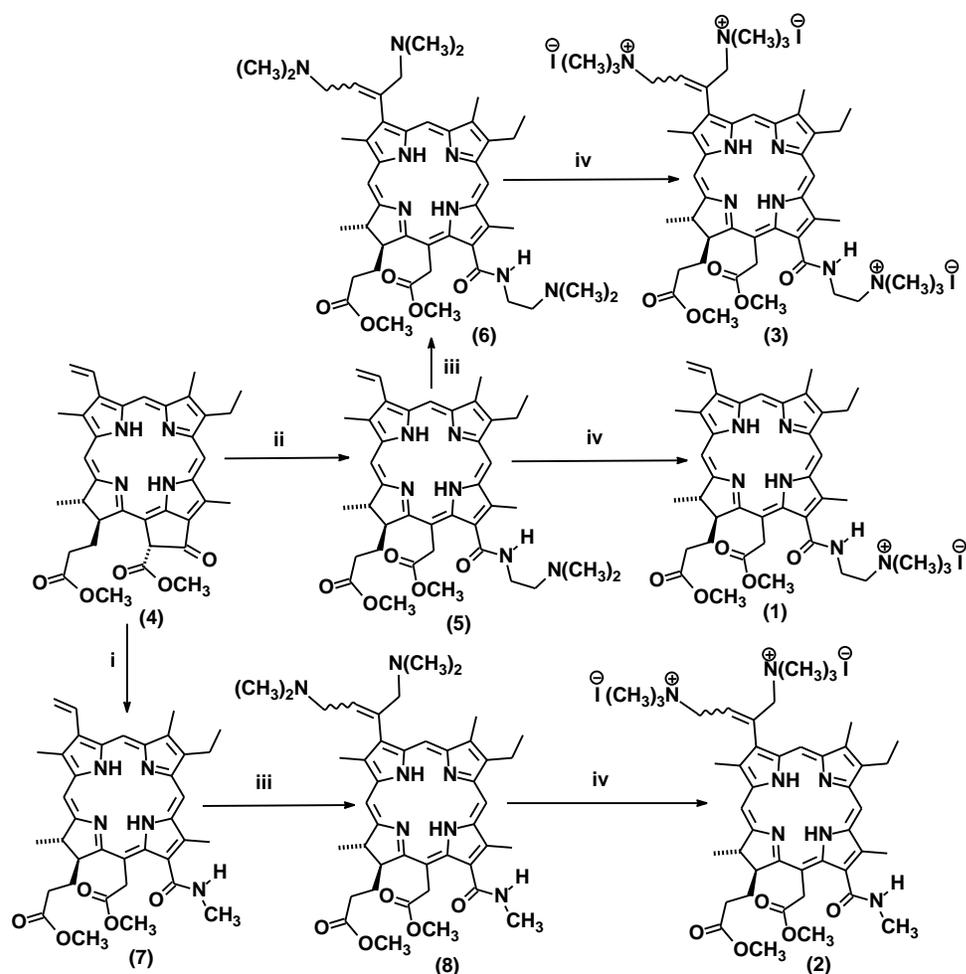


## Interaction of cationic chlorin photosensitizers with non-ionic surfactant Tween 80

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### 1. Synthetic scheme and identification of PSs

To obtain derivatives of chlorin  $e_6$  with one, two or three charged groups (see compounds **1–3** in Scheme S1), we carried out the chemical functionalization of methyl pheophorbide **a** (**4**) according to the scheme illustrated below (see also published procedure<sup>1</sup>).



**Scheme S1** Reagents and conditions: i,  $\text{MeNH}_2$  (aq.), THF, room temperature, 3 h; ii,  $\text{H}_2\text{NCH}_2\text{CH}_2\text{NMe}_2$ ,  $\text{CH}_2\text{Cl}_2$ , room temperature; iii,  $\text{CH}_2(\text{NMe}_2)_2$ , AcOH, THF, reflux, 0.5 h; iv, MeI,  $\text{CH}_2\text{Cl}_2$ , room temperature.







## 2. The PS–surfactant interaction and fluorescence quenching

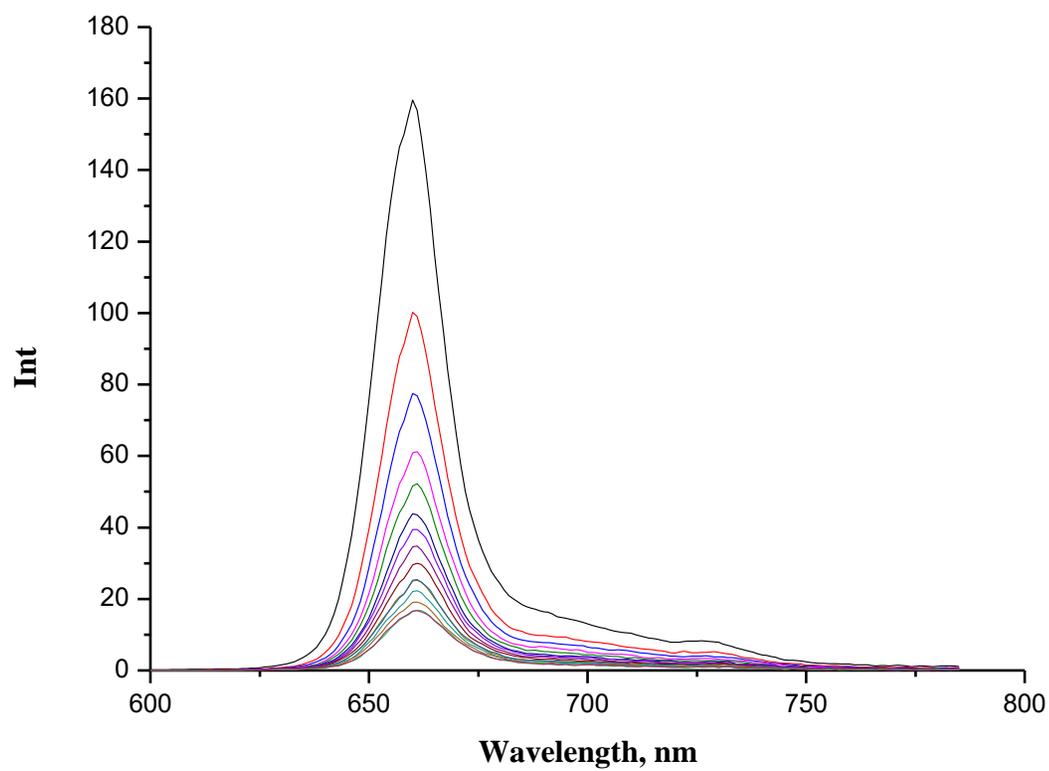
Cationic PSs (compounds **2**, **3**) were dried in vacuum at 353 K for several days. Water was distilled twice and non-ionic surfactant Tween 80 provided by Panreac (Chemical purity) was used as supplied. UV-VIS spectra were obtained at 293 K on a Drawell G9 spectrophotometer in highly dilute pigment solutions ( $\sim 7.3 \mu\text{mol kg}^{-1}$ , see Table S1). Fluorescence spectra were recorded on a CM 2203 spectrofluorimeter (Solar) at a PS concentration of  $1.1 \mu\text{mol kg}^{-1}$  (see Table S2 and Figures S4 and S5). The concentrations of PSs and surfactants were kept constant during the titration with KI solutions.

**Table S1** Spectrophotometric titration of aqueous solutions of compounds **2**, **3** with Tween 80.

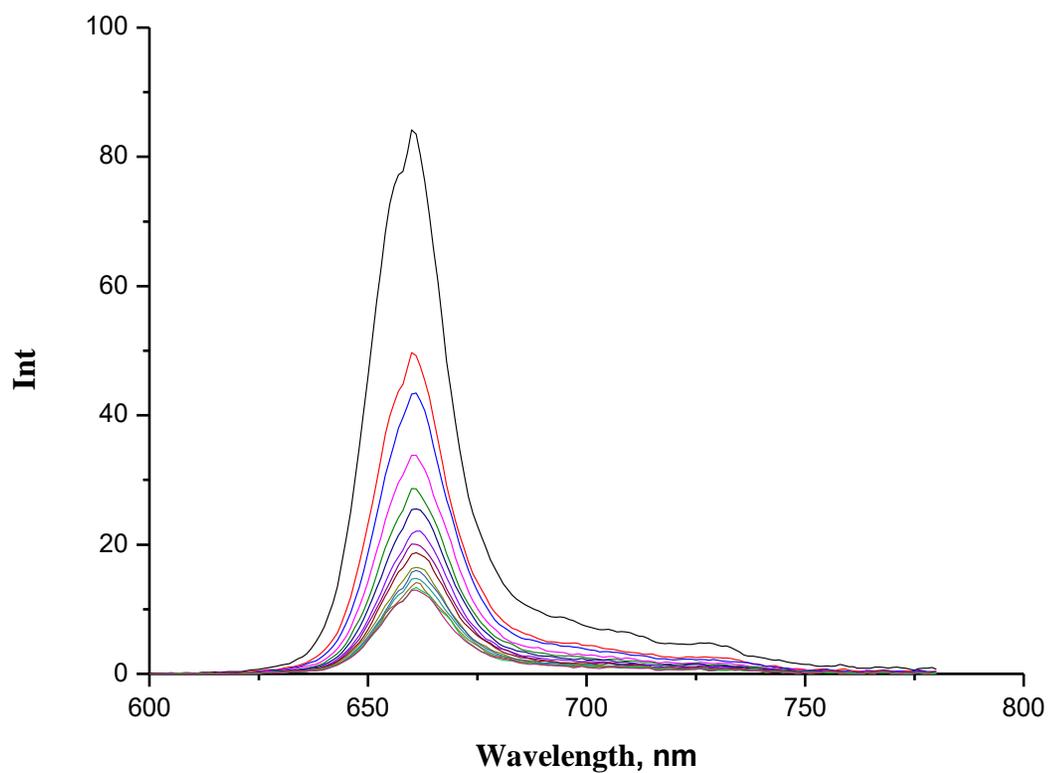
$m_T \times 10^4/\text{mol kg}^{-1}$	$A/\text{arbitrary units}$	$m_T \times 10^4/\text{mol kg}^{-1}$	$A/\text{arbitrary units}$
compound <b>2</b> , $\lambda = 407 \text{ nm}$		compound <b>3</b> , $\lambda = 395 \text{ nm}$	
0	0.545	0	1.29
2.920	0.566	0.06273	1.332
4.380	0.583	0.1131	1.346
5.840	0.596	0.1459	1.349
7.300	0.614	0.2378	1.366
10.95	0.626	0.2619	1.375
14.60	0.635	0.5333	1.387
21.90	0.641	0.5579	1.39
31.00	0.645	0.8748	1.438
36.50	0.649	1.110	1.441
43.80	0.652	1.488	1.479
54.75	0.655	2.215	1.480
73.00	0.657	2.558	1.481

**Table S2** Fluorescence titration of compounds **2** and **3** in aqueous Tween 80 solutions using KI at various PS/surfactant molar ratios.

Compound 2				Compound 3			
PS/Tween 80 = 1 : 60		PS/Tween 80 = 1 : 6000		PS/Tween 80 = 1 : 60		PS/Tween 80 = 1 : 6000	
$m_{\text{KI}}/\text{mol kg}^{-1}$	$F/F_0$						
0	1	0	1	0	1	0	1
0.073171	1.5933	0.073171	1.2487	0.073171	1.6957	0.043530	1.1967
0.14286	2.0603	0.14286	1.4172	0.14286	1.9222	0.080882	1.2252
0.20930	2.6192	0.20930	1.6180	0.20930	2.4711	0.10804	1.2508
0.27273	3.0894	0.27273	1.7638	0.27273	2.9156	0.13209	1.2935
0.33333	3.6430	0.33333	1.9109	0.33333	3.2704	0.37324	1.5960
0.39130	4.0462	0.39130	2.0561	0.44681	3.7830	0.42261	1.7173
0.44681	4.6129	0.50000	2.2760	0.55102	4.1730	0.49525	1.6949
0.55102	5.4099	0.60000	2.5444	0.64706	4.4508	0.57381	1.7863
0.64706	6.3737	0.69231	2.7533	0.73585	5.0682	0.70185	1.9260
0.73585	6.3158	0.77778	2.9924	0.81818	5.2183	0.82885	1.9962
0.81818	7.2421	0.93103	3.3499	0.96610	5.6551	0.90793	2.1020
0.96610	8.3833	1.0645	3.6863				



**Figure S4** Changes in fluorescence spectra ( $\lambda_{\text{exc}} = 405 \text{ nm}$ , 298 K) of compound **2** ( $m_{\text{PS}} = 1.1 \times 10^{-6} \text{ mol kg}^{-1}$ ) in aqueous solution of Tween 80 (PS/Tween 80 = 1 : 60) during titration with 3 M solution of KI (see Table S2).



**Figure S5** Changes in fluorescence spectra ( $\lambda_{\text{exc}} = 405 \text{ nm}$ , 298 K) of compound **3** ( $m_{\text{PS}} = 1.1 \times 10^{-6} \text{ mol kg}^{-1}$ ) in aqueous solution of Tween 80 (PS/Tween 80 = 1 : 60) during titration with 3 M solution of KI (see Table S2).

### References

1. A. V. Kustov, D. V. Belykh, N. L. Smirnova, E. A. Venediktov, T. V. Kudayarova, S. O. Kruchin, I. S. Khudyaeva and D. B. Berezin, *Dyes Pigm.*, 2018, **149**, 553.