Electronic Supplementary Material (ESI) for RSC Advances

Supporting Information

Modulation of the Photophysical Properties of BODIPY Dyes by Substitution at their Meso Position.

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Table S1. Photophysical properties of dyes **1**, **2** and **3** in several solvents ranking from apolar (c-hexane), to polar (ethyl acetate and acetone), to polar/protic (ethanol, methanol and F_3-ethanol). The corresponding data of the unsubstituted chromophore (BDP) are included for comparison.

Solvent	λ_{abs} (nm)	ε_{max} ($10^4 M^{-1}cm^{-1}$)	λ_{flu} (nm)	$\Delta\nu_{St}$ (cm^{-1})	ϕ	τ (ns)	k_{fl} ($10^8 s^{-1}$)	k_{nr} ($10^8 s^{-1}$)
BDP								
F_3-ethanol	497.0	6.1	505.0	325	0.86	8.23	1.04	0.17
methanol	497.0	5.8	507.0	395	0.87	7.33	1.18	0.18
ethanol	498.0	5.6	508.0	385	0.90	7.02	1.28	0.14
acetone	497.5	5.5	507.5	395	0.89	7.12	1.25	0.15
ethyl acetate	498.0	5.9	507.5	370	0.93	6.90	1.34	0.10
c-hexane	503.5	7.6	510.5	265	0.96	6.47	1.48	0.06
Dye 1								
F_3-ethanol	489.0	5.8	498.5	385	0.86	7.95	1.08	0.17
methanol	491.0	5.9	501.5	430	0.88	7.15	1.23	0.16
ethanol	492.0	5.9	502.5	425	0.90	6.84	1.31	0.14
acetone	491.0	5.6	502.0	450	0.92	6.93	1.32	0.11
ethyl acetate	492.0	5.3	502.0	415	0.90	6.62	1.35	0.15
c-hexane	497.0	6.8	505.0	315	0.95	6.23	1.52	0.08
Dye 2								
F_3-ethanol	496.0	2.9	505.5	390	0.85	8.41	1.01	0.18
methanol	497.5	3.3	508.0	415	0.87	7.58	1.14	0.17
ethanol	499.0	3.3	509.5	415	0.89	7.26	1.22	0.15
acetone	498.0	3.2	508.5	420	0.88	7.36	1.19	0.16
ethyl acetate	498.5	2.8	508.5	400	0.94	7.04	1.33	0.08
c-hexane	503.0	3.4	512.0	355	0.92	6.65	1.38	0.12
Dye 3								
F_3-ethanol	490.0	5.5	501.0	450	0.87	8.10	1.07	0.16
methanol	491.0	5.9	502.5	475	0.89	7.42	1.20	0.15
ethanol	492.0	6.0	504.0	475	0.89	7.09	1.25	0.15
acetone	490.5	5.8	503.0	505	0.91	7.16	1.27	0.12
ethyl acetate	491.5	5.4	503.0	465	0.94	6.83	1.37	0.08
c-hexane	496.5	7.0	506.5	385	0.97	6.50	1.49	0.04

absorption (λ_{abs}) and fluorescence (λ_{flu}) wavelength, Stokes shift ($\Delta\nu_{St}$), molar absorption coefficient (ε_{max}), fluorescence quantum yield (ϕ) and lifetime (τ), radiative (k_{fl}) and non-radiative (k_{nr}) rate constant.

Table S2. Quantum mechanical simulation of the absorption transition properties for unsubsituted reference BDP chromophore and compound **5** and **6** in the gas phase. Absorption energy gap (ΔE_{ab}) and wavelength (λ_{ab}), and oscillator strength (f).

	TD-B3LYP			ZINDO		
	BDP	**5**	**6**	BDP	**5**	**6**
ΔE_{ab} (eV)	3.16	3.10	3.12	2.66	2.73	2.72
λ_{ab} (nm)	392	400	398	465	454	456
f	0.30	0.34	0.24	0.88	0.97	0.87

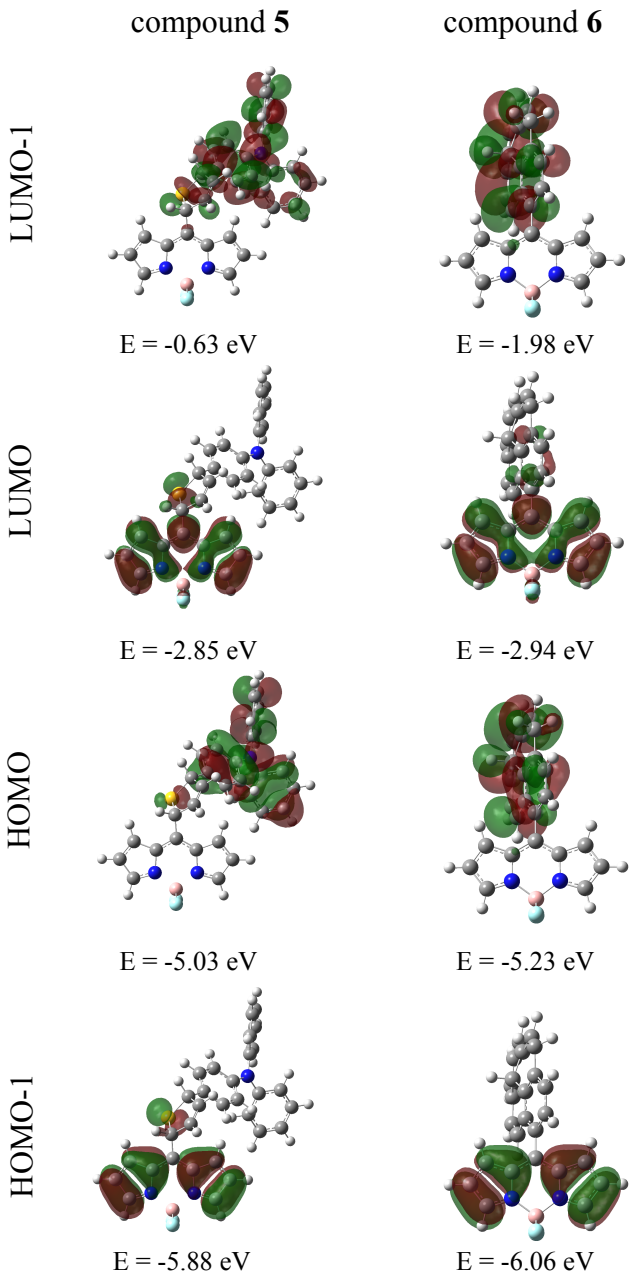

Figure S1. Molecular orbitals (electronic density and energy) of compound **5** and **6**.

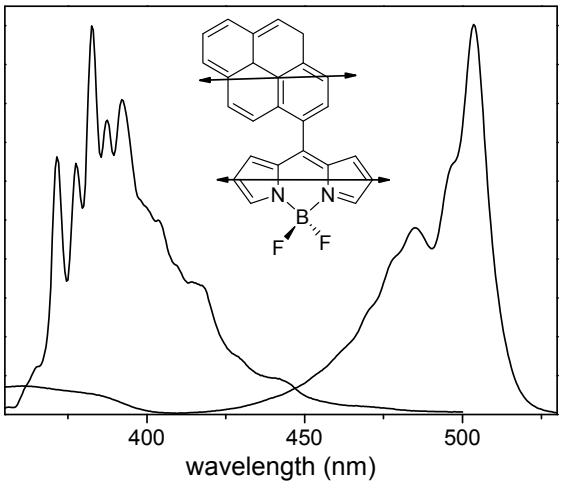

Figure S2. Spectral overlap of the fluorescence emission of the pyrene and the absorption spectrum of the BDP chromophore. The corresponding transition moment orientation of each chromophore in compound **6** is also enclosed.

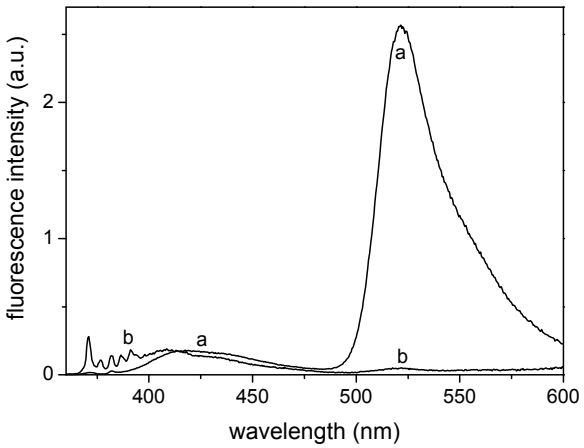

Figure S3. Fluorescence spectra of compound **6** at 298 K (a) and 77 k (b) in a diluted solution of cyclohexane