Supporting Information

6-Hydroxyindole-Based Borondipyrromethene: Synthesis and Spectroscopic Studies

Chunchang Zhao,* Peng Feng,† Jian Cao,† Yulin Zhang, Xuzhe Wang, Yang Yang, Yanfen Zhang, Jinxin Zhang

Key Laboratory for Advanced Materials and Institute of Fine Chemicals, East China University of Science & Technology, Shanghai 200237, P. R. China

zhaocchang@ecust.edu.cn

† These two authors contributed equally

General Methods

All chemical reagents and solvents for synthesis were purchased from commercial suppliers and were used without further purification. All moisture-sensitive reactions were carried out under an atmosphere of argon. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker AV-400 spectrometer with chemical shifts reported in ppm (in $CDCl_3$, TMS as internal standard) at room temperature. Mass spectra were measured on a HP 1100 LC-MS spectrometer.

UV-vis absorption spectra were recorded on a Varian Cary 100 spectrophotometer. Fluorescence spectra were measured with a Varian CARY Eclipse Fluorescence spectrophotometer. Fluorescence quantum yields were determined by comparing the corrected fluorescence spectra with that of Rhodamine B in EtOH (Φ_F 0.89) as the standard. Spectroscopic measurements were made in a quartz cuvette (1 cm path length) at room temperature. Spectral-grade solvents were used for measurements of UV-vis absorption and fluorescence.

Table S1.Absorption data for **BODIPY-OH** and **BODIPY-OMe** in various solvents in the absence or presence of organic bases.

		λ_{ab} (nm)		λ_{ab} (nm)		
Solvent	E_T (N)	**-OH**	**-OMe**	**-OH**+BA	**-OH**+DBN	**-OH**+DBU
water	1.000	546	551	596	598	598
methanol	0.762	548	544	553	611	611
				610		
ethanol	0.654	553		554	624	624
				622		
1-butanol	0.586	558		558	628	628
				625		
2-propanol	0.546	556		556	630	630
				627		
acetonitrile	0.460	542	540	542	634	634
				634		
DMSO	0.444	558	546	645	644	645
		644				
DMF	0.386	553		556	642	642
				642		
dichloromethane	0.309	545	546	549	631	632
benzene	0.111	553		562	580	581
					628	635
toluene	0.099	563	555	566	580	582
					629	633

Table S2. Fluorescence of **BODIPY-OH** and **BODIPY-OMe** in various solvents in the absence or presence of organic bases.

		λ_{em} (nm) [Φ_F]		λ_{em} (nm)[Φ_F]		
Solvent	E_T(N)	**-OH**	**-OMe**	**-OH**+BA	**-OH**+DBN	**-OH**+DBU
water	1.000			632	629	632
					[0.18]	
methanol	0.762	577	567	576	642	647
		[0.25]		643	[0.22]	
ethanol	0.654	580		580	650	653
		[0.30]		652	[0.19]	
1-butanol	0.586	583		583	654	658
		[0.31]		654	[0.19]	
2-propanol	0.546	582		581	656	656
		[0.28]		655	[0.17]	
acetonitrile	0.460	571	567	571	664	670
		[0.22]		666	[0.17]	
DMSO	0.444	583	574	681	675	681
		680			[0.18]	
		[0.34]				
DMF	0.386	583		581	672	676
		[0.31]		674	[0.17]	
dichloromethane	0.309	577	571	581	656	661
		[0.30]			[0.24]	
benzene	0.111	573		583	655	656
		[0.44]			[0.26]	
toluene	0.099	586	573	588	655	661
		[0.40]			[0.24]	

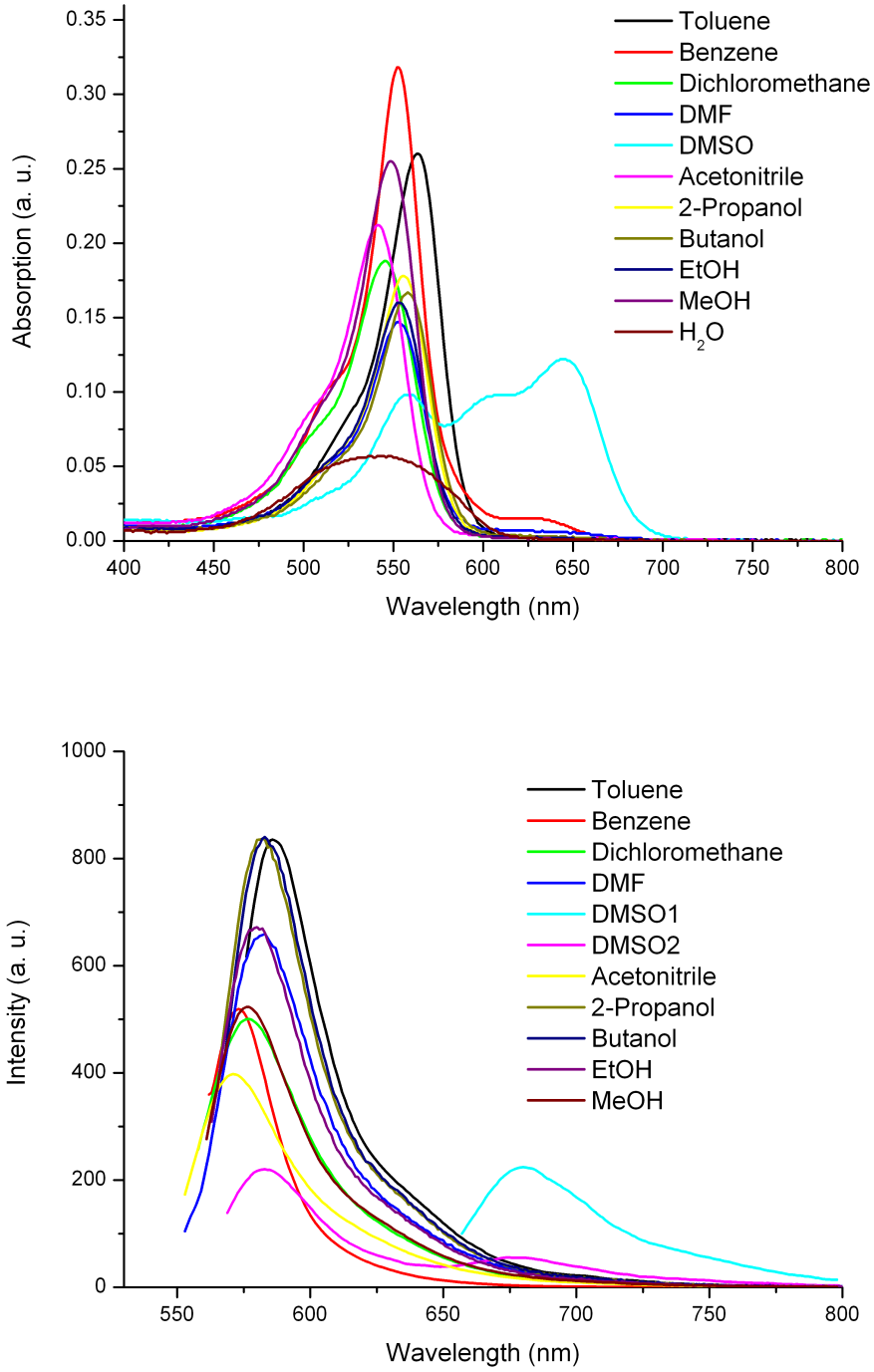

Figure S1. Absorption (top) and fluorescence (bottom) spectra of **BODIPY-OH** in various solvents. DMSO1: fluorescence recorded at the shorter excitation wavelength (λ_{ex} = 558 nm); DMSO2: fluorescence recorded at the second excitation wavelength (λ_{ex} = 644 nm).

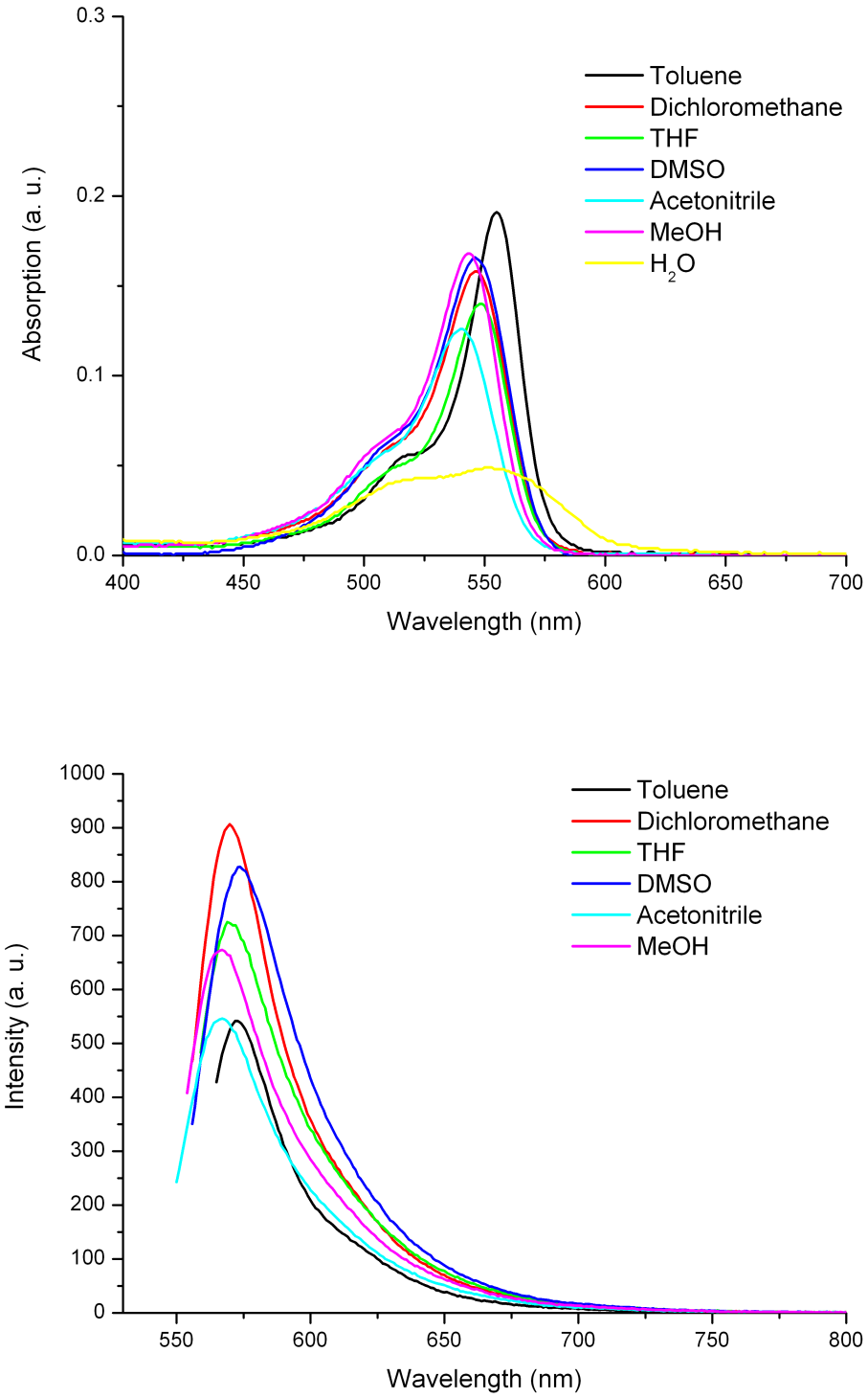

Figure S2 . Absorption and emission spectra of **BODIPY-OMe** in various solvents.

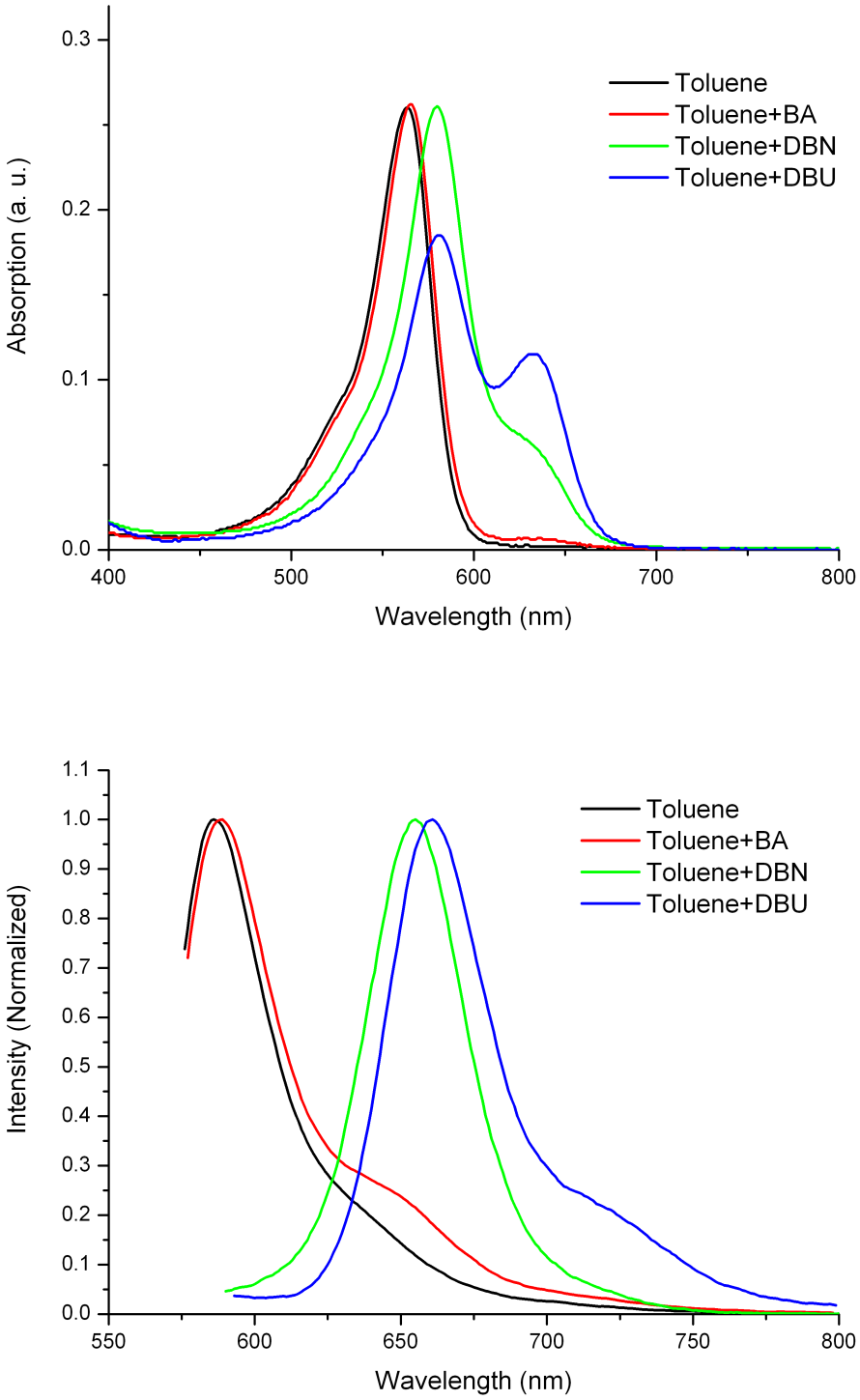

Figure S3. UV-vis absorption and fluorescence spectra of **BODIPY-OH** (5.0×10^{-6} M) in toluene containing organic bases.

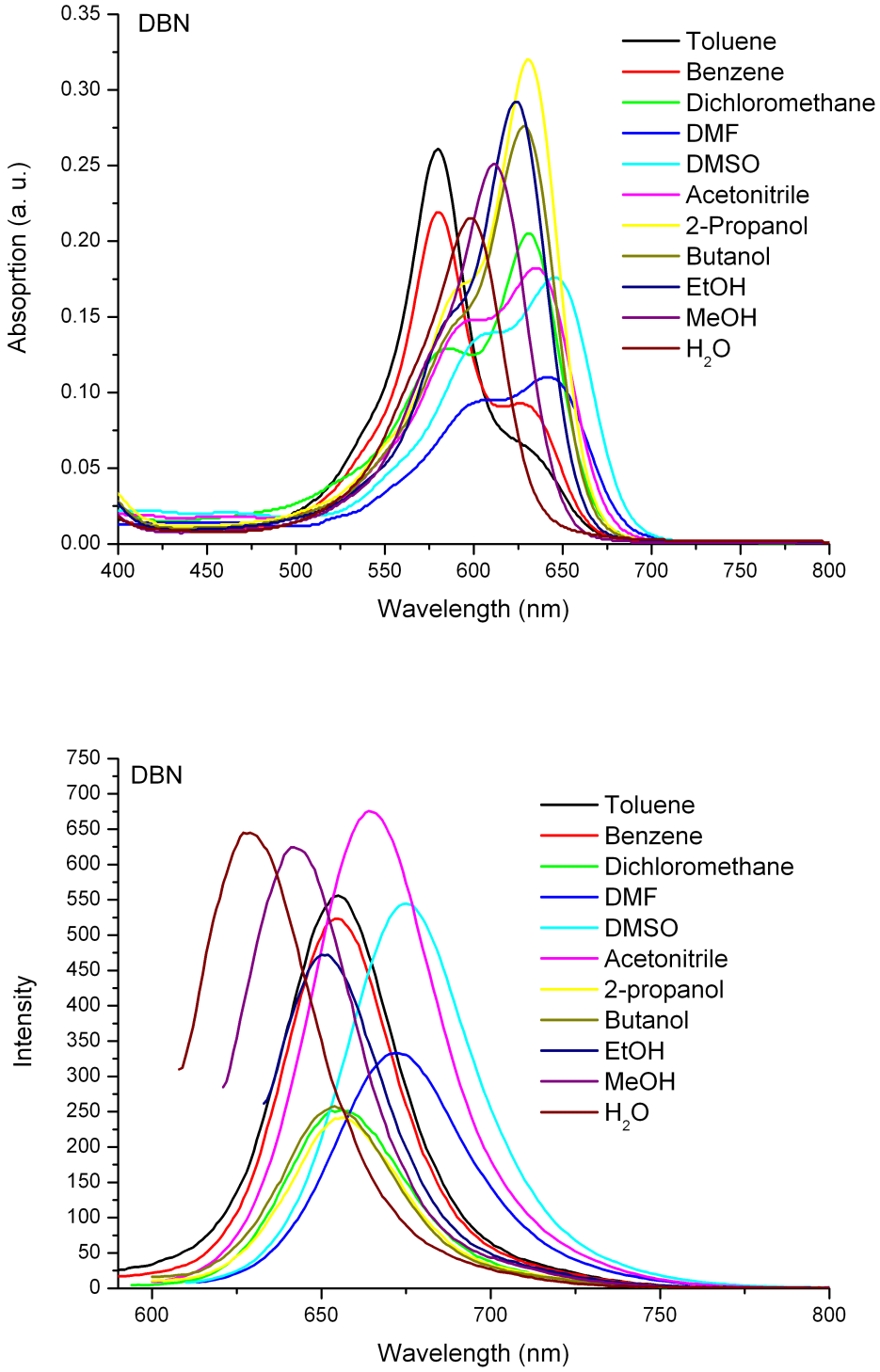

Figure S4. Effects of DBN on the absorption and fluorescence spectra of **BODIPY-OH** (5.0×10^{-6} M).

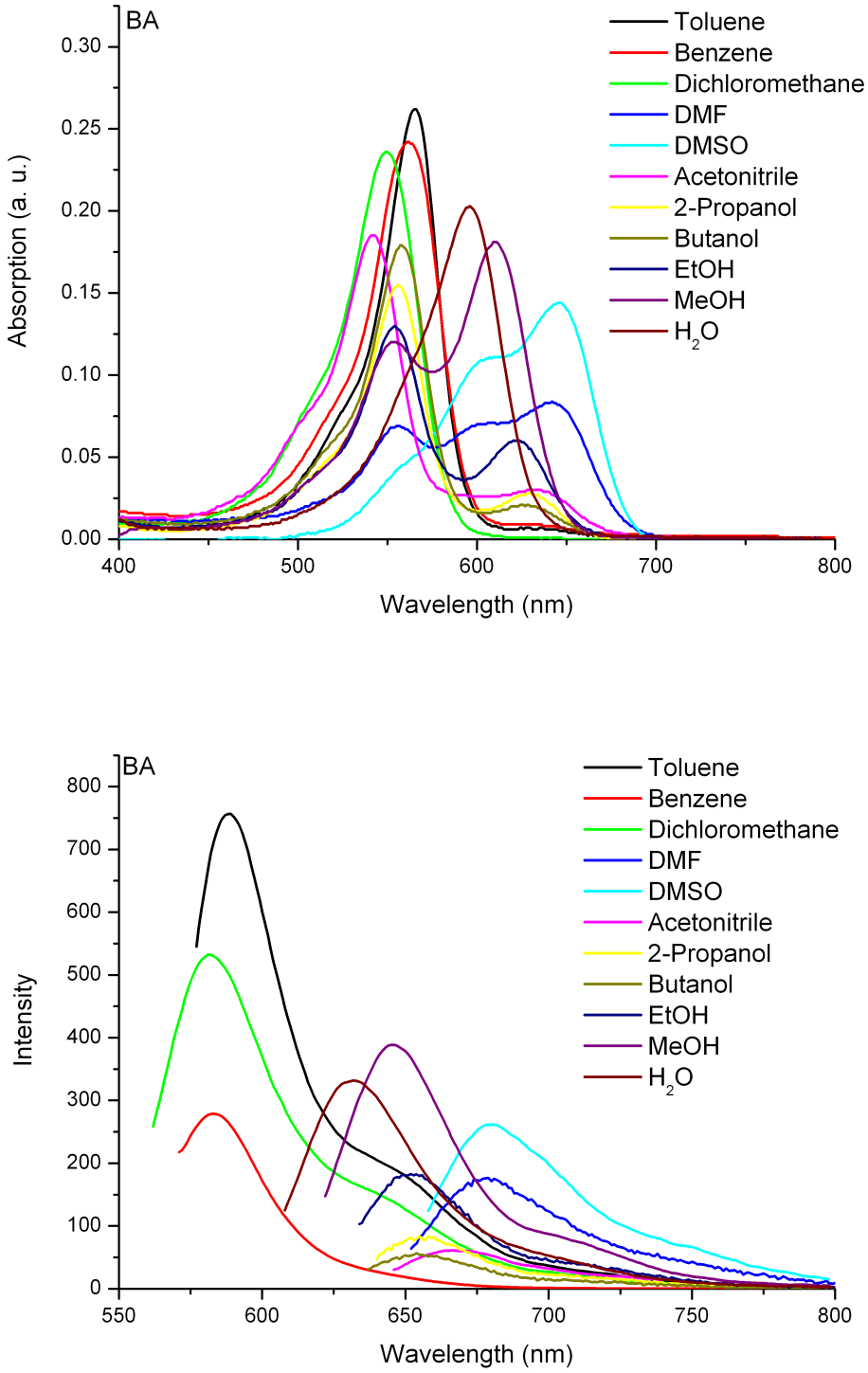

Figure S5. Effects of BA on the absorption and fluorescence spectra of **BODIPY-OH** (5.0×10^{-6} M). Fluorescence spectra were recorded at excitation of the longer absorption maximum.

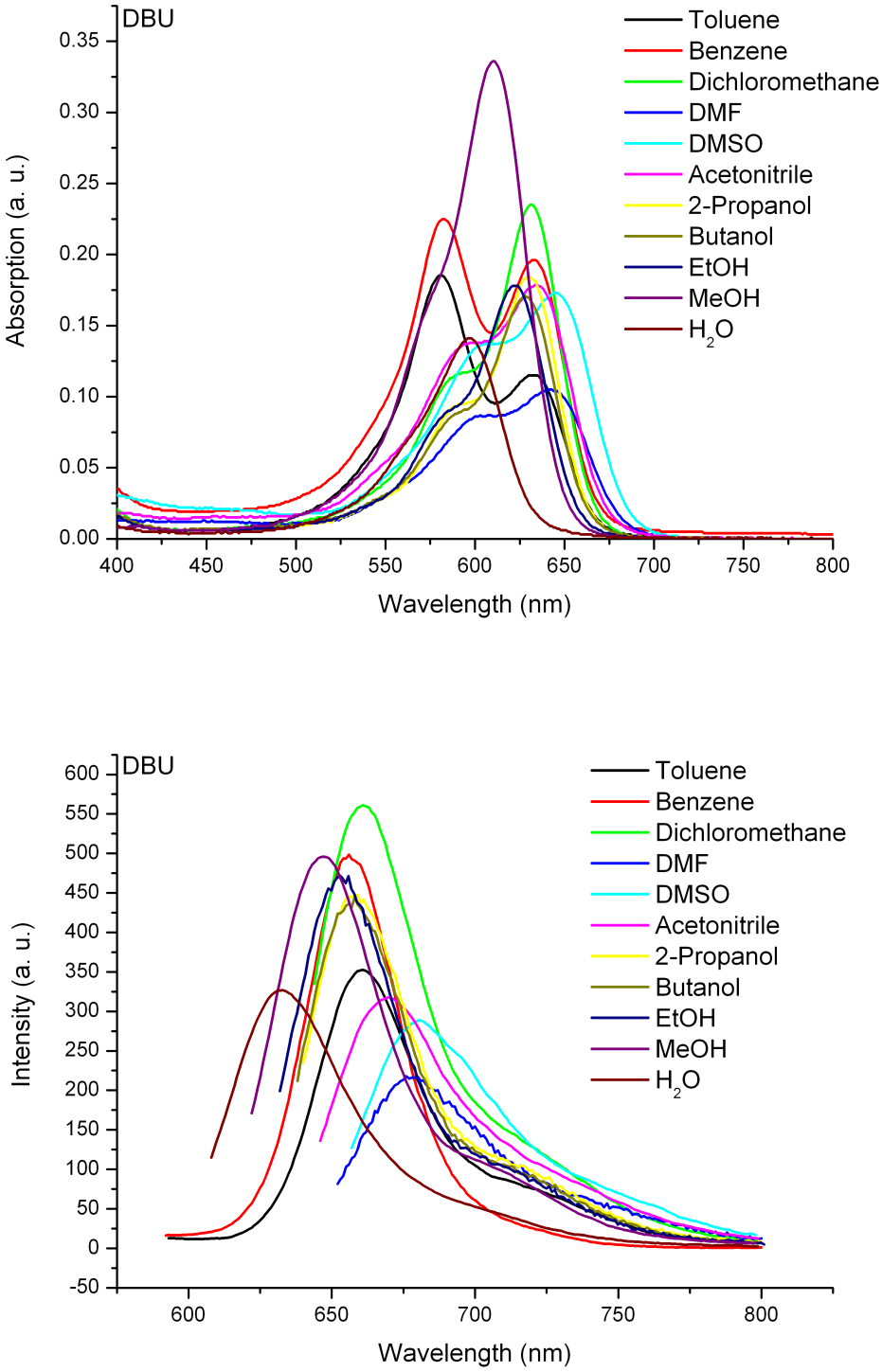

Figure S6. Effects of DBU on the absorption and fluorescence spectra of **BODIPY-OH** (5.0×10^{-6} M).

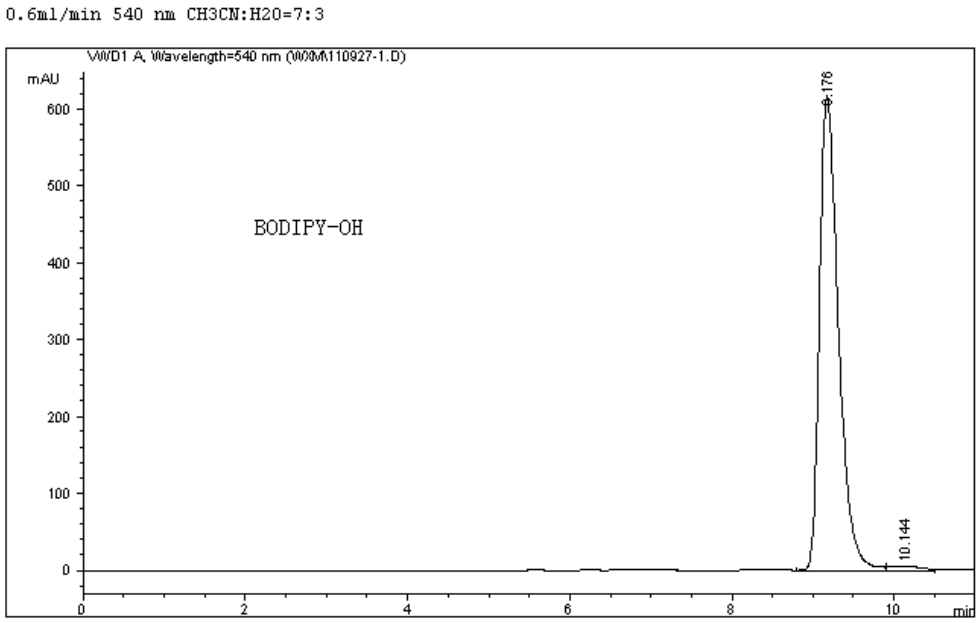

Figure S7. HPLC analysis of BODIPY-OH.

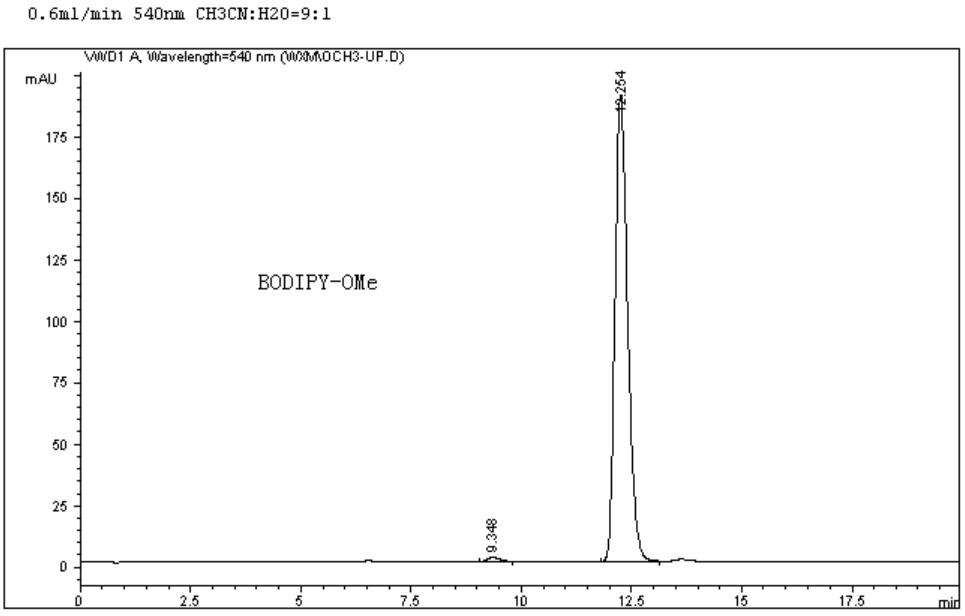

Figure S8. HPLC analysis of BODIPY-OMe.

Table S3. Analytical HPLC conditions for **BODIPY-OH** and **BODIPY-OMe**.

Compound	Rt (min)	elute	Area
BODIPY-OH	9.716	$CH_3CN:H_2O$ = 7:3	98.7537
BODIPY-OMe	12.254	$CH_3CN:H_2O$ = 9:1	99.2292