Supplementary Information

Distribution of Xanthene Dyes in DPPC Vesicles: Rationally Accounting for Drug Partitioning Using a Membrane Model

Italo R. Calori,*[a] Diogo S. Pellosi,[b] Douglas Vanzin,[b] Gabriel B. Cesar,[b] Paulo C. S. Pereira,[b] Mario J. Politi,[c] Noboru Hioka[b] and Wilker Caetano[b]

[a]Departamento de Química, Laboratório de Fotobiologia e Fotomedicina, Faculdade de Filosofia, Ciências e Letras de Ribeirão Preto, Universidade de São Paulo, 14040-901 Ribeirão Preto-SP, Brazil

[b]Departamento de Química, Núcleo de Pesquisa em Sistemas Fotodinâmicos, Universidade Estadual de Maringá, 87020-900 Maringá-PR, Brazil

[c]Departamento de Bioquímica, Laboratório de Cinética Rápida e Fototermia, Universidade de São Paulo, 05513-970 São Paulo-SP, Brazil

The Förster distance (cm) is given by the equation S1:

$$R_0 = 8.8 \times 10^{-5}(k^2 n^{-4} Q_D J) \quad (S1)$$

where k^2 is the factor describing the relative orientation in space of the transition dipoles of the donor and acceptor, n is the refractive index of the medium, Q_d is the fluorescence quantum yield of the donor in the absence of the acceptor, and J is the overlap integral between the donor emission and acceptor absorption, as given by equation S2:

$$J = \int_0^\infty F_d(\lambda)\varepsilon_\alpha(\lambda)\lambda^4 d\lambda \quad (S2)$$

where F_d is the corrected fluorescence intensity of the donor at wavelength λ to $\lambda + \Delta\lambda$ with the total intensity normalized to unity, and ε_α is the molar absorptivity of the acceptor in absence of the donor (in L mol^{-1} cm^{-1}). Equation S3 gives the efficiency of energy transfer.

$$E = 1 - \left(\frac{F_{da}}{F_d}\right) = 1 - \left(\frac{\tau_{da}}{\tau_d}\right) \quad (S3)$$

*e-mail: italocalori@hotmail.com

where F_{da} and F_d correspond to the static fluorescence intensities of the donor in the presence and absence of acceptor, respectively, and τ_{da} and τ_d correspond to the fluorescence lifetime of the donor in the presence and absence of the acceptor, respectively.

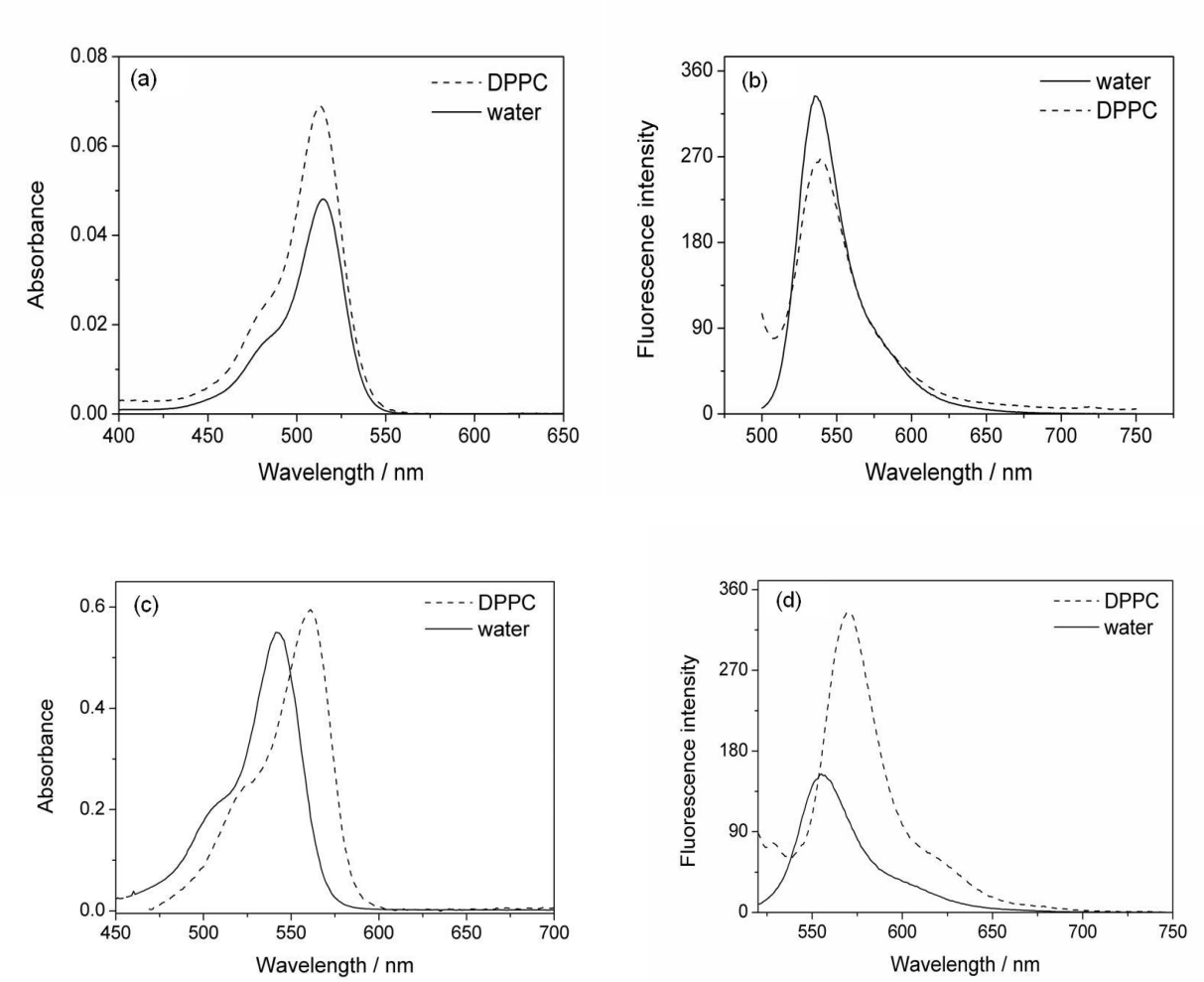


Figure S1. Absorption (5.00×10^{-6} mol L^{-1}) of (a) EOS and (c) RBB; fluorescence emission (5.00×10^{-7} mol L^{-1}) spectra of (b) EOS and (d) RBB in water (solid line) and DPPC vesicle (dashed line) suspension (7.5×10^{-4} mol L^{-1}). The excitation wavelength used was 480 and 500 nm for EOS and RBB, respectively. pH 7.25, I = 0.10 mol L^{-1} at 30.0 °C.

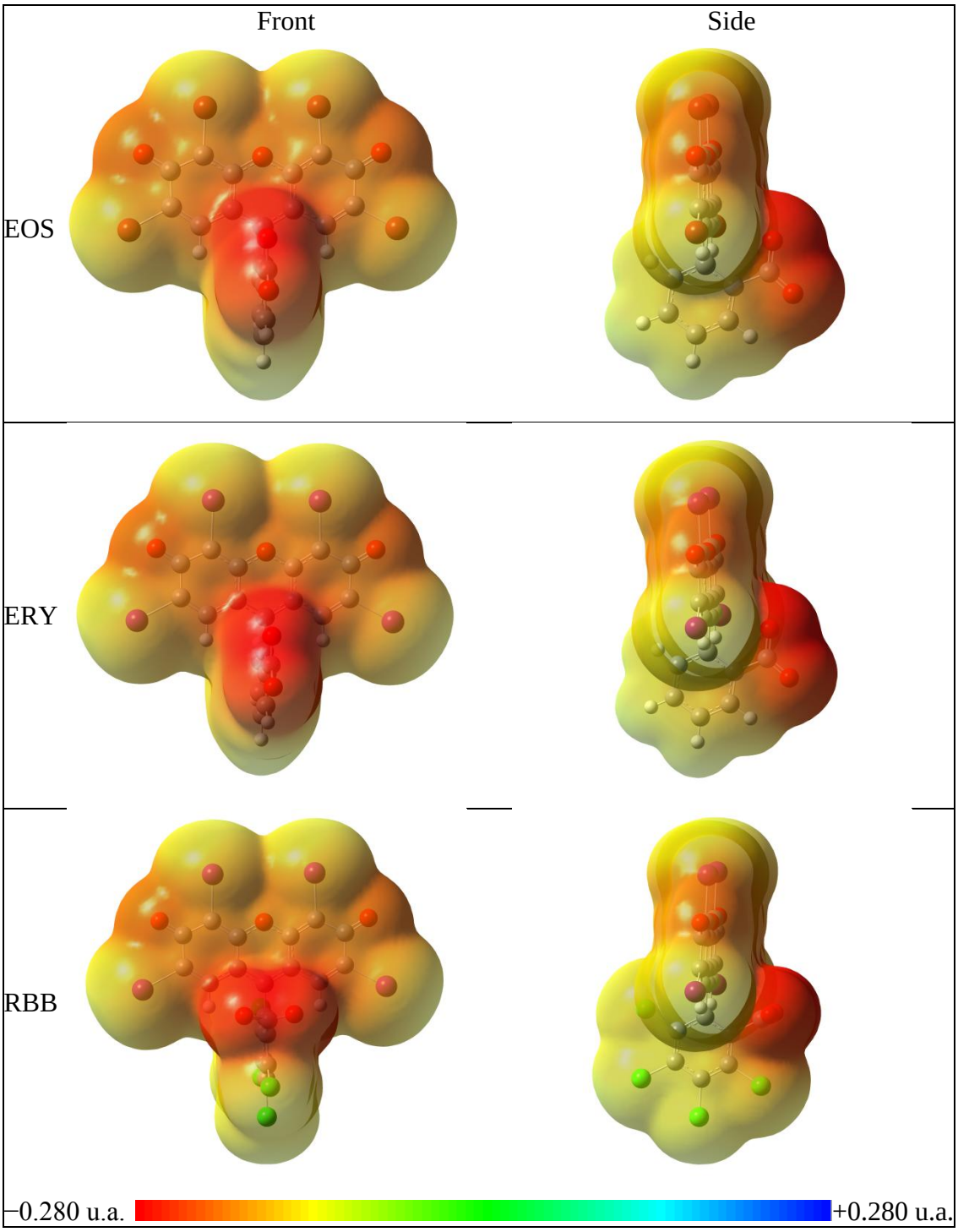


Figure S2. Electrostatic potential maps to EOS, ERY and RB generated with electron density from total SCF density, mapped with ESP.

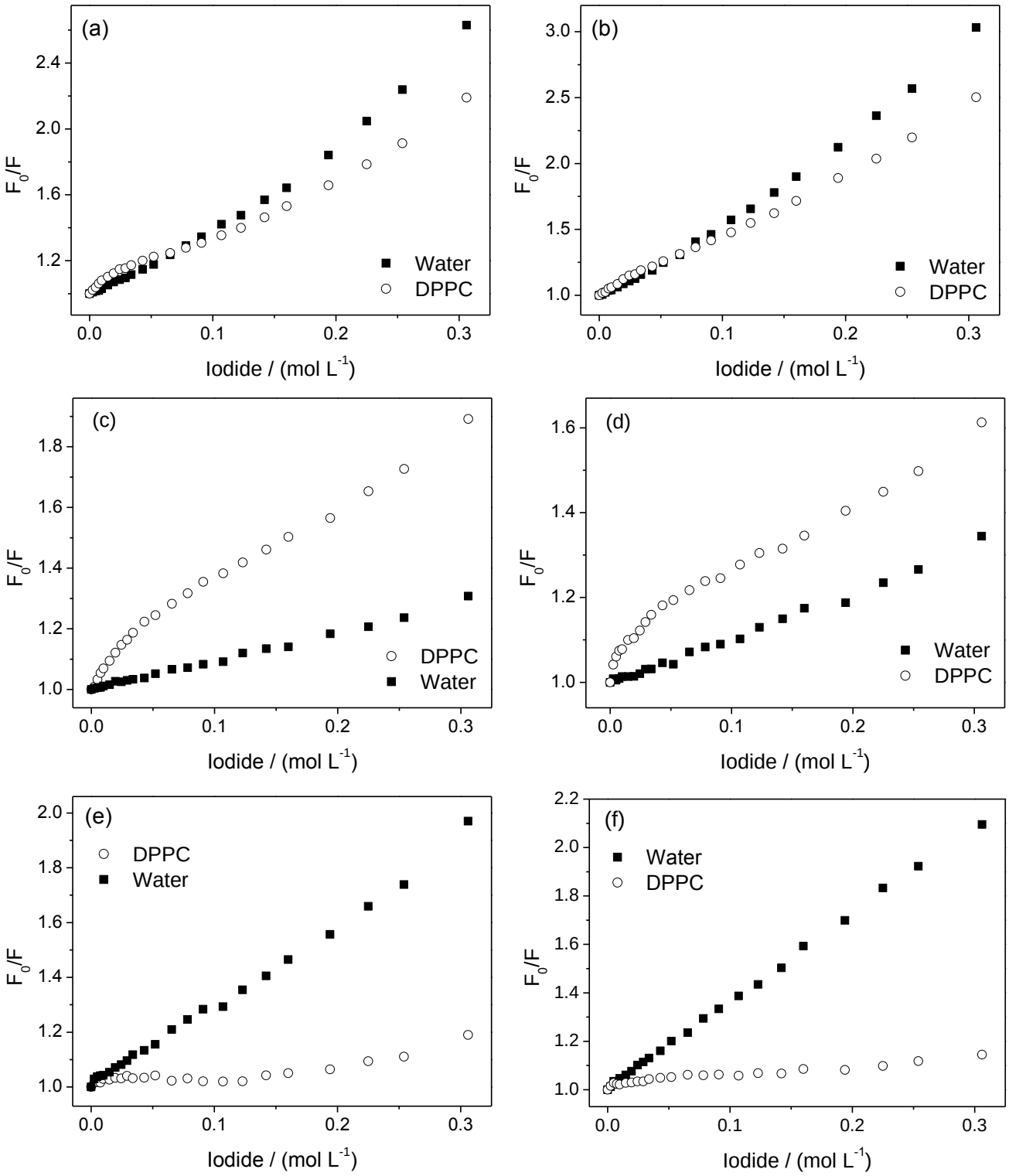
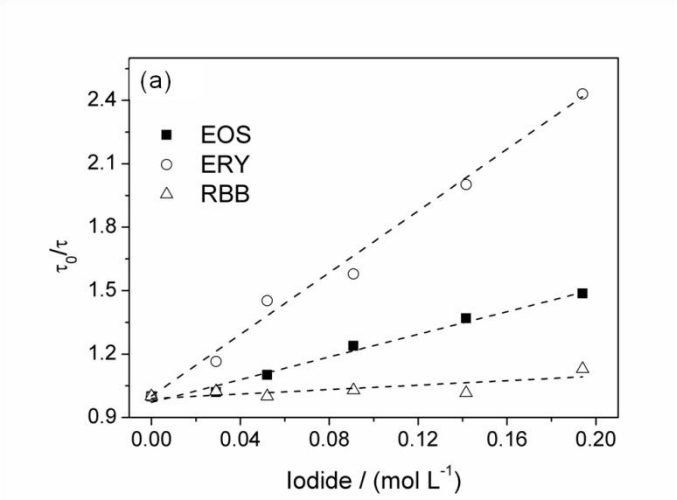


Figure S3. Stern-Volmer plot for EOS (a) 30.0 °C and (b) 50.0 °C; ERY (c) 30.0 °C and (D) 50.0 °C; RBB (e) 30.0 °C and (f) 50.0 °C using iodide as quencher: steady-state measurements in water (filled square) and in DPPC vesicle (empty circle) suspension. The excitation wavelength used was 480, 495 and 500 nm for EOS, ERY and RBB, respectively.



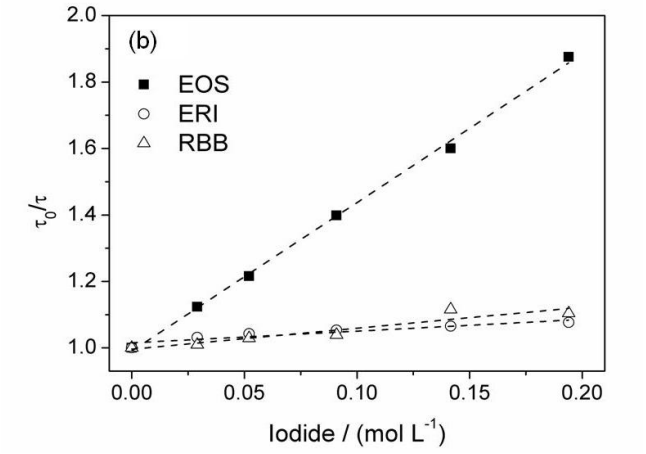


Figure S4. Stern-Volmer plot for EOS (filled square), ERY (empty circle) and RBB (empty triangle) at (a) 30.0 °C; (b) 50.0 °C using iodide as quencher: time-resolved measurements in DPPC vesicle suspension. The excitation wavelength used was 480, 495 and 500 nm for EOS, ERY and RBB, respectively.

Table S1. Fluorescence lifetime of XD (5.0×10^{-6} mol L^{-1}) in water (30 °C) and DPPC vesicles (30 and 50 °C) suspension (1.2×10^{-3} mol L^{-1})

XD	Water		DPPC		
	τ (30°C) / ns	χ^2	τ (30°C) / ns	τ (50°C) / ns	χ^2
EOS	1.19	0.89	0.94	0.86	0.795 (30 °C) 0.795 (50 °C)
ERI	0.16	1.17	0.13	0.66	0.688 (30 °C) 0.736 (50 °C)
RBB	1.44	0.77	2.15	2.49	0.842 (30 °C) 0.799 (50 °C)

Table S2. Fluorescence quantum yield (Φ_F) of XDs in water (30.0 °C) and DPPC vesicles (30.0 and 50.0 °C) suspension. The excitation wavelength used was 480, 495 and 500 nm for EOS, ERY and RBB, respectively

XD	λ_{exc} / nm	Φ_f Water[a]	Φ_f DPPC	
		30.0 °C	30.0 °C	50.0 °C
EOS	480	0.20	0.249 ± 0.001	0.266 ± 0.005
ERY	490	0.02	0.090 ± 0.001	0.108 ± 0.004
RBB	500	0.02	0.079 ± 0.003	0.089 ± 0.003

[a]Reference 1.

Reference

1. Pellosi, D. S.; Estevao, B. M.; Semensato, J.; Severino, D.; Baptista, M. S.; Politi, M. J.; Hioka, N.; Caetano, W.; *J. Photochem. Photobiol., A* **2012**, *247*, 8.