

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^{b*} 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

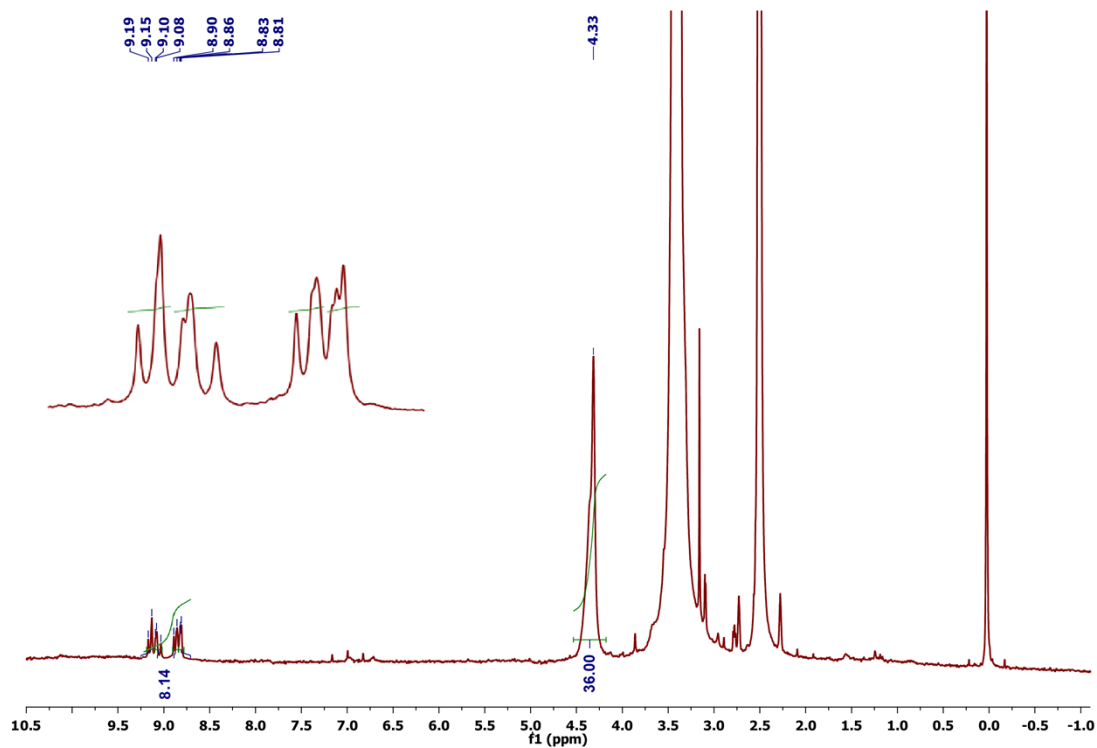


Fig. S1 ^1H NMR (300.13 MHz) spectrum of **1a** in $\text{DMSO-}d_6$.

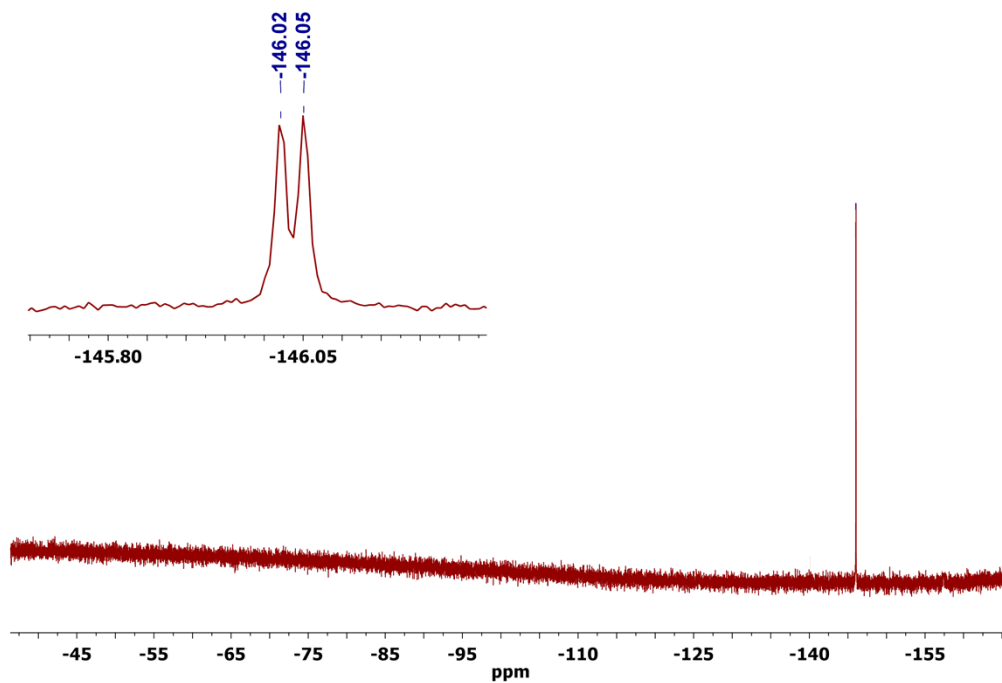


Fig. S2 ^{19}F NMR (282.38 MHz) spectrum of **1a** in $\text{DMSO-}d_6$.

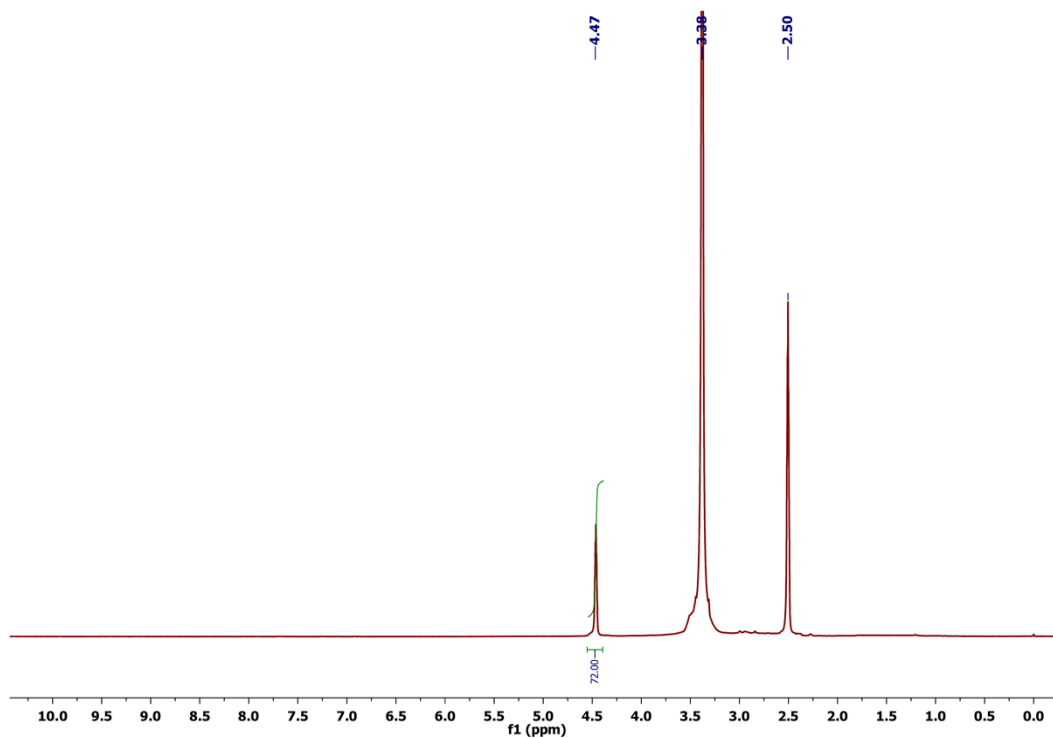


Fig. S 3 ¹H NMR (300.13 MHz) spectrum of **2a** in DMSO-*d*₆.

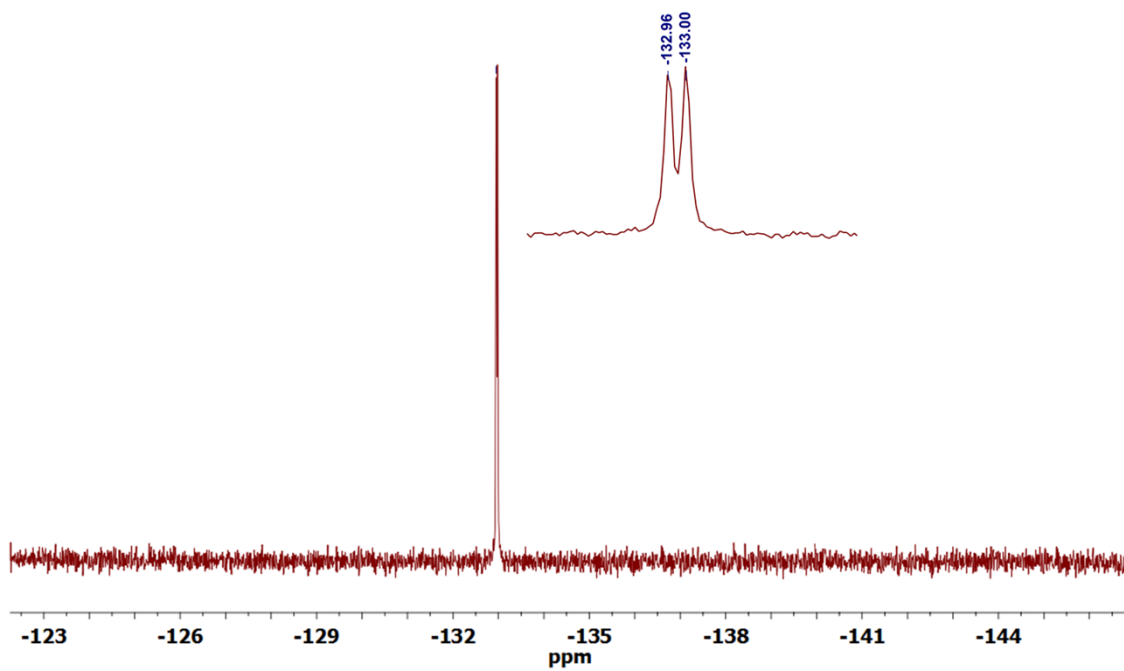


Fig. S4 ¹⁹F NMR (282.38 MHz) spectrum of **2a** in DMSO-*d*₆.

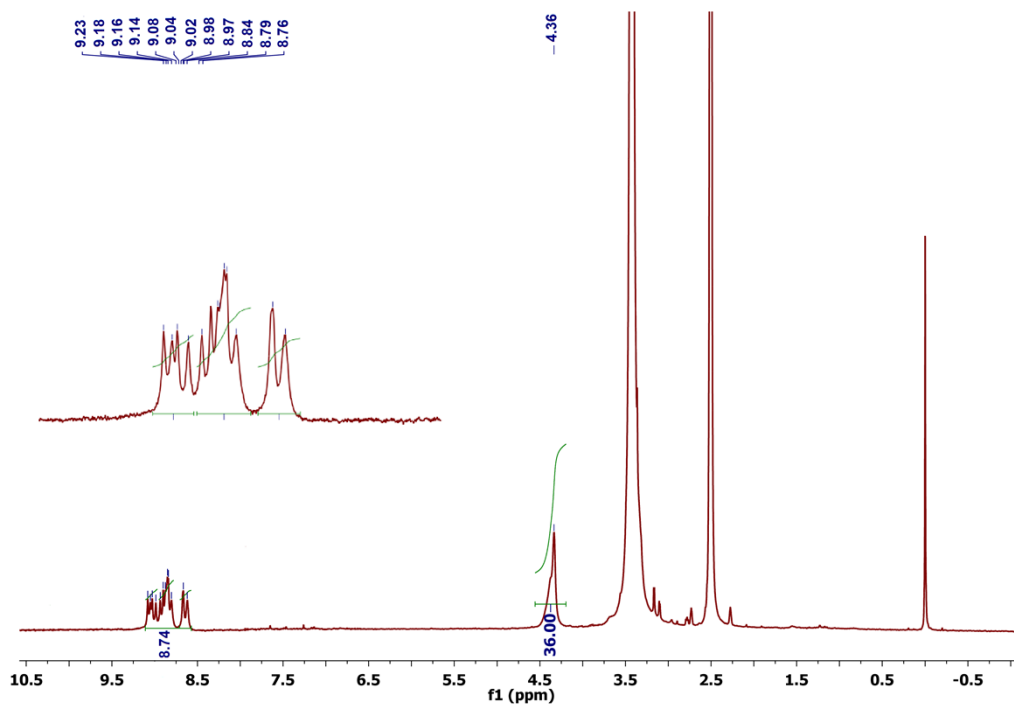


Fig. S5 ^1H NMR (300.13 MHz) spectrum of **3a** in $\text{DMSO-}d_6$.

2. MALDI-TOF MSs

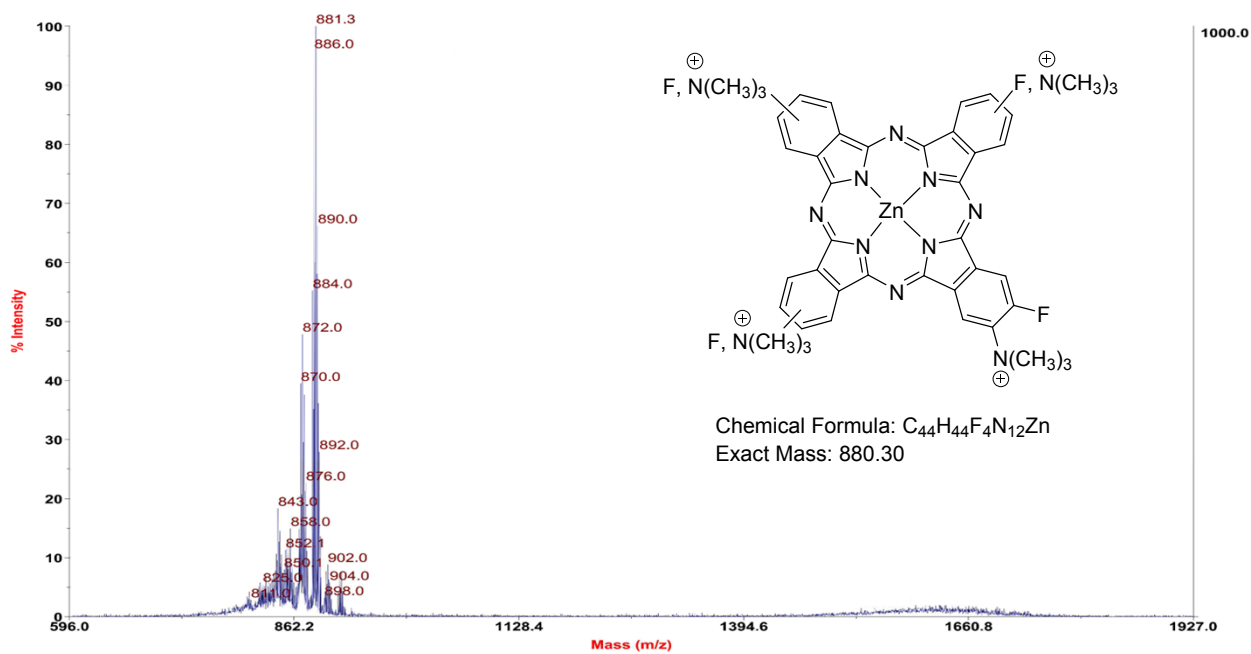


Fig. S6 MALDI-TOF MS spectrum of **1a**.

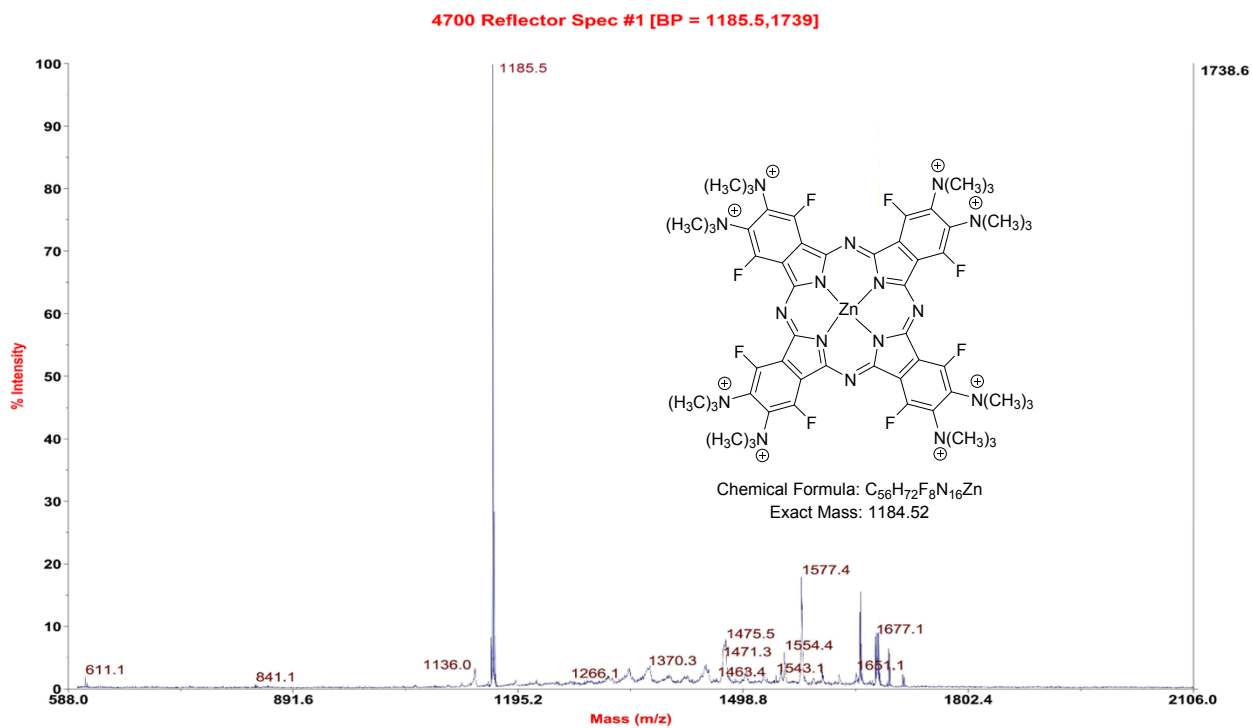


Fig. S7 MALDI-TOF MS spectrum of **2a**.

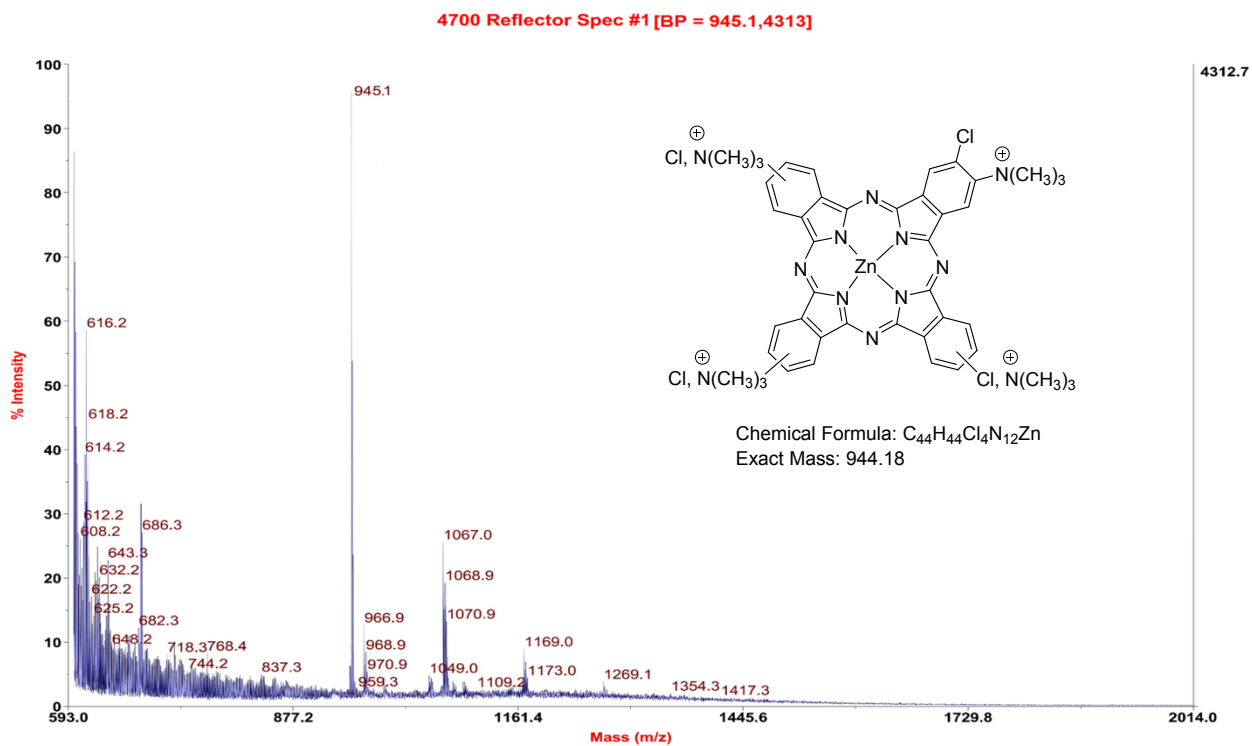


Fig. S8 MALDI-TOF MS spectrum of **3a**.

3. Solubility studies in DMSO and PBS

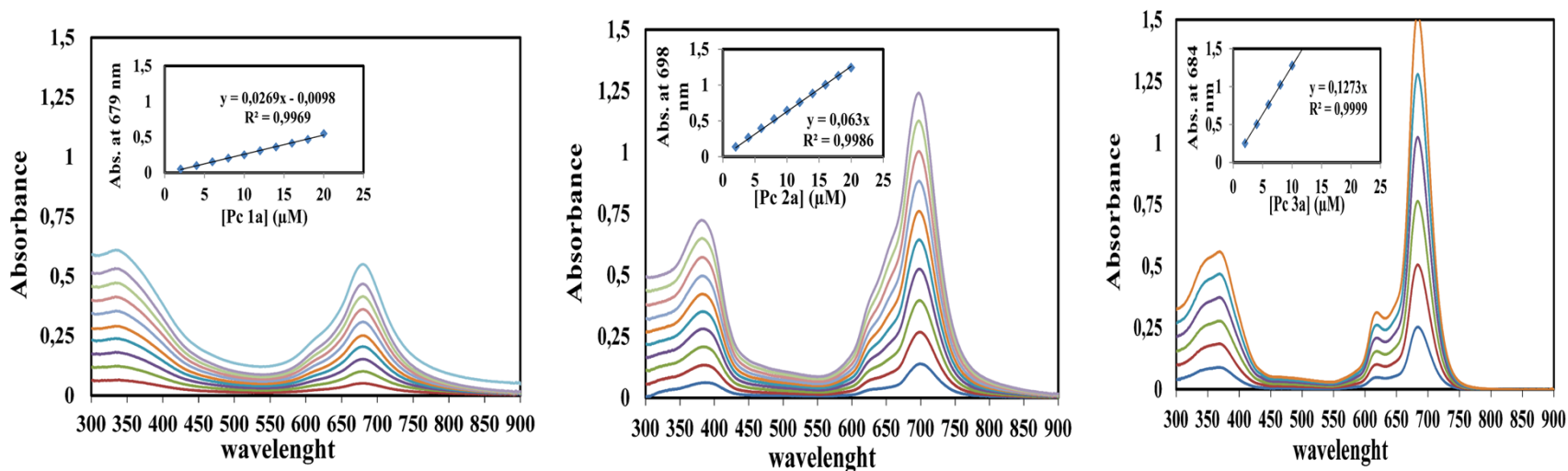


Fig. S9 UV-visible spectra of the phthalocyanines **1a**, **2a** and **3a** in DMSO at different concentrations. The regression graphics represent absorbance of the Q-band of each Pc in DMSO *versus* concentrations.

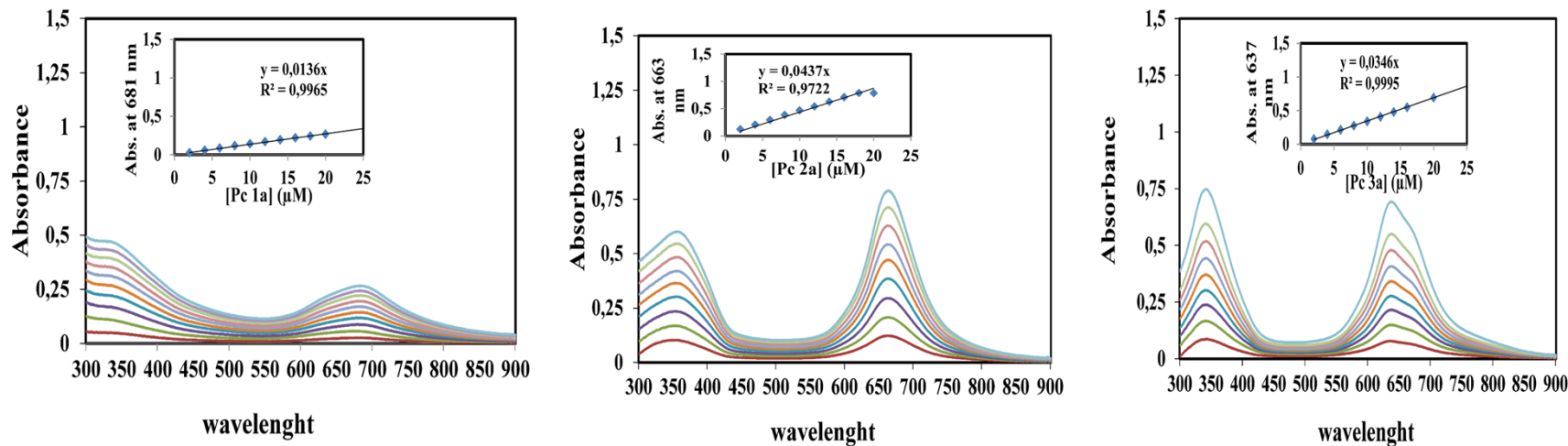


Fig. S10 UV-visible spectra of the phthalocyanines **1a**, **2a** and **3a** in PBS at different concentrations. The regression graphics represent absorbance of the Q-band of each Pc in PBS *versus* concentrations.

4. Absorption bands of the Pcs and emission bands of the light sources

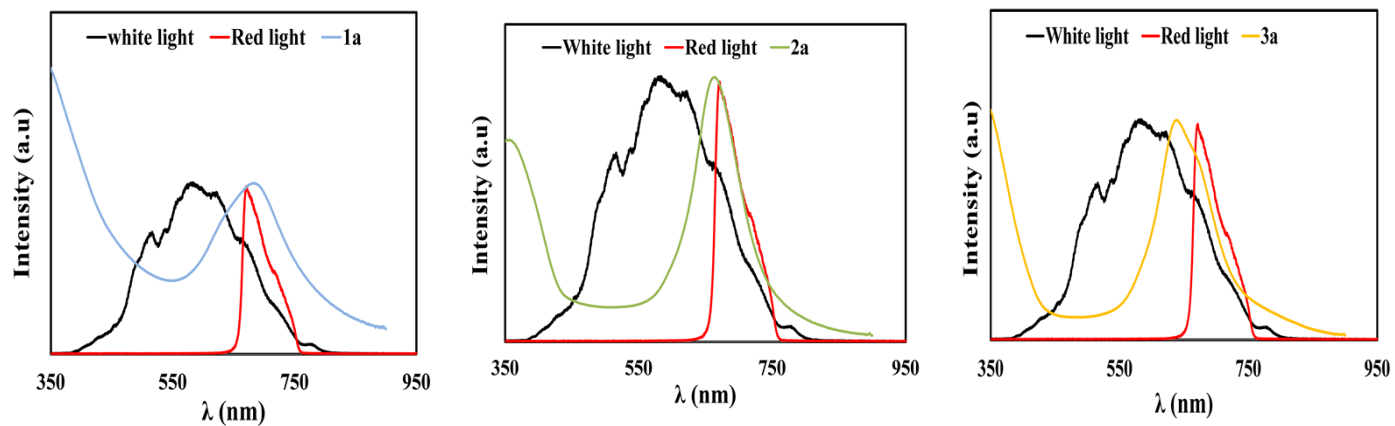


Fig. S11 UV- Normalized UV-Vis spectra of Pcs **1a**, **2a** and **3a** in PBS and white and red light source emission.