Supplementary Information for:

Negative Thermal Quenching of Photoluminescence from Liquid-Crystalline Molecules in Condensed Phases

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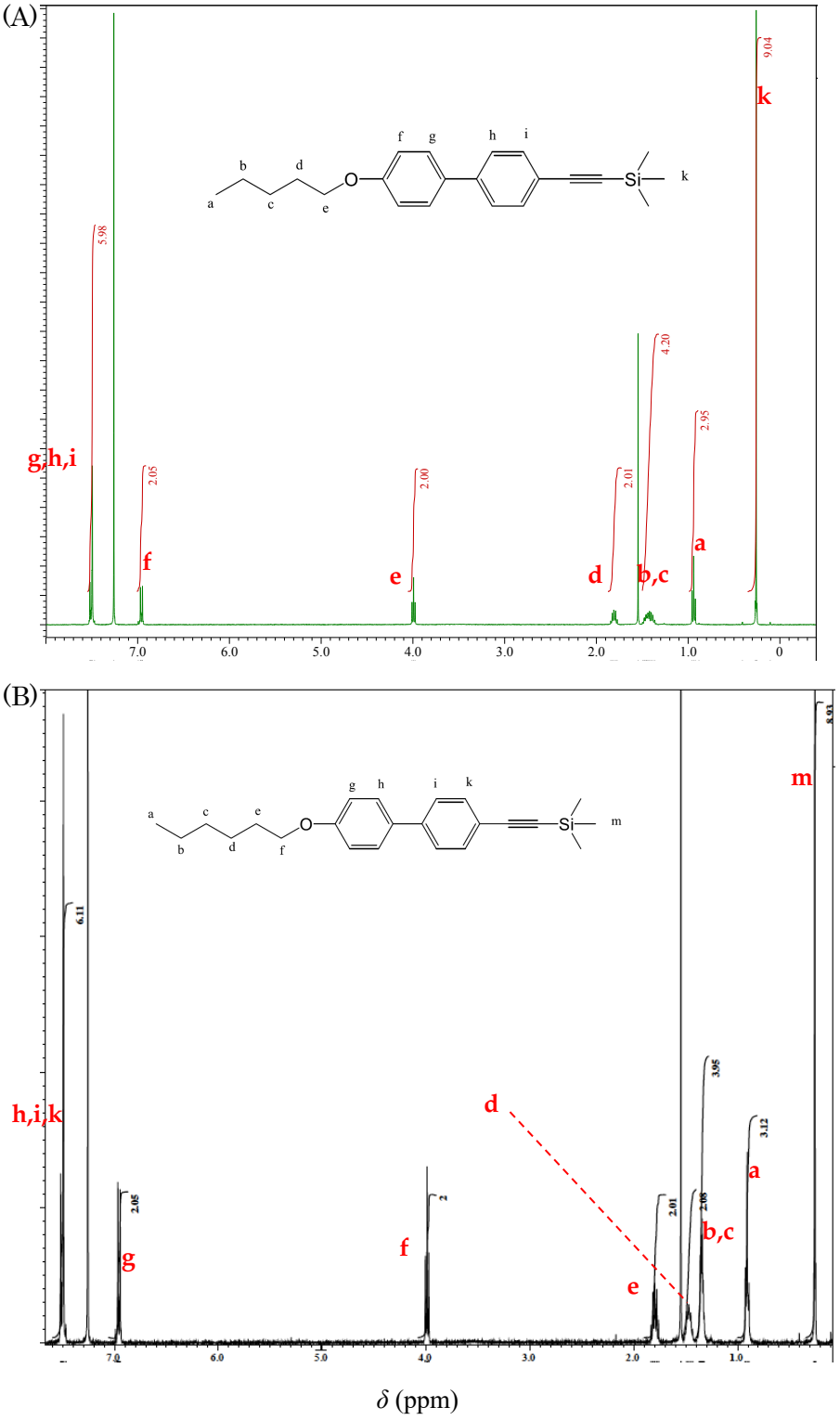
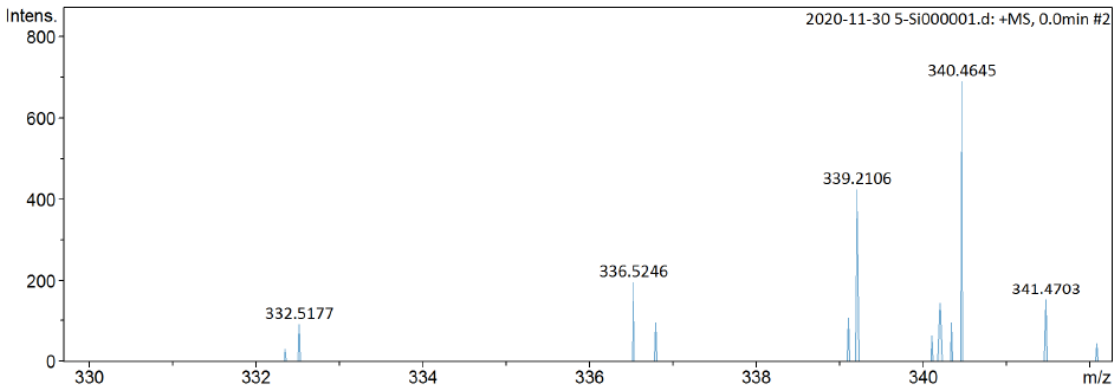


Figure S1. ^{1}H NMR spectra for compounds **5-BPTMS** (A) and **6-BPTMS** (B) in $CDCl_3$.

(A)



m/z

(B)

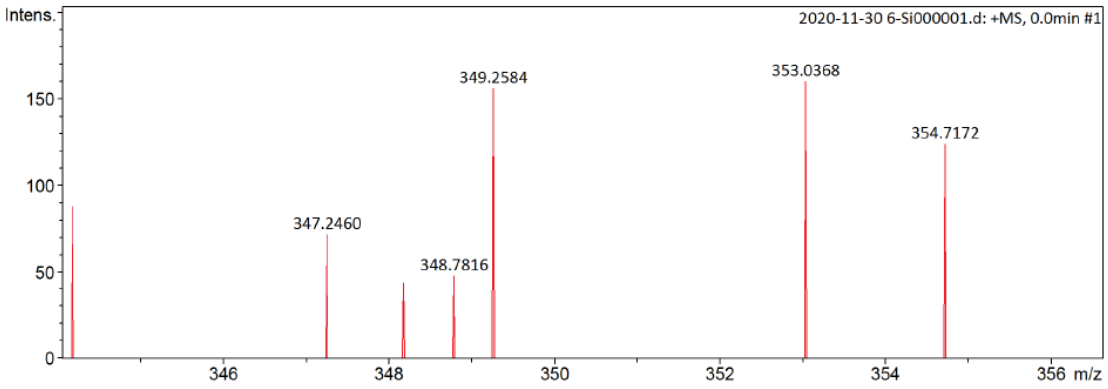


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Figure S2. ESI-MS spectra for **5-BPTMS** (A) and **6-BPTMS** (B).

Table S1. Crystallographic data of compounds **5-BPTMS** and **6-BPTMS** obtained at room temperature.

Compounds	**5-BPTMS**	**6-BPTMS**
Radiation type	Mo Kα	Mo Kα
Wavelength (Å)	0.71073	0.71073
Empirical formula	$C_{22}H_{28}OSi$	$C_{23}H_{30}OSi$
Formula weight	336.53	350.58
Temperature (K)	293	293(2)
Crystal habit	needle	plate
Crystal color	colorless	colorless
Crystal system	triclinic	triclinic
Space group	*P*–1	*P*–1
a (Å)	9.7958(4)	10.6202(10)
b (Å)	11.3838(5)	15.6239(14)
c (Å)	19.2863(8)	21.913(2)
α (deg)	90.456(2)	70.612(3)
β (deg)	98.942(2)	81.599(3)
γ (deg)	97.185(2)	79.479(3)
V (Å^3)	2107.04(15)	3357.8(5)
Z	4	6
ρ (g cm^{-3})	1.061	1.032
R [$F^2 > 2\sigma(F^2)$]	0.0750	0.1157
wR (F^2)	0.2229	0.3550

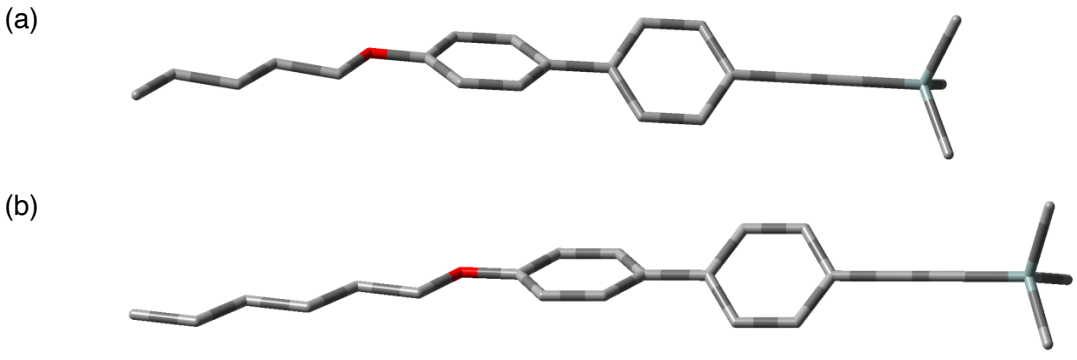
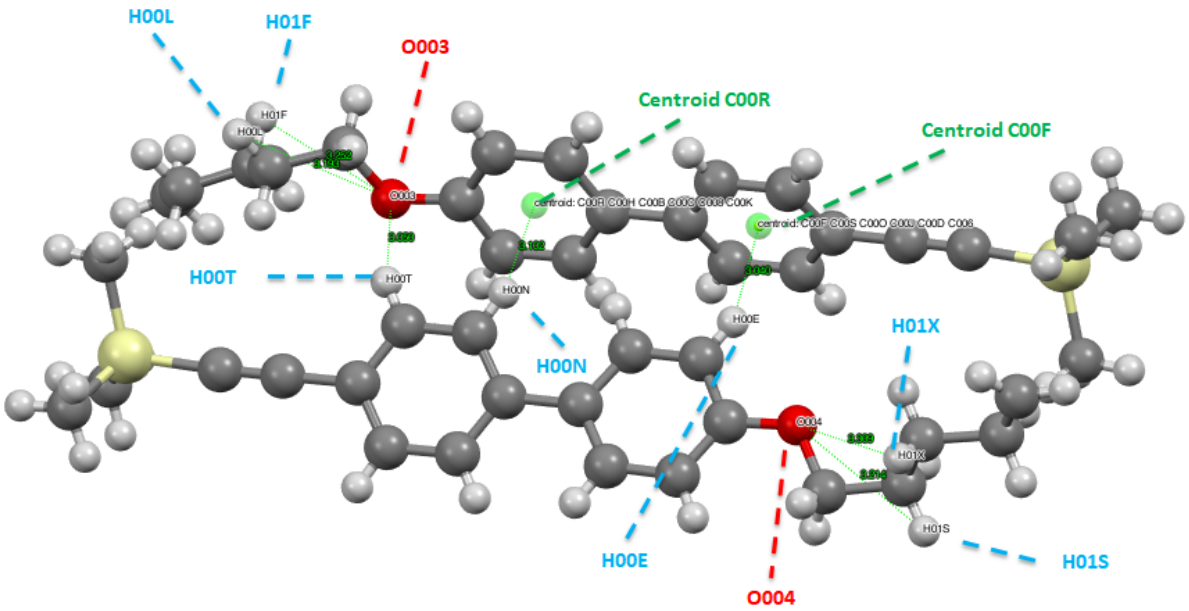
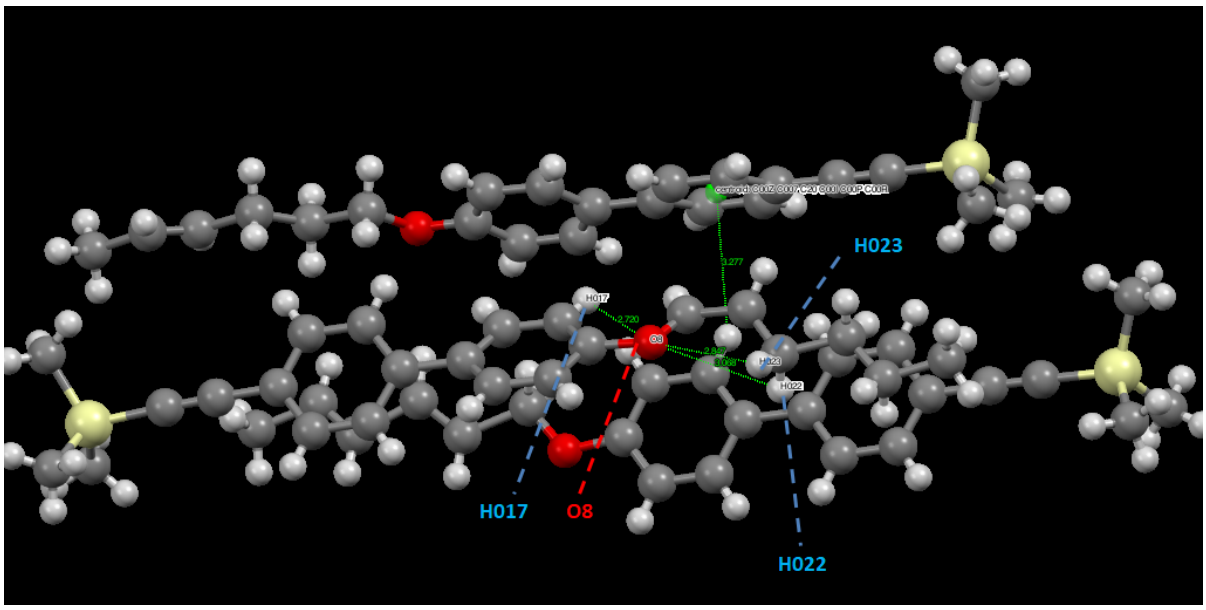


Figure S3. Calculated molecular structure of **5-BPTMS** and **6-BPTMS** optimized by DFT calculation employing B3LYP hybrid functionals with 6-311+G(d,p) basis sets. Atom color legend: grey, C; white, H; red, O; grayish blue, Si.



Molecular Interaction between the atoms	Distances (Å)
O004 – H01X	3.309
O004 – H01S	3.214
O003 – H00T	3.050
O003 – H00L	3.193
O003 – H01F	3.252
Centroid C00F – H00E	3.040
Centroid C00R – H00N	3.102

Figure S4. Molecular structure of compound **5-BPTMS**. Atom color legend: gray, C; white, H; red, O; yellow, Si.



Molecular Interaction between the atoms	Distances (Å)
O8-H017	2.720
O8-H023	2.847
O8-H022	3.068

Figure S5. Molecular structure of compound **6-BPTMS**. Atom color legend: gray, C; white, H; red, O; yellow, Si.

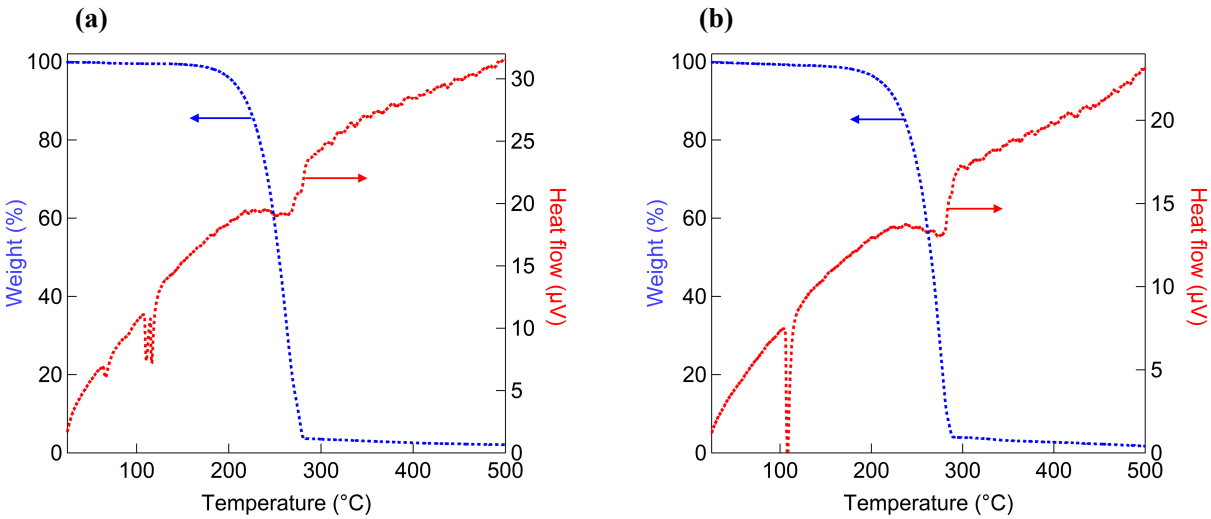


Figure S6. TG/DTA thermograms of **5-BPTMS** (a) and **6-BPTMS** (b) recorded under nitrogen atmosphere: heating rate of 5 °C min^{-1}.

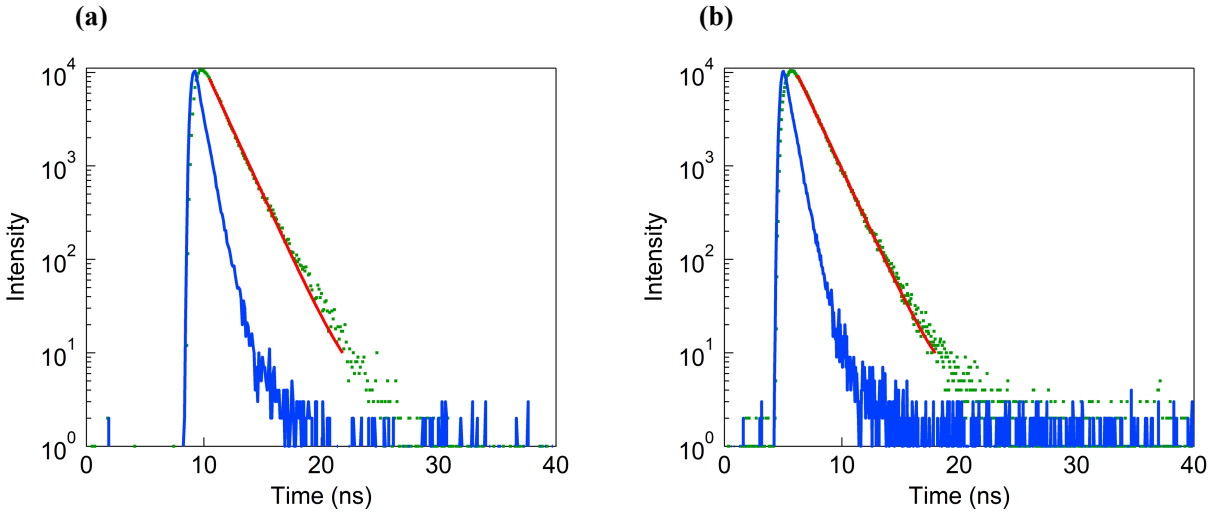


Figure S7. Luminescence decay profile of **5-BPTMS** (a) and **6-BPTMS** (b) at 380 nm (λ_{ex} = 280 nm) in Cry at room temperature: green, observed luminescence decay; red, fitting curve; blue, instrument response function.

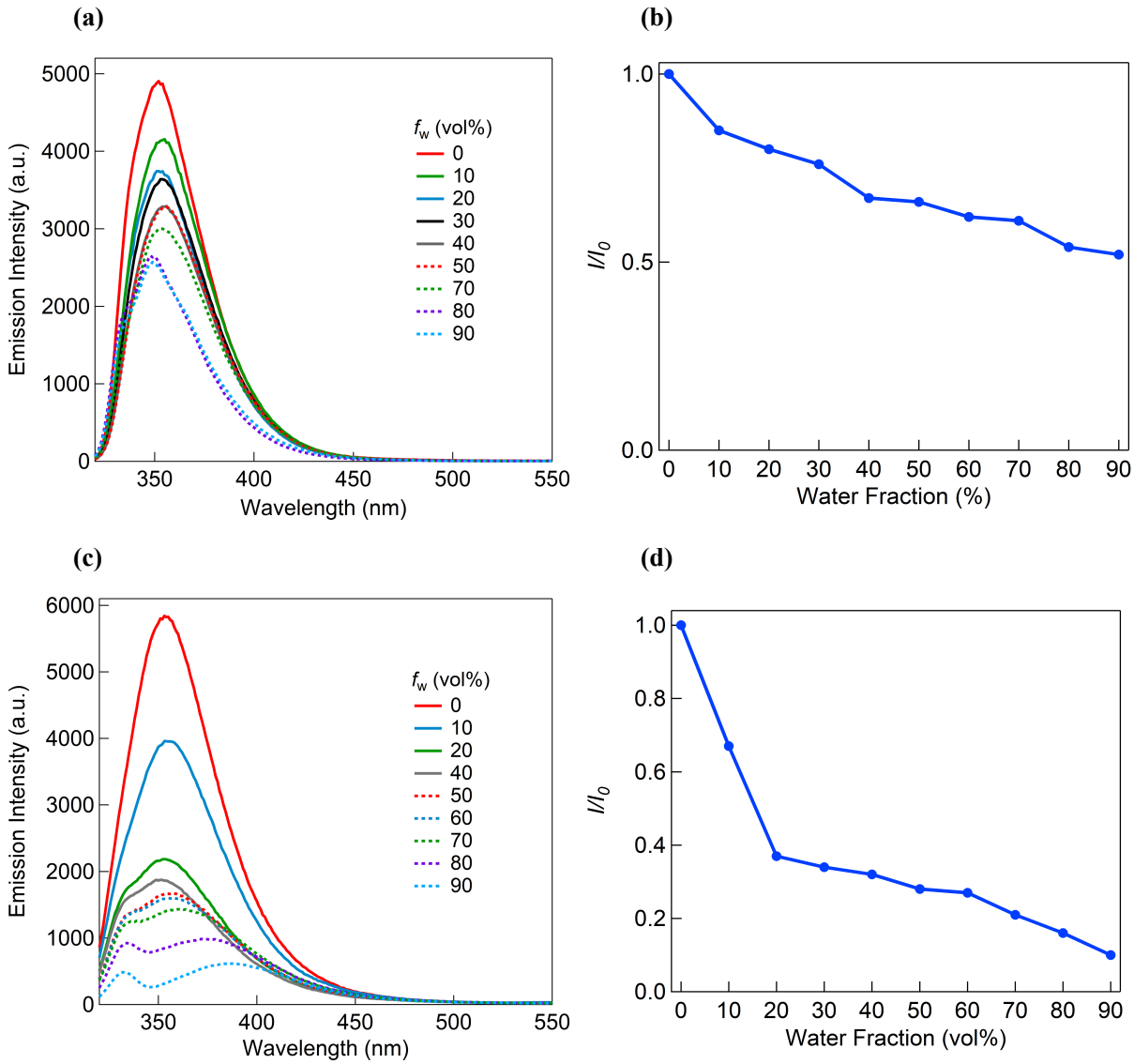


Figure S8. (a),(c) Luminescence spectra of compound **5-BPTMS** (a) and **6-BPTMS** (c) in THF/water mixtures with different water fractions (f_w) (λ_{ex} = 296 nm). (b),(d) Relative fluorescence intensity (I/I_0) of the compound **5-BPTMS** (a) and **6-BPTMS** (c) at 350 nm in THF/water mixtures as a function of f_w (λ_{ex} = 296 nm). I_0 is defined as the fluorescence intensity of the compounds in pure THF.