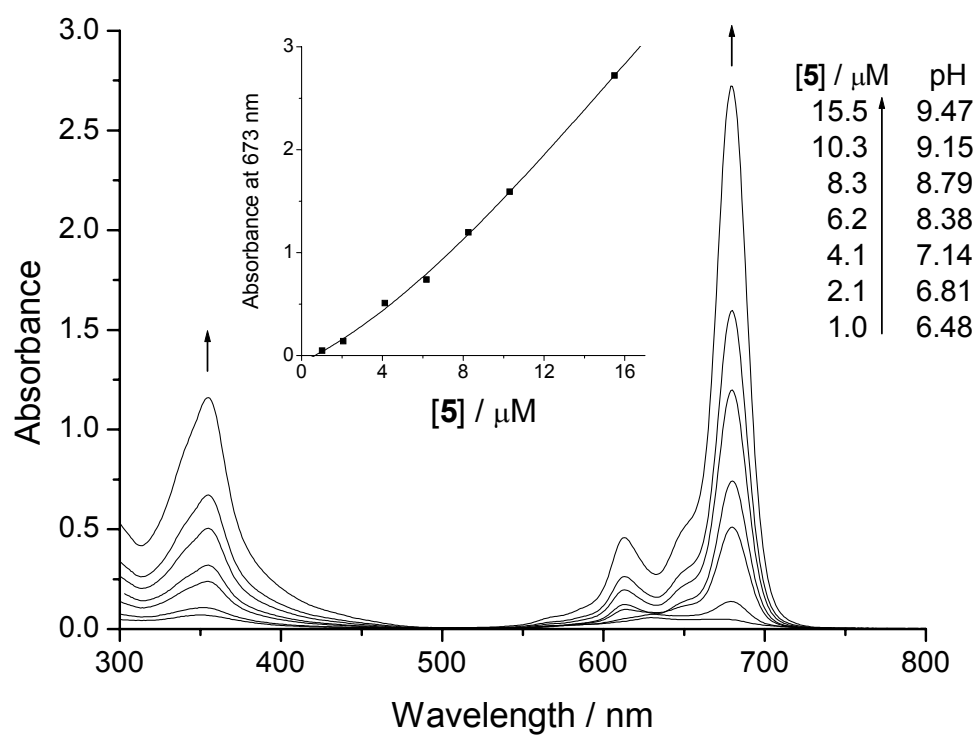


Fig. S2 UV-Vis spectra of **5** in the presence of NaOH (about 1.3 equiv. per COOH group) in water. The inset shows the plot of the Q-band absorbance vs. the concentration of **5**.

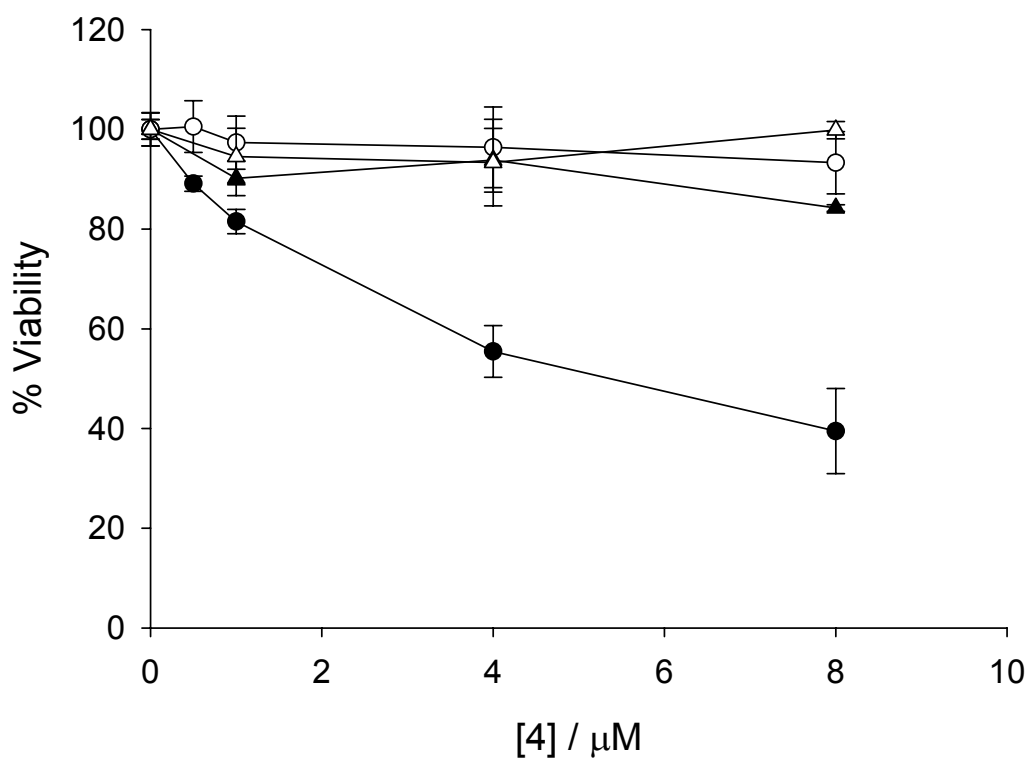


Fig. S3 Effect of **4** on HepG2 (triangles) and J774 (circles) in the absence (open symbols) and presence (closed symbols) of light. For the latter, the cells were illuminated with a red light ($\lambda > 610 \text{ nm}$, 40 mW cm^{-2} , 48 J cm^{-2}). Data are expressed as mean \pm SD ($n = 3$).