Electronic Supplementary Material (ESI) for Soft Matter.

Supplementary Information

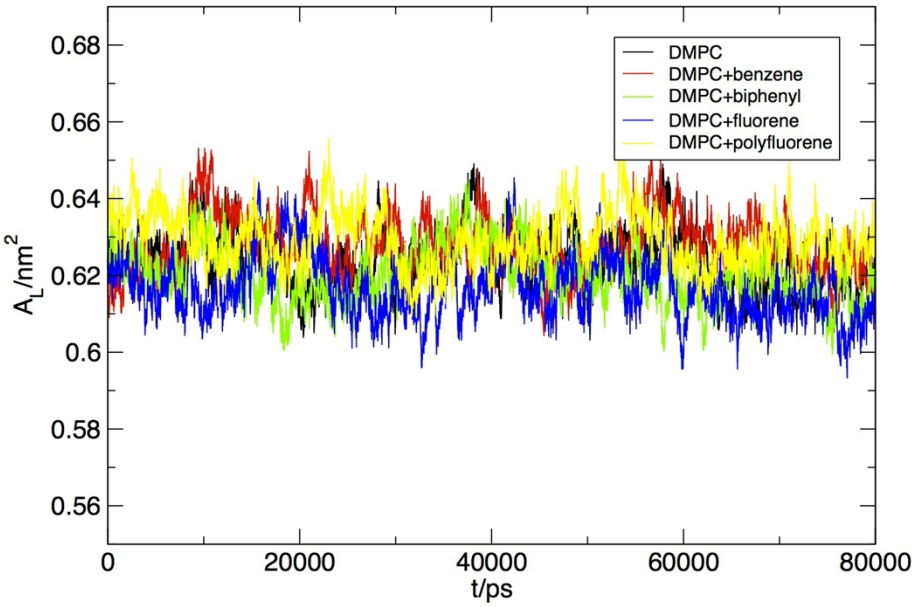
From molecular modelling to photophysics of neutral oligo- and polyfluorenes incorporated into phospholipid bilayers

By M. J. Tapia,[1]* M. Monteserín,[1] H. D. Burrows,[2] J. A. S. Almeida,[2] A. A. C. C. Pais,[2] J. Pina,[2] J. S. Seixas de Melo,[2] S. Jarmelo,[2] J. Estelrich[3]

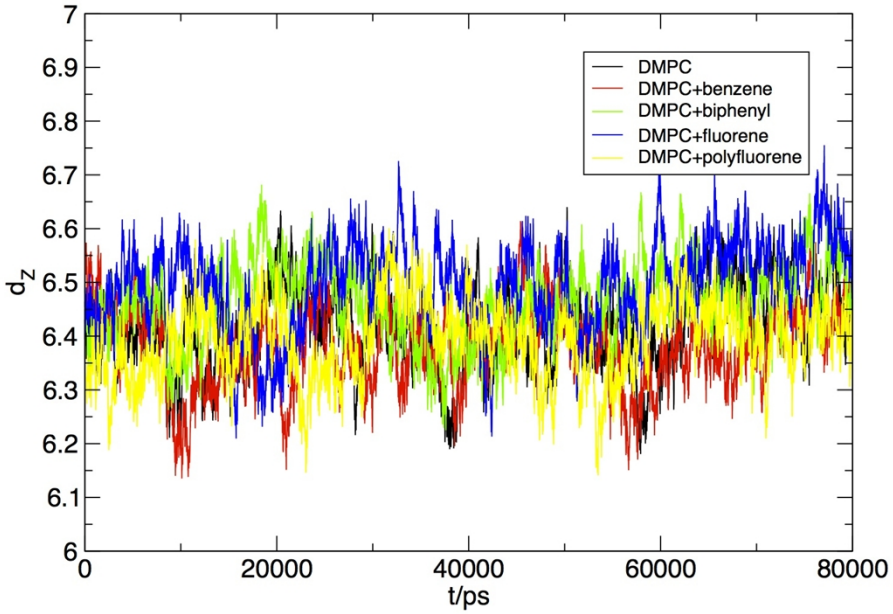
[*] Dr. M. J. Tapia
Departamento de Química
Universidad de Burgos
Plaza Misael Bañuelos, Burgos 09001, Spain.
E-mail: mjtapia@ubu.es

Molecular dynamics simulation

[1] Departamento de Química, Universidad de Burgos, Plaza Misael Bañuelos s/n, 09001 Burgos, Spain
[2] Centro de Química de Coimbra (CQC), Department of Chemistry, University of Coimbra, 3004-535 Coimbra, Portugal
[3] Facultat de Farmàcia, Universitat de Barcelona, Avda. Joan XXIII s/n 08028 Barcelona, Catalonia, Spain



(a)



(b)

Figure S1 – Area per lipid (a) and bilayer thickness (b) for the fully hydrated DMPC bilayer in the absence and presence of a single molecule of the indicated solute.

Diferential Scanning calorimetry

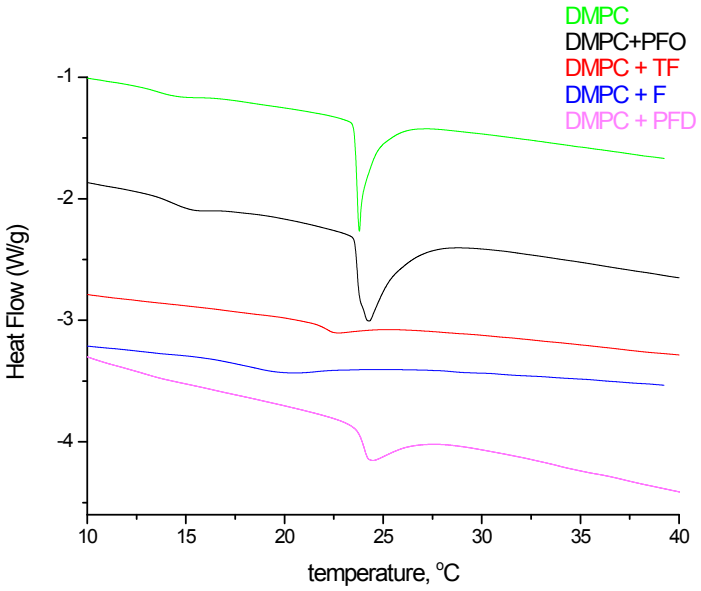


Figure S2. Experimental DSC thermograms for aqueous DMPC (3.69×10^{-2} M, green) and DMPC/probes ratio 2:1 (PFO in black, TF in red, fluorene in blue and PFD in pink)

Spectroscopic properties of fluorenes in different solvents

Chloroform

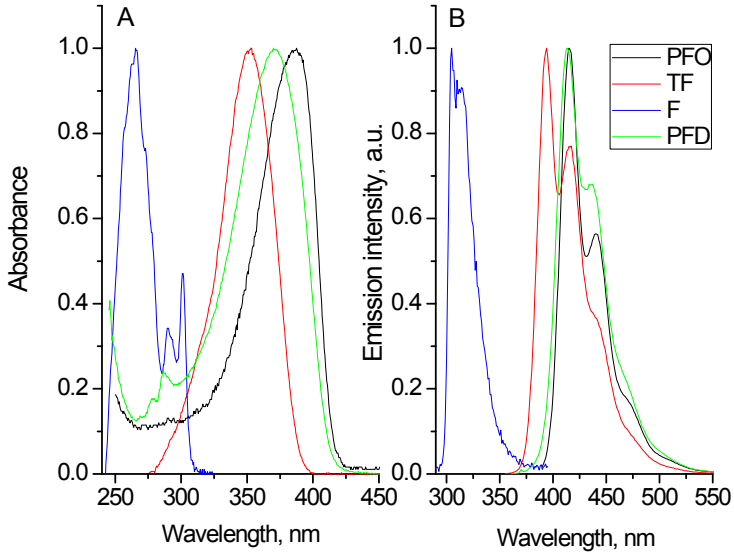


Figure S3. Normalized absorption (A) and emission (B) spectra of F (blue, 9.2×10^{-6} M), TF (red, 1×10^{-5} M), PFD (green, 1×10^{-5} M) and PFO (black, 1×10^{-5} M) (in repeat units for the polymers) in chloroform.

Cyclohexane

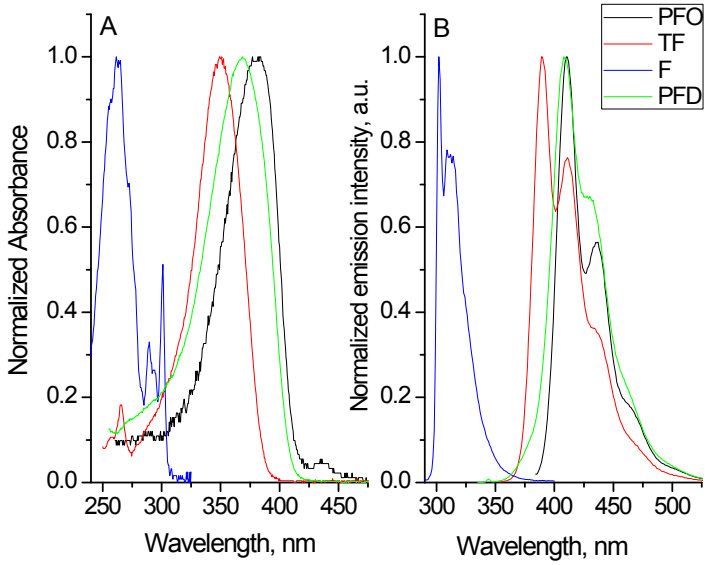


Figure S4. Normalized absorption (A) and emission (B) spectra of F (8.0×10^{-6} M, blue), TF (1.0×10^{-5} M, red), PFD (1.0×10^{-5} M, green) and PFO (4.0×10^{-6} M, black) in cyclohexane.

Ethanol

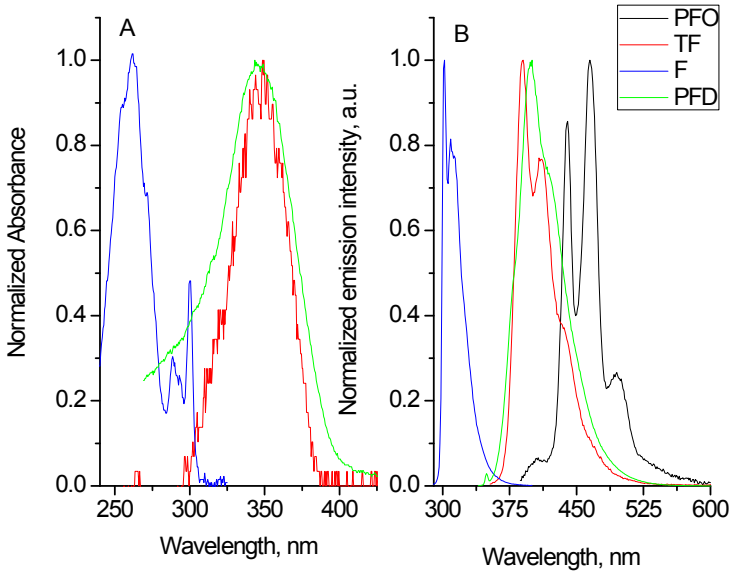


Figure S5. Normalized absorption (A) and emission (B) spectra of F (9.6×10^{-6} M, blue), TF (1.0×10^{-5} M, red), PFD (filtered, green) and PFO (1.0×10^{-5} M, black) in ethanol. The absorbance of PFO in ethanol is so low that the spectrum cannot be registered.

Effect of organic solvents and DMPC

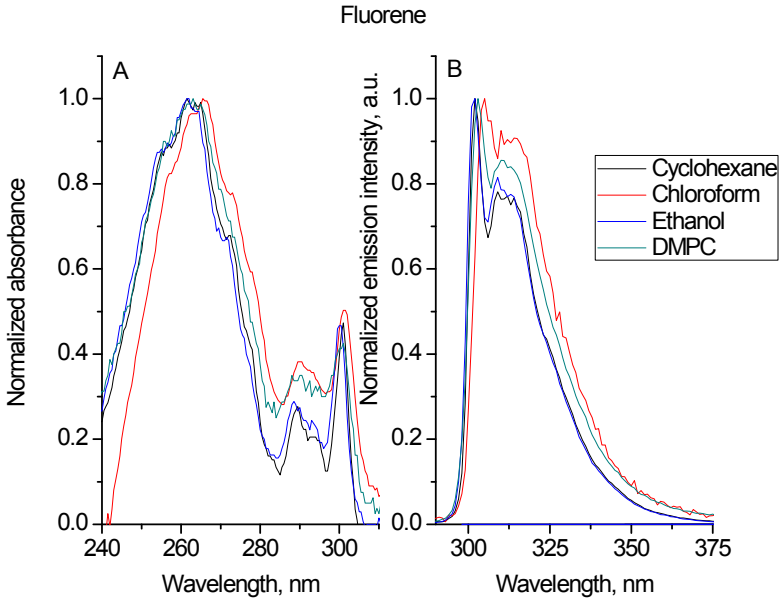


Figure S6. Normalized absorption (A) and emission (B) spectra of F in cyclohexane (black, 8.0×10^{-6} M), chloroform (red, 9.2×10^{-6} M), ethanol (blue, 9.6×10^{-6} M) and DMPC (8.7×10^{-6} M green).

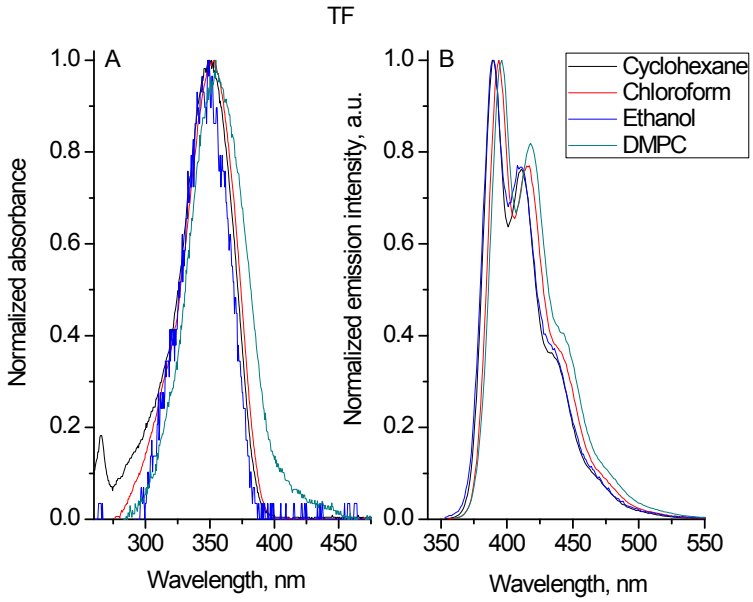


Figure S7. Normalized absorption (A) and emission (B) spectra of TF (1.0×10^{-5} M) in cyclohexane (black), chloroform (red), ethanol (blue) and DMPC (green).

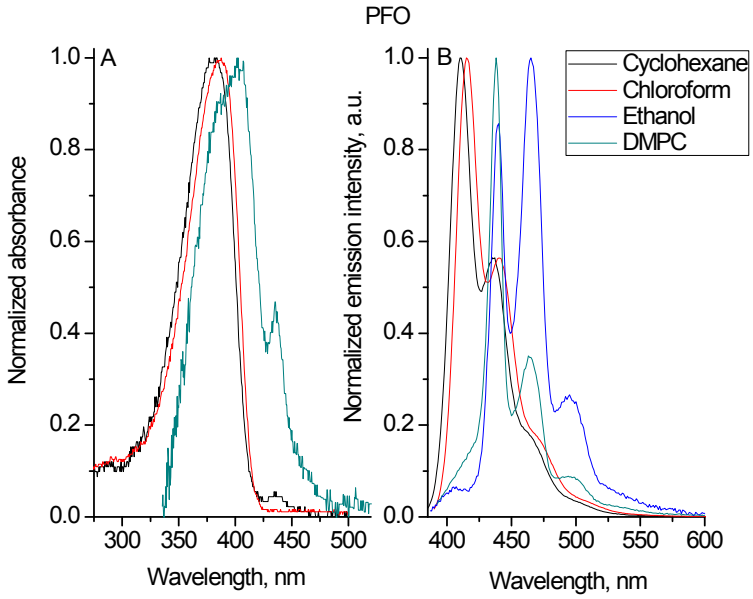


Figure S8. Normalized absorption (A) and emission (B) spectra of PFO (1.0×10^{-5} M) in cyclohexane (black), chloroform (red), ethanol (blue) and DMPC (green).

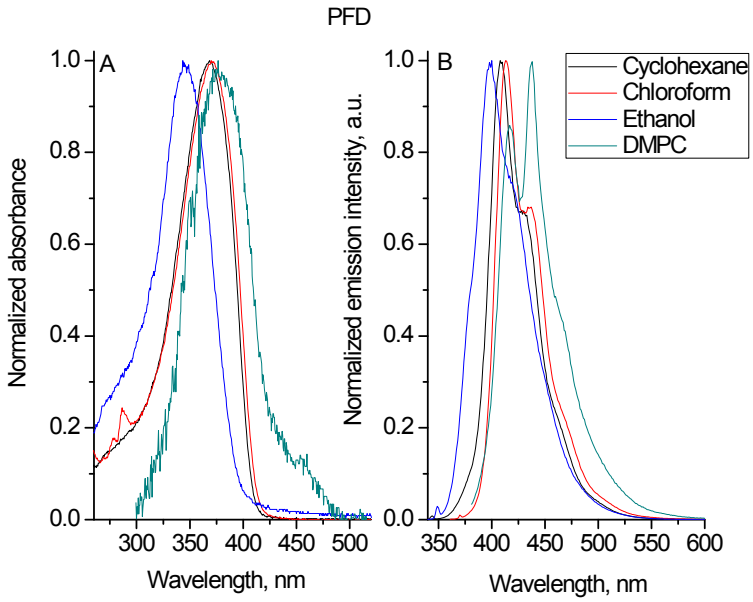


Figure S9. Normalized absorption (A) and emission (B) spectra of PFD (1.0×10^{-5} M) in cyclohexane (black), chloroform (red), ethanol (blue) and DMPC (green).

Time-resolved emission

Table S1. Decay time (τ_i), pre-exponential factors (a_i), chi-squared (χ^2) of F in DMPC (9.38×10^{-5} M) at 25 ºC. Excitation wavelength at 282 nm and average values.

Wavelength, nm			315		
F	τ_1, ps	τ_2, ps	a_1	a_2	χ^2
1.85×10^{-6}	2690	6270	0.302	0.698	0.93
2.77×10^{-6}	3150	6490	0.335	0.665	0.91
3.63×10^{-6}	2660	6300	0.290	0.710	1.03
4.61×10^{-6}	2550	6140	0.241	0.759	1.02
5.60×10^{-6}	2460	6130	0.294	0.706	0.98
6.59×10^{-6}	3070	6340	0.357	0.643	0.99
7.58×10^{-6}	3200	6120	0.335	0.665	0.90
8.57×10^{-6}	3580	6930	0.408	0.592	0.89
9.55×10^{-6}	3210	6060	0.447	0.553	0.90
1.05×10^{-5}	3910	7260	0.616	0.710	1.06

Average	
τ_1, ps	3048.0 ± 466.5
τ_2, ps	6404.0 ± 393.5
a_1	0.362 ± 0.107
a_2	0.670 ± 0.061

Table S2. Decay time (τ_i), pre-exponential factors (a_i), chi-squared (χ^2) of TF in DMPC (9.58×10^{-5} M) at 25 ºC. Excitation wavelength at 392 nm and average values.

Wavelength, nm			400			420			440		
TF	τ_1, ps	τ_2, ps	a_1	a_2	χ^2	a_1	a_2	χ^2	a_1	a_2	χ^2
1.34×10^{-5}	120	440	0.146	0.854	1.05	0.127	0.873	1.03	0.108	0.892	1.05
2.68×10^{-5}	80	390	0.122	0.878	1.03	0.113	0.888	1.03	0.075	0.924	1.03
4.03×10^{-5}	70	500	0.089	0.911	1.07	0.073	0.927	1.02	0.036	0.964	1.05
4.70×10^{-5}	60	530	0.09	0.91	1.02	0.078	0.92	1.01	0.05	0.948	1.02
5.37×10^{-5}	80	440	0.101	0.899	0.95	0.085	0.913	1.00	0.069	0.929	1.01
6.04×10^{-5}	70	490	0.08	0.92	1.05	0.069	0.93	0.98	0.032	0.967	1.05
6.70×10^{-5}	100	510	0.084	0.916	1.08	0.065	0.934	1.06	0.025	0.972	1.07
7.38×10^{-5}	60	530	0.076	0.924	1.05	0.074	0.925	0.96	0.027	0.971	0.99
8.05×10^{-5}	60	500	0.078	0.921	1.06	0.08	0.919	1.01	0.048	0.95	1.06
1.21×10^{-4}	50	460	0.087	0.912	0.98	0.091	0.908	1.00	0.057	0.941	1.00

Average		400	420	440
τ_1, ps	75.0 ± 21.2			
τ_2, ps	479.0 ± 45.3			
a_1		0.095 ± 0.022	0.085 ± 0.019	0.053 ± 0.026
a_2		0.904 ± 0.022	0.914 ± 0.019	0.946 ± 0.025

Table S3. Decay time (τ_i), pre-exponential factors (a_i), chi-squared (χ^2) of PFD in DMPC (9.55×10^{-5} M) at 25 ºC. Excitation wavelength at 378 nm and average values.

Wavelength, nm				440				475			
PFD	τ_1, ps	τ_2, ps	τ_3, ps	a_1	a_2	a_3	χ^2	a_1	a_2	a_3	χ^2
2.32×10^{-6}	39.7	180.5	681.1	0.840	0.125	0.035	1.05	0.801	0.151	0.048	1.05
3.09×10^{-6}	32.5	277.7	908.1	0.743	0.106	0.151	1.11	0.773	0.088	0.139	1.09
3.86×10^{-6}	43.1	198.2	725.1	0.528	0.374	0.097	1.02	0.478	0.404	0.118	0.96
4.64×10^{-6}	54.9	206.8	636.4	0.479	0.441	0.080	1.09	0.412	0.480	0.108	1.03
5.41×10^{-6}	60.6	236.1	668.0	0.522	0.384	0.094	1.09	0.429	0.445	0.126	1.06
6.18×10^{-6}	39.8	214.2	780.0	0.703	0.196	0.101	1.06	0.656	0.224	0.119	1.04
6.95×10^{-6}	66.6	226.1	714.0	0.651	0.269	0.080	1.02	0.589	0.300	0.111	1.02
8.04×10^{-6}	34.7	113.9	695.6	0.840	0.126	0.033	1.01	0.808	0.151	0.041	1.04
9.22×10^{-6}	44.8	245.4	845.4	0.538	0.264	0.199	1.02	0.493	0.299	0.208	1.02
1.08×10^{-5}	43.8	198.2	595.9	0.438	0.474	0.088	1.06	0.383	0.504	0.113	1.07

Average		440	475
τ_1, ps	46.0 ± 11.1		
τ_2, ps	209.7 ± 43.7		
τ_3, ps	724.9 ± 95.3		
a_1		0.628 ± 0.148	0.582 ± 0.167
a_2		0.276 ± 0.137	0.305 ± 0.149
a_3		0.096 ± 0.049	0.113 ± 0.046

Table S4. Decay time (τ_i), pre-exponential factors (a_i), chi-squared (χ^2) of PFO in DMPC (9.56×10^{-5} M) at 25 ºC. Excitation wavelength at 392 nm and average values.

Wavelength, nm			440			500		
PFO	τ_1, ps	τ_2, ps	a_1	a_2	χ^2	a_1	a_2	χ^2
1.39×10^{-6}	130	260	0.363	0.632	0.98	0.508	0.467	1.08
2.79×10^{-6}	120	280	0.327	0.666	1.07	0.479	0.499	1.07
4.89×10^{-6}	120	260	0.293	0.701	0.99	0.487	0.482	1.04
6.27×10^{-6}	110	240	0.327	0.669	1.03	0.495	0.482	1.07
8.35×10^{-6}	90	220	0.189	0.803	1.06	0.482	0.482	1.07
9.75×10^{-6}	130	270	0.199	0.799	1.00	0.456	0.531	1.08
1.25×10^{-5}	110	240	0.024	0.926	1.02	0.199	0.721	1.03

Average		440	500
τ_1, ps	115.7 ± 13.9		
τ_2, ps	252.9 ± 20.6		
a_1		0.246 ± 0.118	0.444 ± 0.109
a_2		0.742 ± 0.104	0.523 ± 0.089