Electronic Supplementary Material (ESI) for Photochemical & Photobiological Sciences

Supplementary Information

Modulation of the spectroscopic property of Bodipy derivates through tuning the molecular configuration

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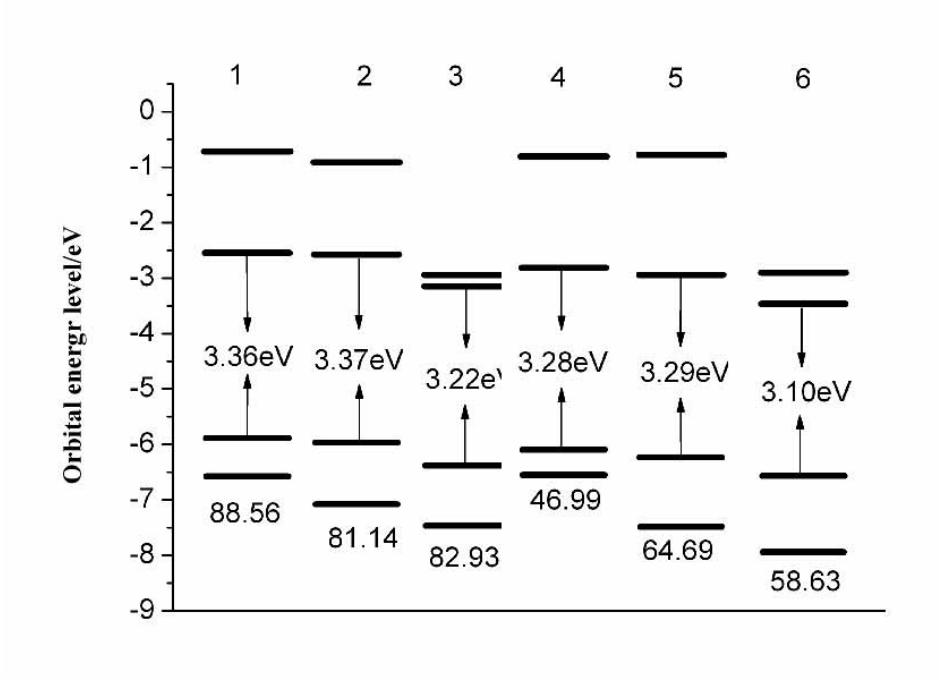

Figure S1. The orbital energies from HOMO to LUMO for Bodipy compounds **1**-**6**.

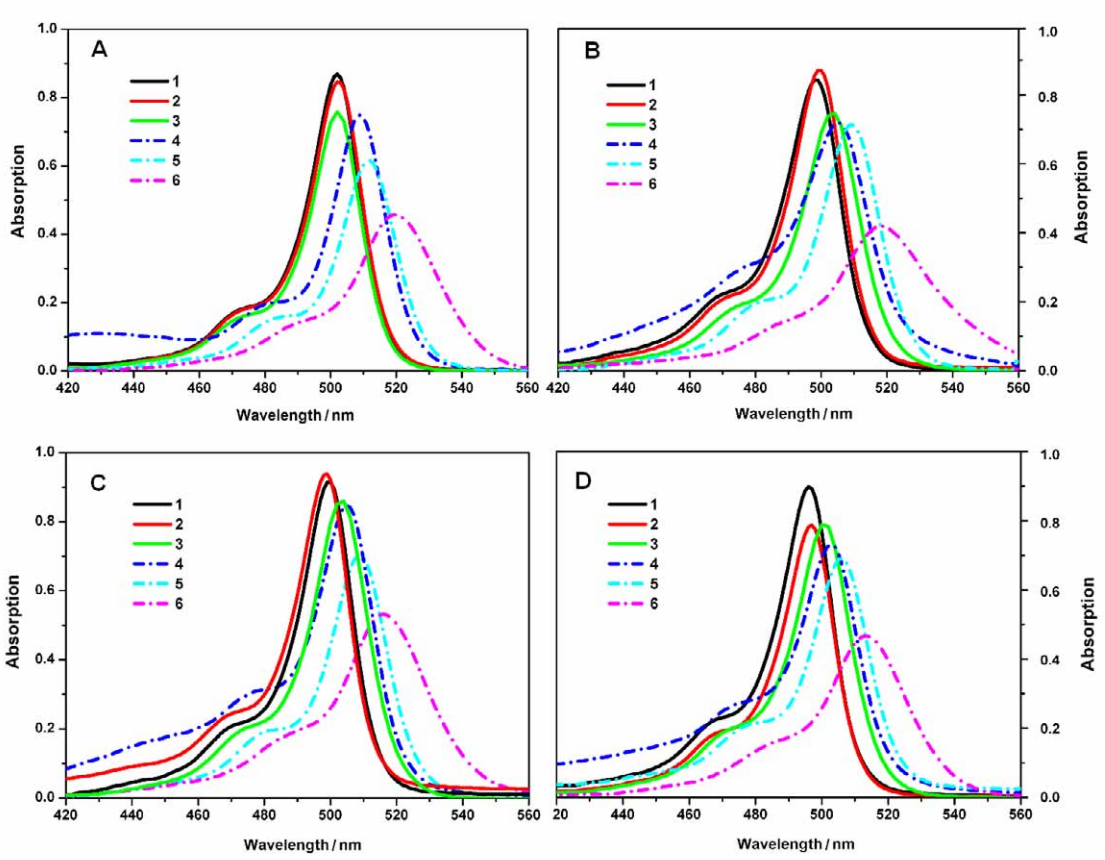

Figure S2. The electronic absorption spectra of **1-6** at the concentration of 1×10^{-5} M in toluene (A), DMF (B), THF (C), and MeOH (D), respectively.

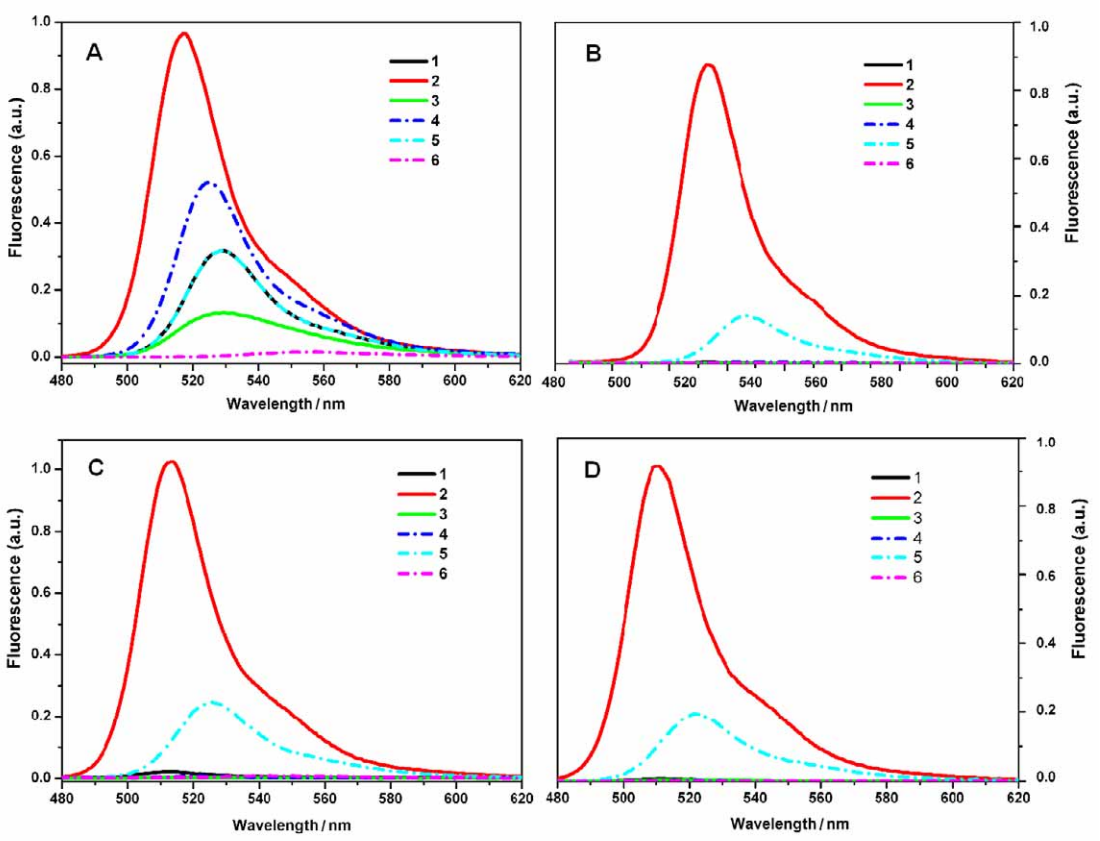

Figure S3. The fluorescence emission spectra of **1-6** at the concentration of 1×10^{-5} M in toluene (A), DMF (B), THF (C), and MeOH (D), respectively, with the excitation wavelength of 450 nm.

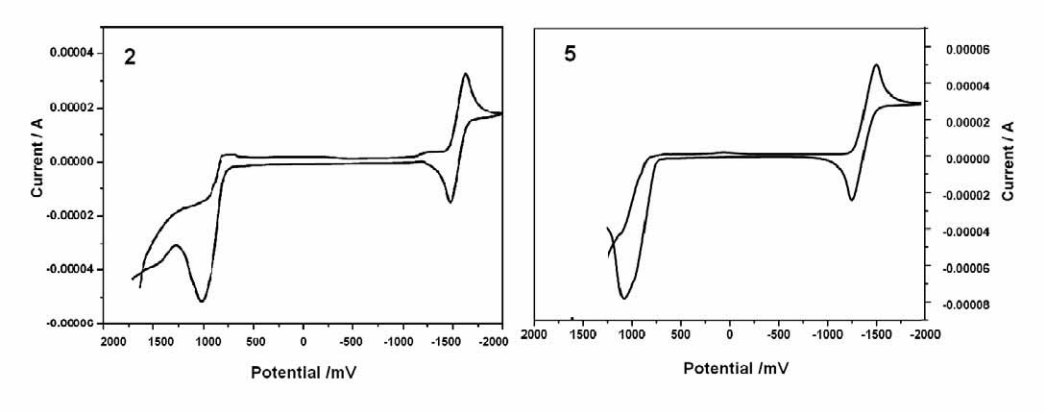

Figure S4. Cyclic voltammetry of CH_3-substituted **2** and **5** in CH_2Cl_2 containing 0.1 M $[NBu_4][ClO_4]$ at the scan rate of 20 mV s^{-1}.

Table S1. The spectral parameters of Bodipy compounds **1**-**6** in different solvents.

compounds	solvent	λ_{Abs} (max/nm)	λ_{em} (max/nm)	$\Delta\lambda_{max\upsilon}$ (cm^{-1})	Φ_f
1	CH_3CN	495	512	17	0.021
	MeOH	496	511	15	0.003
	DMF	498	512	14	0.023
	THF	499	512	13	0.006
	CH_2Cl_2	500	513	13	0.491
	toluene	502	516	14	0.558
2	CH_3CN	496	510	14	0.461
	MeOH	497	510	13	0.559
	DMF	499	513	14	0.505
	THF	500	513	13	0.502
	CH_2Cl_2	500	514	14	0.600
	toluene	502	517	15	0.720
3	CH_3CN	500	519	19	0.015
	MeOH	501	520	19	0.004
	DMF	503	523	20	0.001
	THF	503	526	23	0.002
	CH_2Cl_2	505	527	22	0.009
	toluene	507	528	21	0.143
4	CH_3CN	502	520	18	0.008
	MeOH	503	520	17	0.007
	DMF	505	522	17	0.004
	THF	505	522	17	0.002
	CH_2Cl_2	507	523	16	0.198
	toluene	509	525	16	0.394
5	CH_3CN	506	521	15	0.189
	MeOH	506	521	15	0.111
	DMF	509	524	15	0.152
	THF	509	525	16	0.214
	CH_2Cl_2	510	526	16	0.292
	toluene	512	529	17	0.414
6	CH_3CN	513	547	34	0.011
	MeOH	513	550	37	0.006
	DMF	515	556	41	0.004
	THF	516	557	41	0.014
	CH_2Cl_2	518	555	37	0.002
	toluene	520	557	37	0.005