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Supporting Information

Synthesis, theoretical calculations and laser flash photolysis studies of selected amphiphilic porphyrin derivatives used as biofilms photodegradative materials

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Equations employed

The fluorescence quantum yield values of the porphyrin complexes alone or their conjugates were recorded using a comparative method reported in literature with equation 1.[1]

$$\Phi_F = \Phi_{F(Std)} \frac{F \, . \, A_{Std} \, . \, n^2}{F_{Std} \, . \, A \, . \, n^2_{Std}} \tag{1}$$

In this equation F and F_{Std} are the area under the emission curves of the sample and standard, respectively. A and A_{Std} are the absorbance values corresponding to the excitation wavelength of the studied samples and standard, respectively. n and n_{Std} express the refractive index of the solvents used to prepare the solution of the studied samples and standard, respectively. The TPP was used as a standard with the value: $\Phi_F = 0.14$.[2]

The determination of the singlet oxygen quantum yields (Φ_Δ) values of the prepared Ps and nanoconjugates were carried out following a UV/Vis spectroscopic method in DMSO. The monitoring was done spectroscopically following the photobleaching of 9, 10-dimethylanthracene (DMA) as a singlet oxygen scavenger. TPP (Φ_Δ = 0.52 in DMSO) [3] was utilized as standard for comparative purpose using equation 2.

$$\Phi_\Delta = \Phi_\Delta^{Std} \frac{R \, I_{abs}^{Std}}{R^{Std} \, I_{abs}} \tag{2}$$

Where Φ_Δ^{Std} is the singlet oxygen quantum yield for the standard, R and R^{Std} are the DMA photobleaching rates in the presence of Ps derivatives under investigation and the standard, respectively. I_{abs} and I_{abs}^{Std} are the rates of light absorption by the Ps derivative and standard, respectively. I_{abs} is determined by Eq. 3.

$$I_{abs} = \frac{\alpha . A . I}{N_A} \tag{3}$$

Where α is the fraction of light absorbed, A is the cell area irradiated, N_A is Avogadro's constant and I is the light intensity.

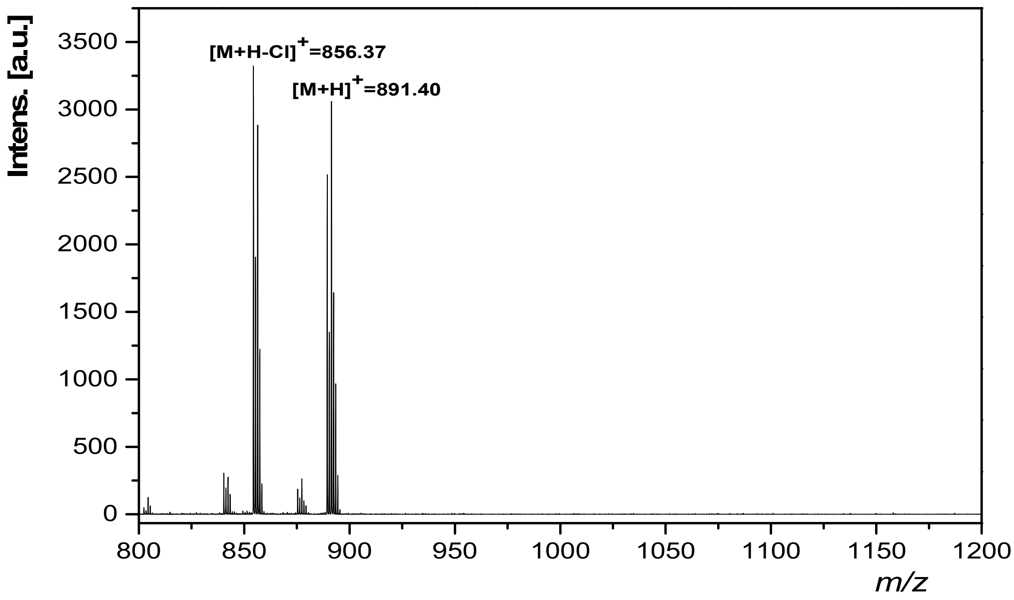


Fig. S1 Mass spectrum of complex **2**.

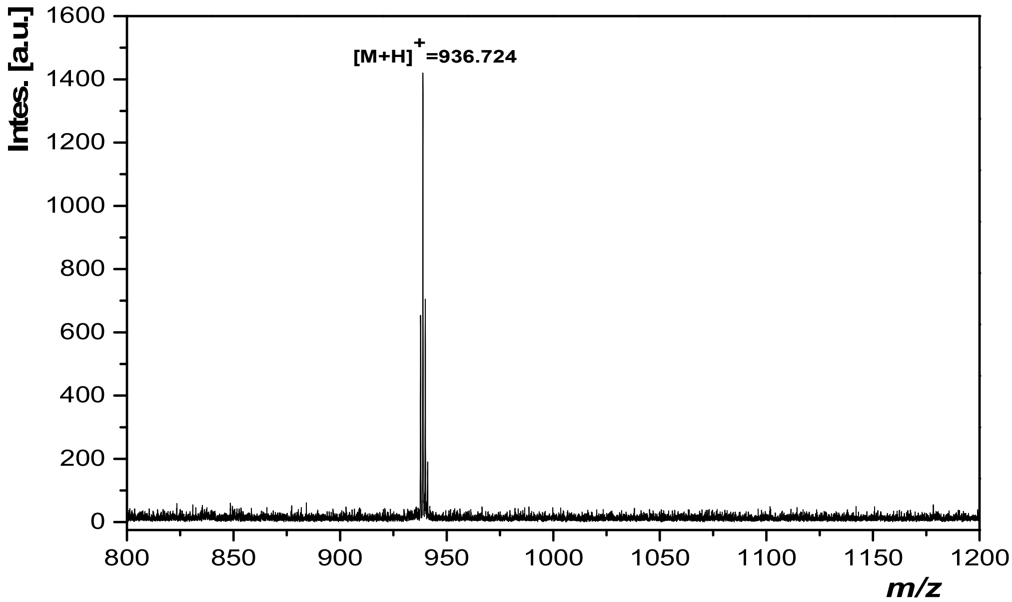


Fig. S2 Mass spectrum of complex **3**.

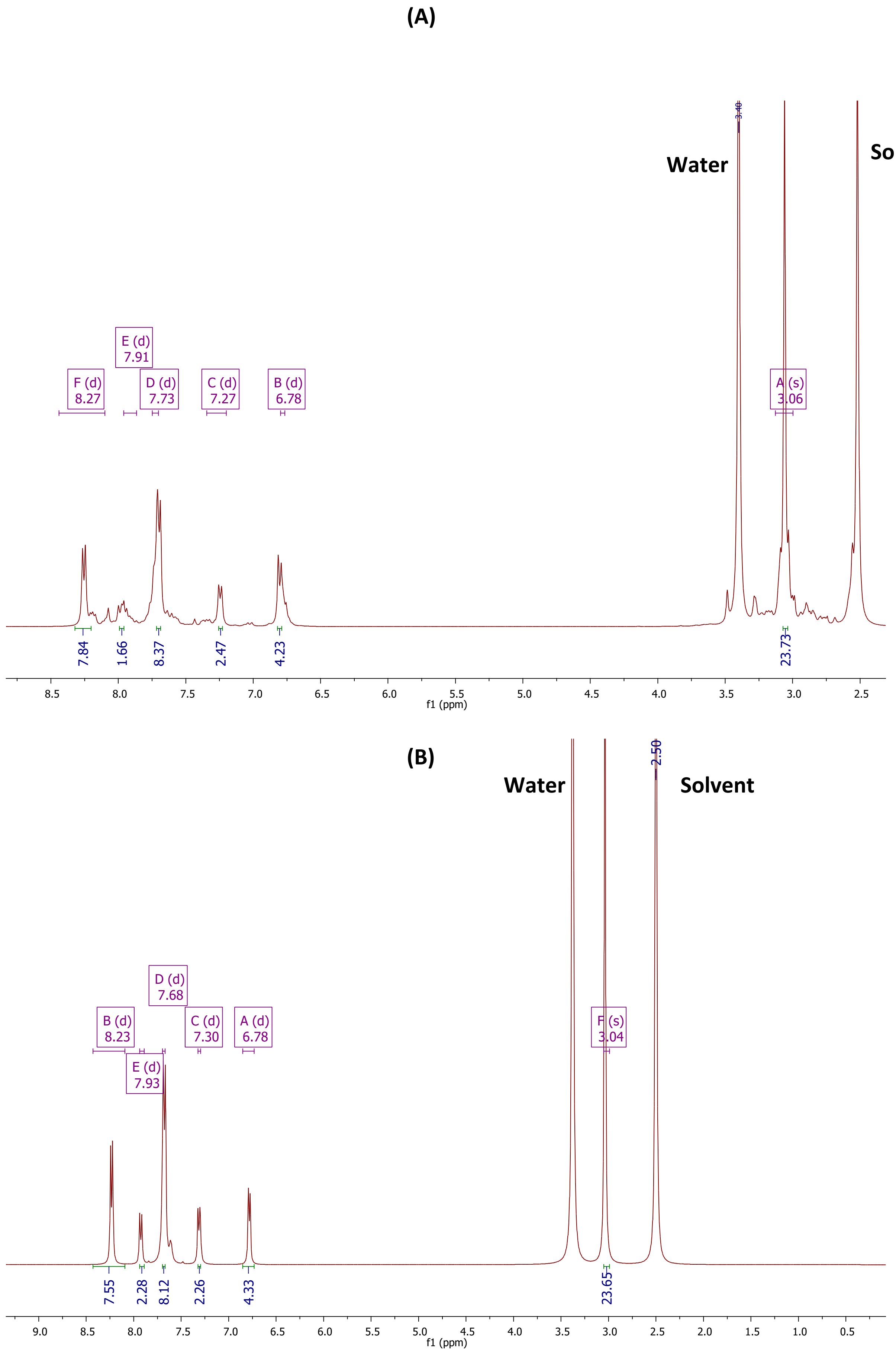
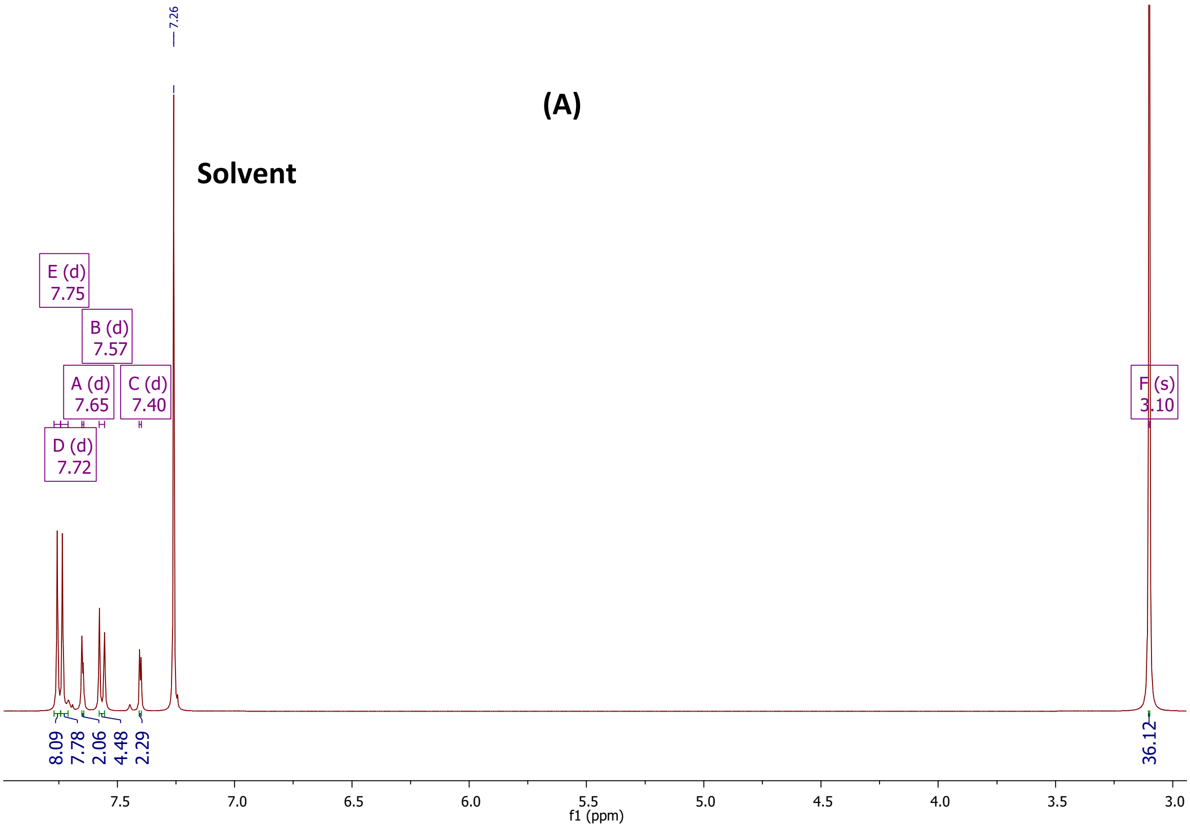


Fig. S3 ^{1}H NMR spectrum (400 MHz, DMSO-*d6*) of complex (**A**) **3** and (**B**) **2**



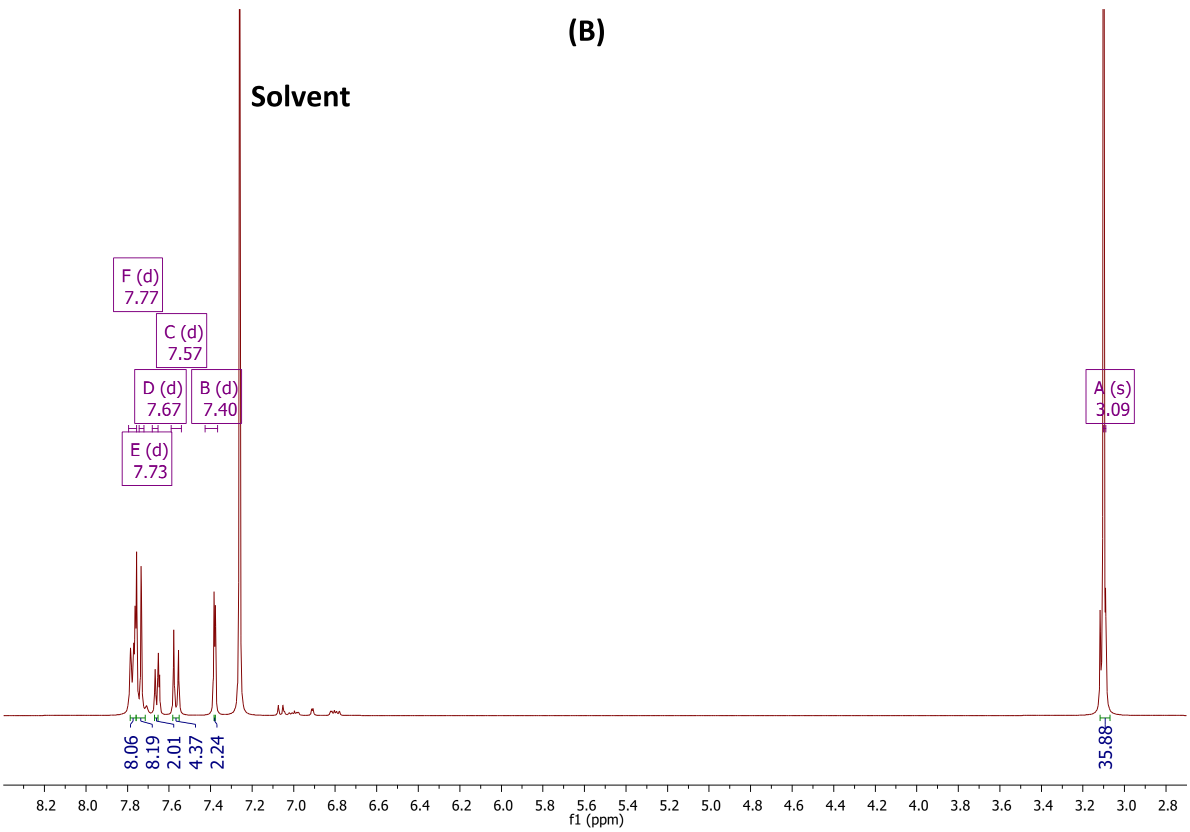
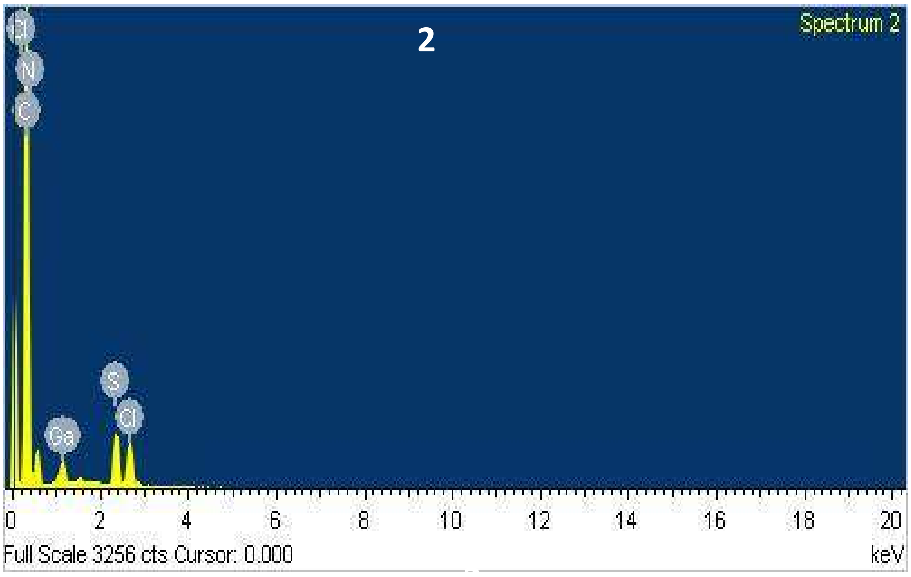
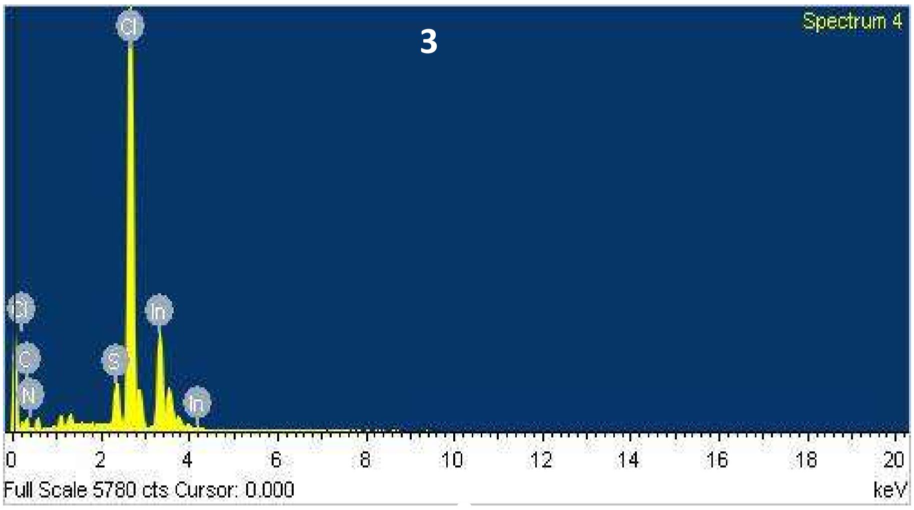


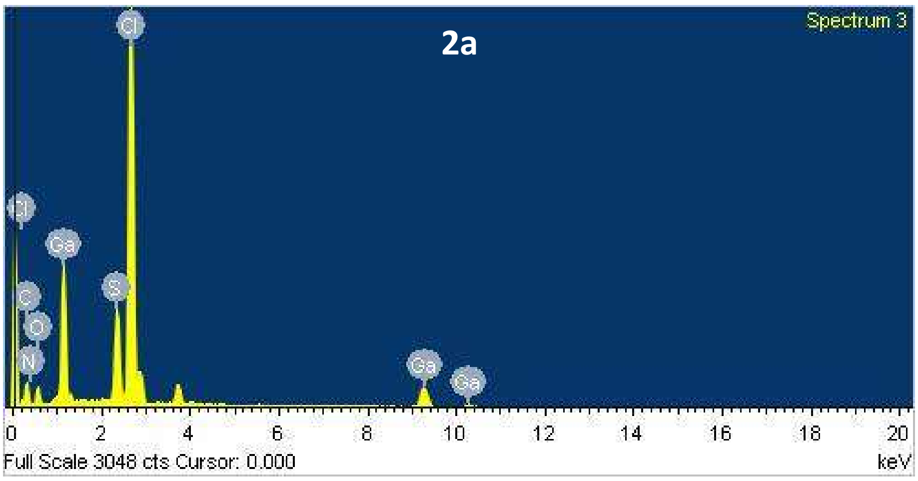
Fig. S4 ^{1}H NMR spectrum (400 MHz, $CDCl_3$) for complex (**A**): **2a** and (**B**) **3a**.



2
Spectrum 2
Cl
N
C
S
Cl
Ga
0 2 4 6 8 10 12 14 16 18 20
Full Scale 3256 cts Cursor: 0.000
keV



3
Spectrum 4
Cl
In
Si
C
N
S
In
0 2 4 6 8 10 12 14 16 18 20
Full Scale 5780 cts Cursor: 0.000
keV



2a
Spectrum 3
Cl
Cl
Ga
C
O
N
S
Ga
Ga
0 2 4 6 8 10 12 14 16 18 20
Full Scale 3048 cts Cursor: 0.000
keV

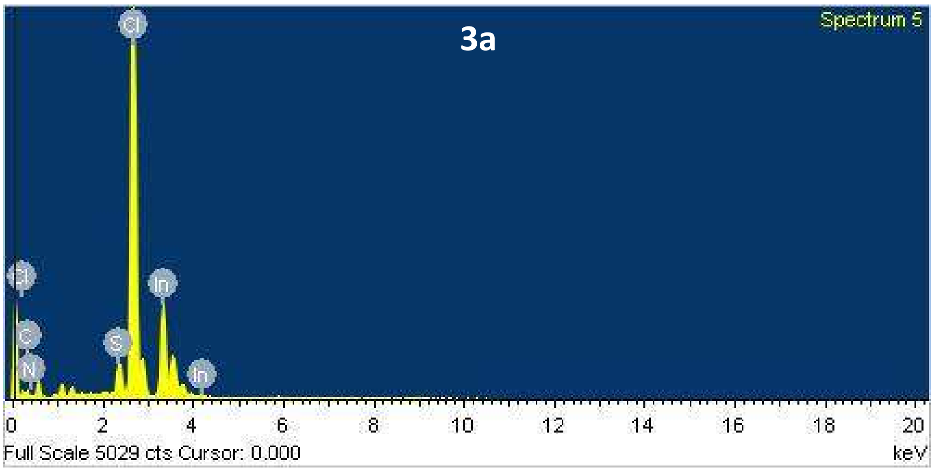


Fig. S5. EDX spectra for elemental analysis of the synthesized complexes **2**, **3**, **2a** and **3a**

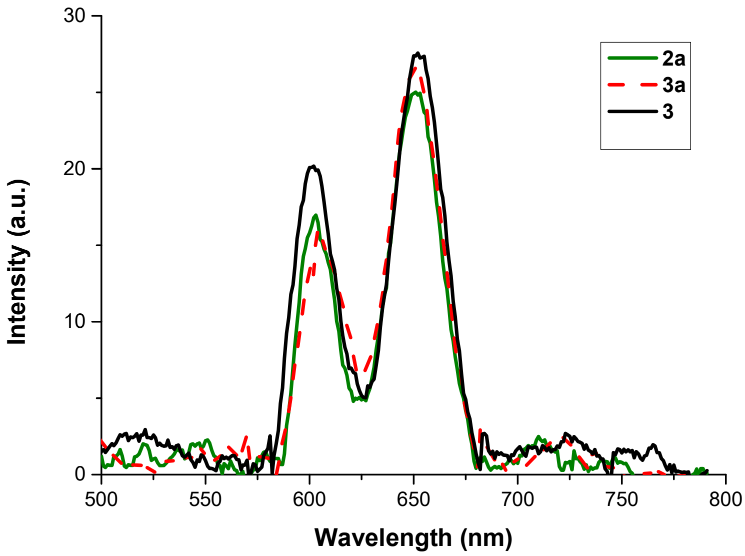
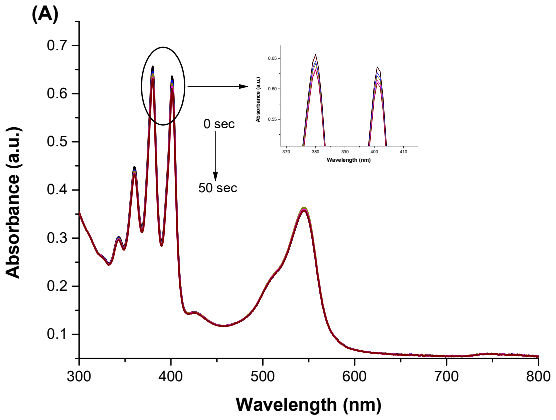
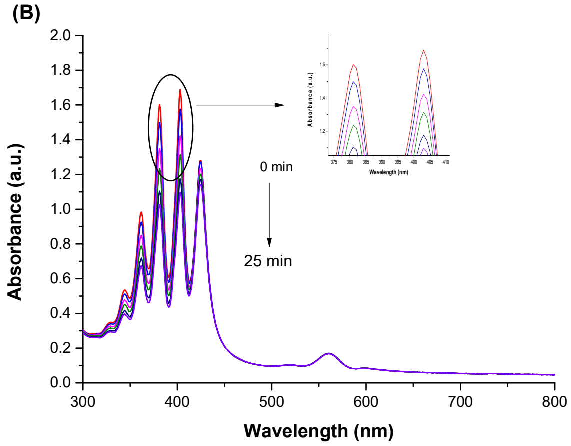
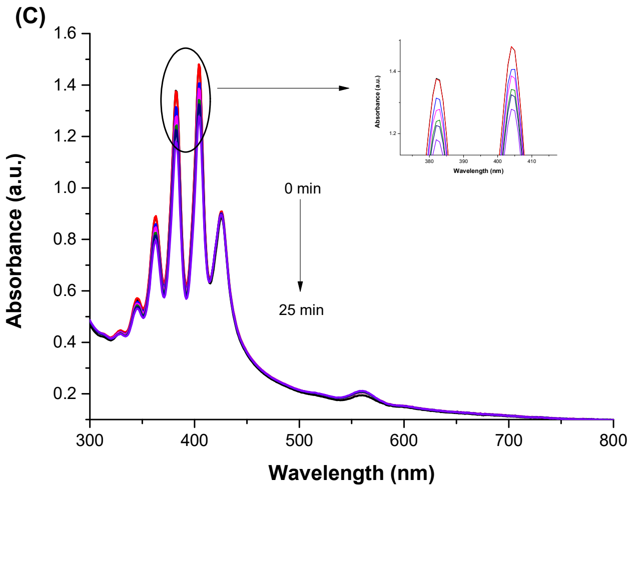


Fig. S6 Typical emission spectra of Porphyrins (**2a, 3a** and **3**) in DMSO


(A)
0 sec
50 sec
Absorbance (a.u.)
Wavelength (nm)


(B)
0 min
25 min
Absorbance (a.u.)
Wavelength (nm)


(C)
0 min
25 min
Absorbance (a.u.)
Wavelength (nm)

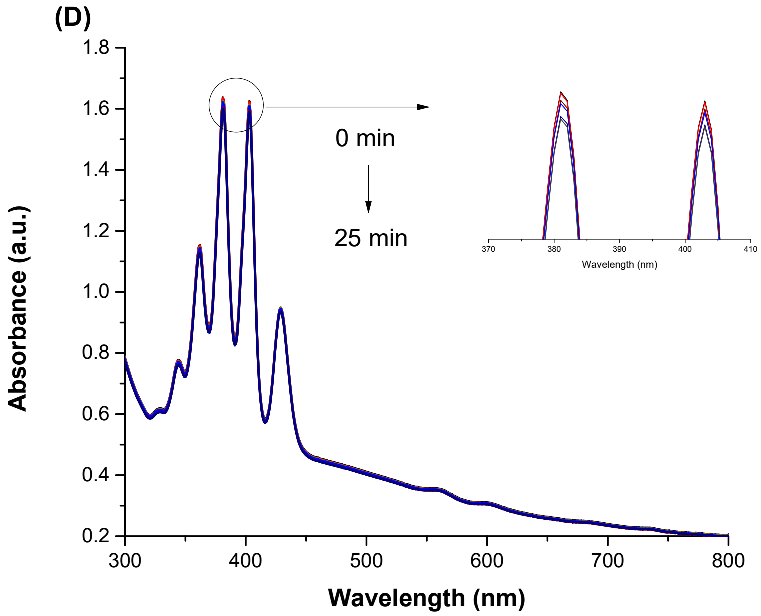
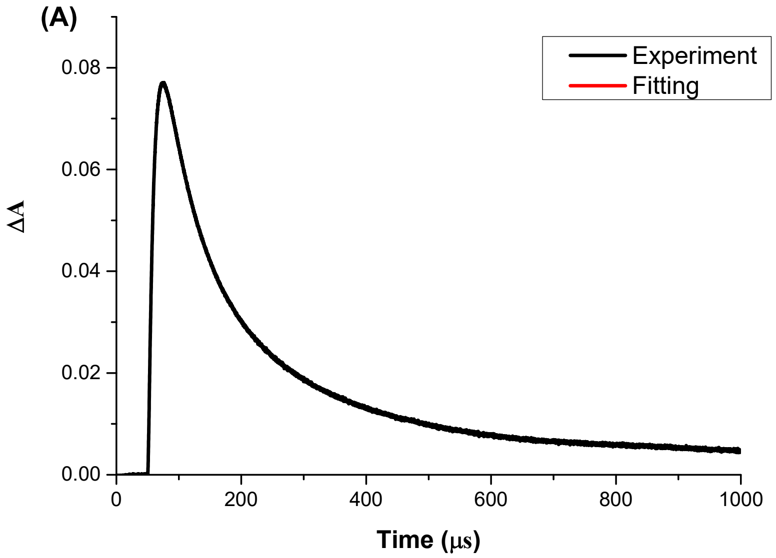


Fig. S7 Typical photodegradation spectra of ADMA **(A)** in the presence of RB; (**B**) in the presence of **3a;** (**C**) in the presence of **2a;** (**D**) in the presence of **2** in water (DMSO:PBS, 1:99 v/v).



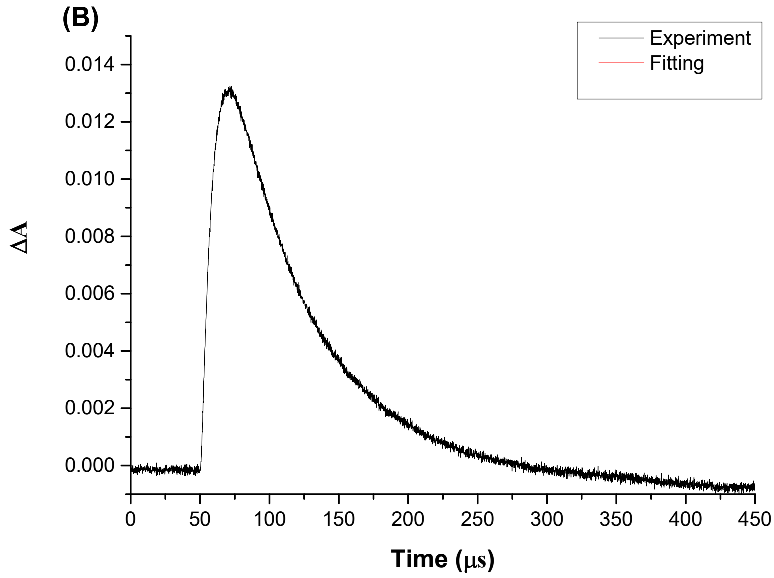


Fig. S8 Transient decay curve (λ_{exc} = 425 nm) of (**A**) **2a,** and (**B**) **3a** in degassed DMSO (as an examples)

Table S1 Conductivity or specific conductance of the quaternized porphyrin derivatives at 25 °C.

Sample	Conductivity (μS/cm)
Water alone	213.7 ± 0.6
2a (14 mg in 3mL water)	451.7 ± 1.2
3a (14 mg in 3mL water)	426.7 ± 1.2

References

1. A. Ogunsipe, J.Y. Chen and T. Nyokong, *New. J. Chem*., 2004, **7**, 822-827.

2. J.S. Hsiao, B.P. Krueger, R.W. Wagner, T.E. Johnson, J.K. Delaney, D.C. Mauzerall, G.R. Fleming, J.S. Lindsey, D.F. Bocian, R.J. Donohoe, *J. Am. Chem. Soc*., 1996, **118**, 11181-11193.

3. A.R. Da Silva, A.C. Pelegrino, A.C. Tedesco, R.A. Jorge, *J. Braz. Chem. Soc*., 2008, **19**, 491-501.