Supporting information for

Photodynamic inactivation of *Escherichia coli* with cationic ammonium Zn(II)phthalocyanines

Deisy M. G. C. Rocha,* a,b N. Venkatramaiah,* a,c Maria. C. Gomes, a,b Adelaide Almeida, b Maria A. F. Faustino, a Filipe A. Almeida Paz, c Ângela Cunha,* and João P. C. Tomé a,d

*a*QOPNA and Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal.

*b*Department of Biology and CESAM, University of Aveiro, 3810-193 Aveiro, Portugal.

*c*CICECO Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal.

*d*Department of Organic and Macromolecular Chemistry, Ghent University, B-9000 Gent, Belgium

*Corresponding authors: Angela Cunha: acunha@ua.pt; João P. C. Tomé: jtome@ua.pt

Table of Contents

1. NMRs of the compounds..........................................................................................................................2
2. MALDI-TOF MSs ........................................................................................................................................4
3. Solubility studies in DMSO and PBS........................................................................................................6
4. Absorption bands of the Pcs and emission bands of the light sources..............................................7
1. NMRs of the compounds

**Fig. S1** $^1$H NMR (300.13 MHz) spectrum of 1a in DMSO-$d_6$.

**Fig. S2** $^{19}$F NMR (282.38 MHz) spectrum of 1a in DMSO-$d_6$. 
Fig. S3 $^1$H NMR (300.13 MHz) spectrum of 2a in DMSO-$d_6$.

Fig. S4 $^{19}$F NMR (282.38 MHz) spectrum of 2a in DMSO-$d_6$. 
Fig. S5 $^1$H NMR (300.13 MHz) spectrum of 3a in DMSO-$d_6$.

2. MALDI-TOF MSs

Fig. S6 MALDI-TOF MS spectrum of 1a.

Chemical Formula: $C_{44}H_{44}F_4N_{12}Zn$

Exact Mass: 880.30
**Fig. S7** MALDI-TOF MS spectrum of 2a.

**Chemical Formula:** C_{56}H_{72}F_{8}N_{16}Zn

**Exact Mass:** 1184.52

---

**Fig. S8** MALDI-TOF MS spectrum of 3a.

**Chemical Formula:** C_{44}H_{44}Cl_{4}N_{12}Zn

**Exact Mass:** 944.18
3. Solubility studies in DMSO and PBS

**Fig. S9** UV-visible spectra of the phthalocyanines 1a, 2a and 3a in DMSO at different concentrations. The regression graphics represent absorbance of the Q-band of each Pc in DMSO versus concentrations.

**Fig. S10** UV-visible spectra of the phthalocyanines 1a, 2a and 3a in PBS at different concentrations. The regression graphics represent absorbance of the Q-band of each Pc in PBS versus concentrations.
4. Absorption bands of the Pcs and emission bands of the light sources

Fig. S11 UV-Normalized UV-Vis spectra of Pcs 1a, 2a and 3a in PBS and white and red light source emission.