Supporting Information

Interfacial pH and polarity detection of amphiphilic self-assemblies using a single Schiff-base molecule

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Table S1: Fluorescence transient decay parameters of SBOH-Z-SBOH (5.0 μM) with residual of fitting (χ^2) in aqueous buffer solution at different pH values. Excitation and emission wavelengths were 450 and 500/530 nm respectively.

pH	Life time (ns)	χ^2
7.0	0.47 –	1.02
9.8	0.51 4.31	1.05
11.0	4.79 –	1.01

Table S2: Electronic excitation wavelength (nm), oscillator strengths (f_{cal}), absorption maxiam (λ_{max}) and extinction coefficient (ε) of non-ionic ($SBOH^0$-Z-$SBOH^0$), partially zwitterionic ($SBOH^0$-Z-$SBOH^{\pm}$), di-anionic (SBO^--Z-SBO^-) forms obtained by the TD-DFT/B3LYP/6-31G++(d,p) calculation on ground state geometries in various solvent with CPCM dielectric solvation model. The experimentally obtained UV-Vis absorption (Obs/Abs) parameters for SBOH-Z-SBOH are depicted for comparison.

	Form	**Solvent**	**λ_{max} (nm)**	**f_{cal}**	**$\varepsilon\times10^{-4}$ ($M^{-1}cm^{-1}$)**
TD-DFT	$SBOH^0$-Z-$SBOH^0$	THF	315	0.160	0.887
	$SBOH^0$-Z-$SBOH^{\pm}$	Water	385 315	0.132 0.098	0.657 0.582
	SBO^--Z-SBO^-	Water	390	0.203	1.205
Obs/Abs	SOBH-Z-SOBH	THF	330	-	1.005
		Buffer, pH 7.0	420 330		0.629 0.454
		Buffer, pH 11.0	395		1.103

Table S3: The correlation time (τ_c) with residual of single exponential fitting (χ^2) for SBOH-Z-SBOH (5.0 μM) obtained from fluorescence anisotropic decays in presence of different self-assembled systems at pH 10.5.

system	**τ_c (ns)**	**χ^2**
Buffer	0.63	1.02
CTAB	1.90	1.03
DDAB	2.01	0.98
TX-100	1.02	1.09
DOPC	1.11	1.03

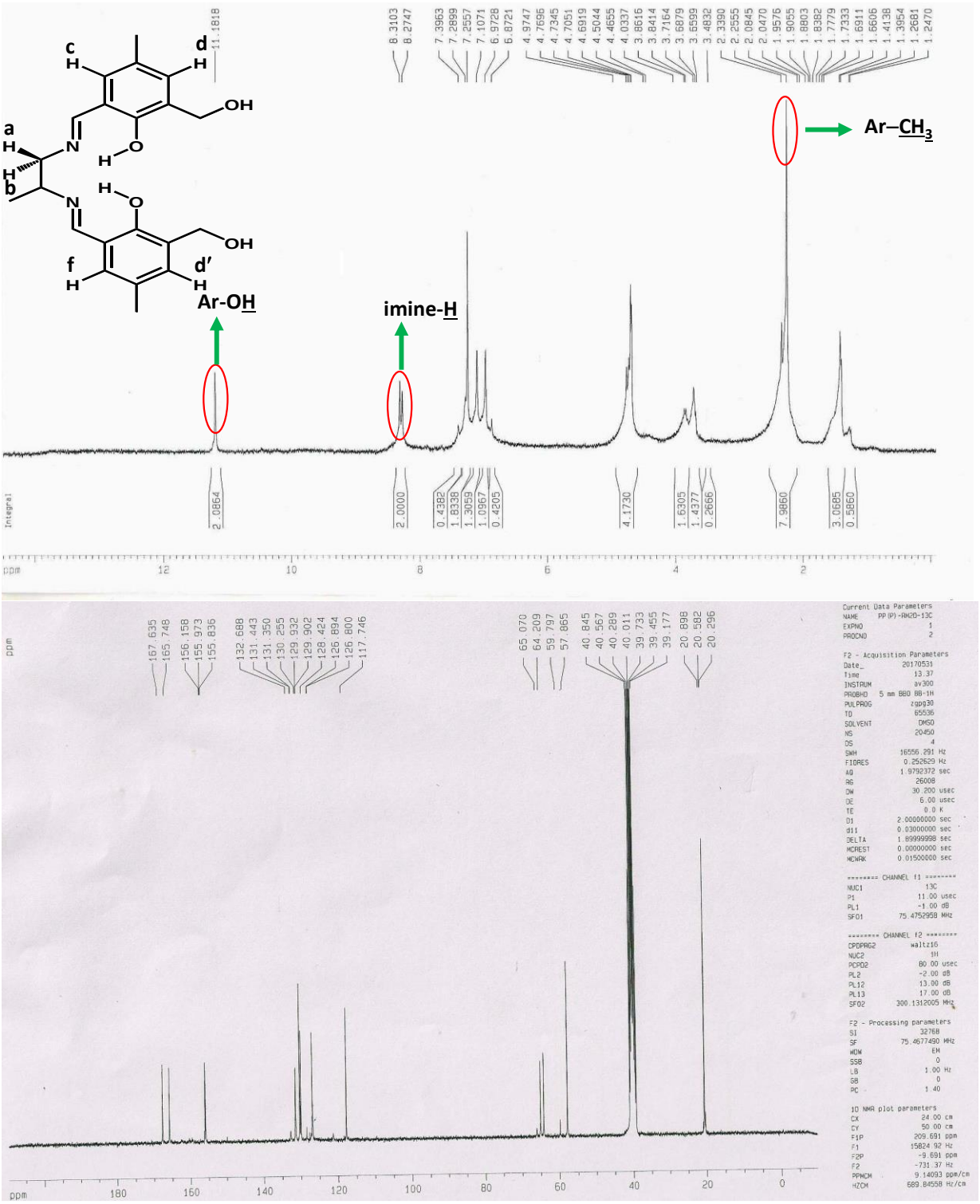

Fig. S1. ^{1}H and ^{13}C NMR spectra of SBOH-Z-SBOH in $CDCl_3$ and DMSO-d_6 respectively.

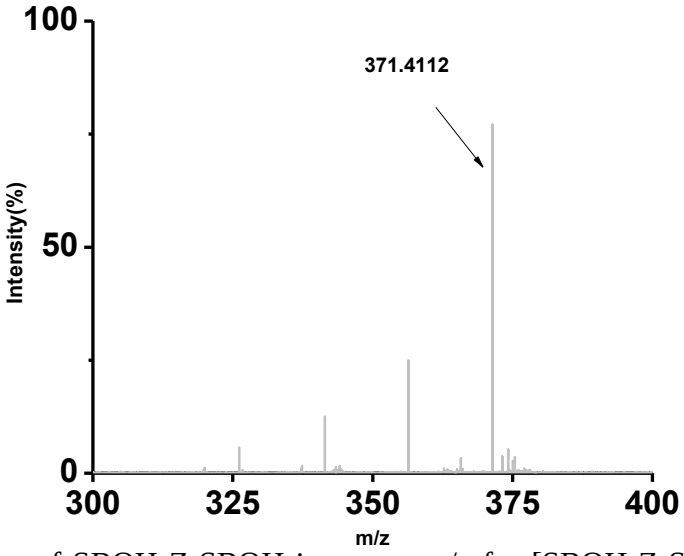

Fig. S2. ESI-MS$^+$ spectra of SBOH-Z-SBOH in water: m/z for [SBOH-Z-SBOH+H]$^+$: obs'd – 371.4112, cal'd – 371.44848)

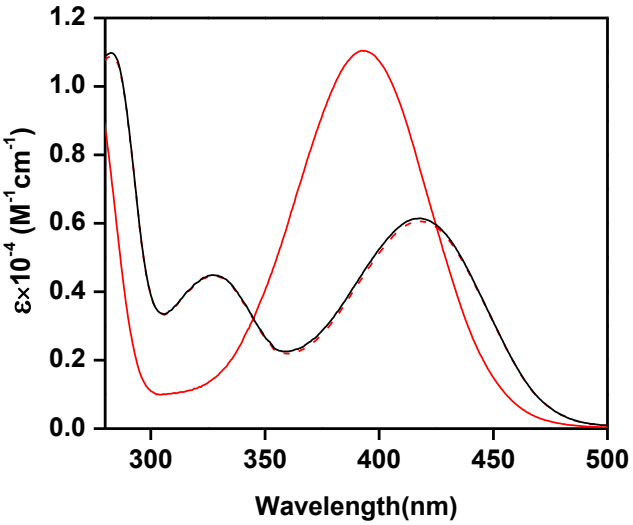

Fig. S3. pH dependent UV-Vis absorption spectral changes of SBOH-Z-SBOH (5.0 μM) in buffer medium. The pH was increased from 7.0 (black) to 12.0 (red) by an addition of 0.1 M NaOH and subsequently decreased to 7.0 (red, broken) by an addition of 0.1 M HCl in 20 mM tris-HCl buffer.

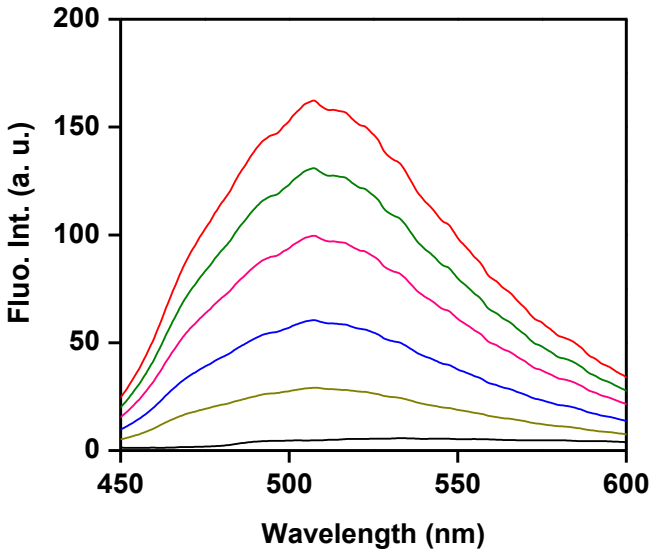

Fig. S4. Fluorescence spectra of SBOH-Z-SBOH (5.0 μM) in buffer/THF mixed medium at different dielectric constants (wt % of THF in the mixtures are depicted in bracket): black, 8.0 (1.0); dark yellow, 18.3 (0.8); blue, 32.0 (0.6); pink, 48.2 (0.4); green, 64.6 (0.2); and red, 78.5 (0.0).

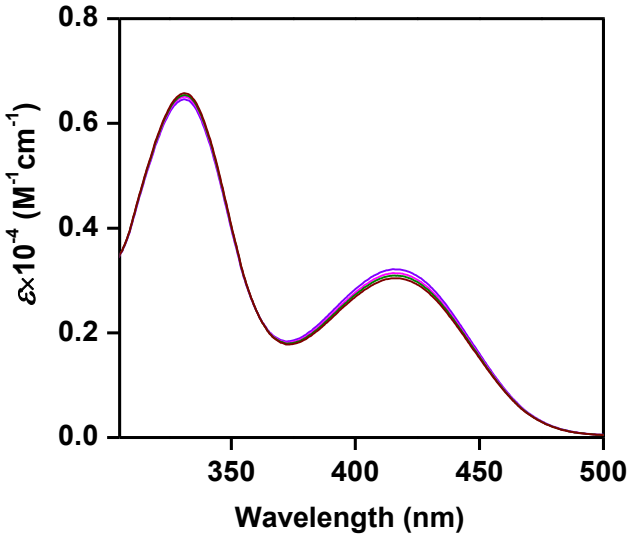

Fig. S5. UV-Vis absorption spectra of SBOH-Z-SBOH (5.0 μM) in 1:1 THF/buffer solution at different pH: violet, 5.5; brown, 7.0; pink, 8.0; green, 10.0.

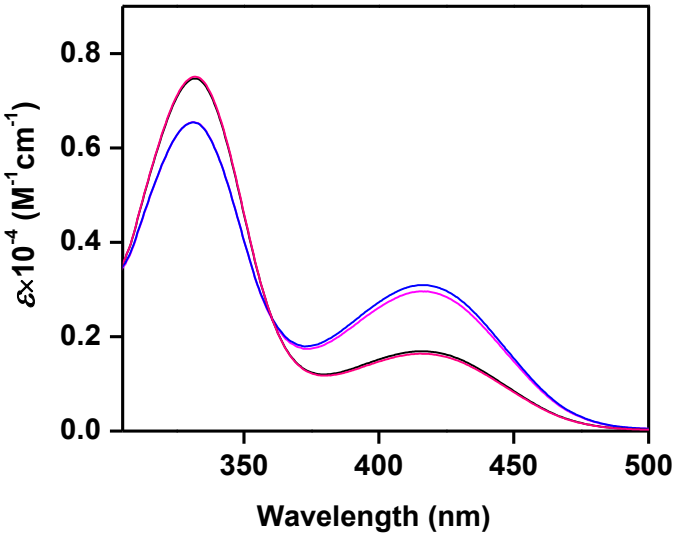

Fig. S6. Solvent composition dependent UV-Vis absorption spectra of SBOH-Z-SBOH (5.0 μM): pink, acetonitrile (κ ~ 37.5); blue, THF/water mixture (52.5% (w/w) THF in the mixture, κ ~ 37.5); red, THF/water mixture (70% (w/w) THF in the mixture, κ ~ 24.5); black, EtOH (κ ~ 24.5).

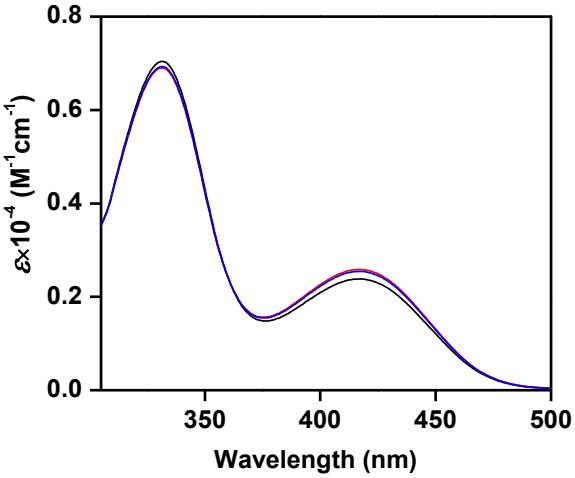

Fig. S7. UV-Vis absorption spectra of SBOH-Z-SBOH (5.0 μM) under identical κ (~ 37.5) at pH 8.0: red, buffer/EtOH mixed medium (75% (w/w) EtOH in the mixture); blue, acetonitrile; black, buffer/glycerol mixed medium (80% (w/w) glycerol in the mixture).

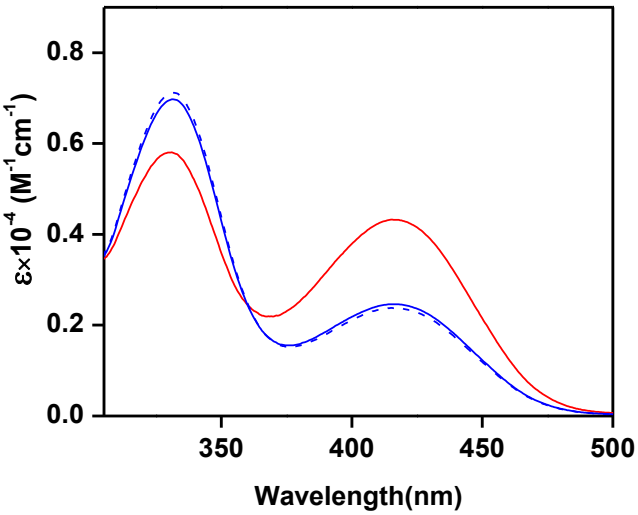

Fig. S8. Solvent dielectric constant (κ) dependent UV-Vis absorption spectral change of SBOH-Z-SBOH (5.0 μM). The κ was increased for the mixed MeOH medium from 33.0 (blue) for pure MeOH to 55.0 (red) by an addition of water (50% (w/w) of water in the MeOH/water mixture) and subsequently decreased to 33.0 (broken, blue) by addition of THF (48 and 26% (w/w) of THF and water in THF/water/MeOH mixture, respectively).

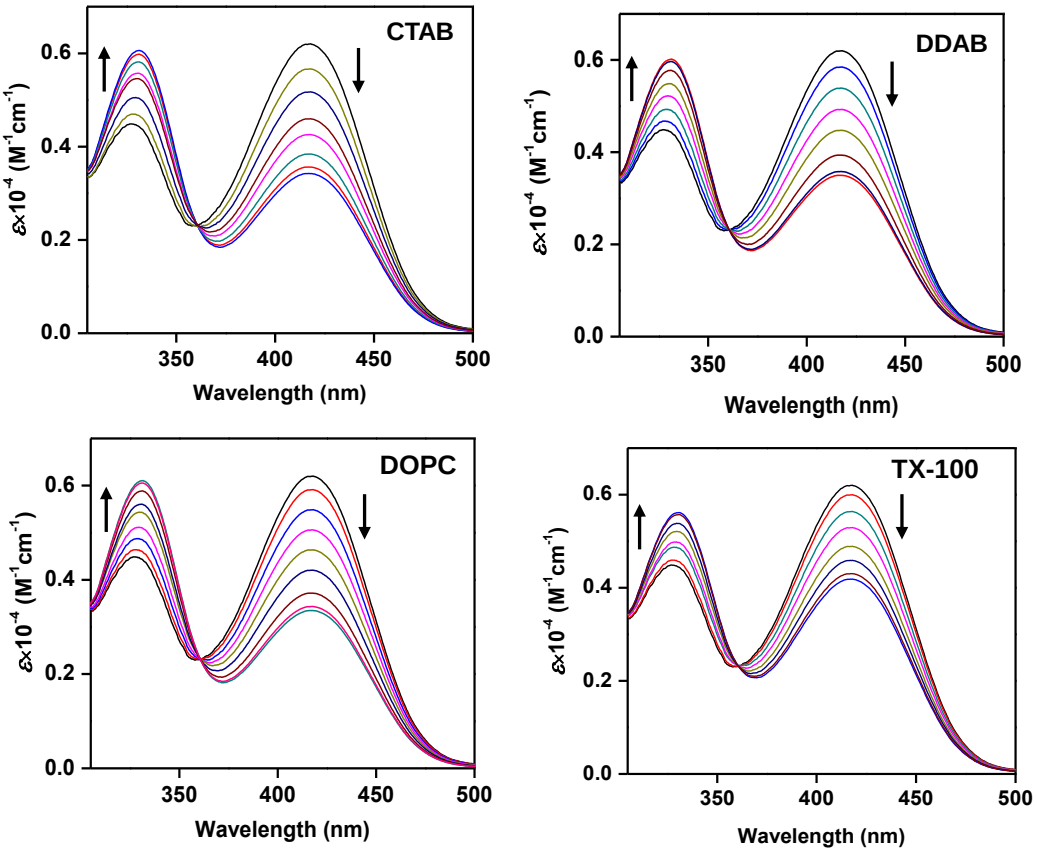

Fig. S9. UV-Vis absorption spectra of SBOH-Z-SBOH (5.0 μM) in presence of increasing concentration of different self-assembled systems in 20 buffer, pH 7.0: CTAB (0–5.0 mM), DDAB (0–3.0 mM), TX-100 (0–6.0 mM) and DOPC (0–4.0 mM).

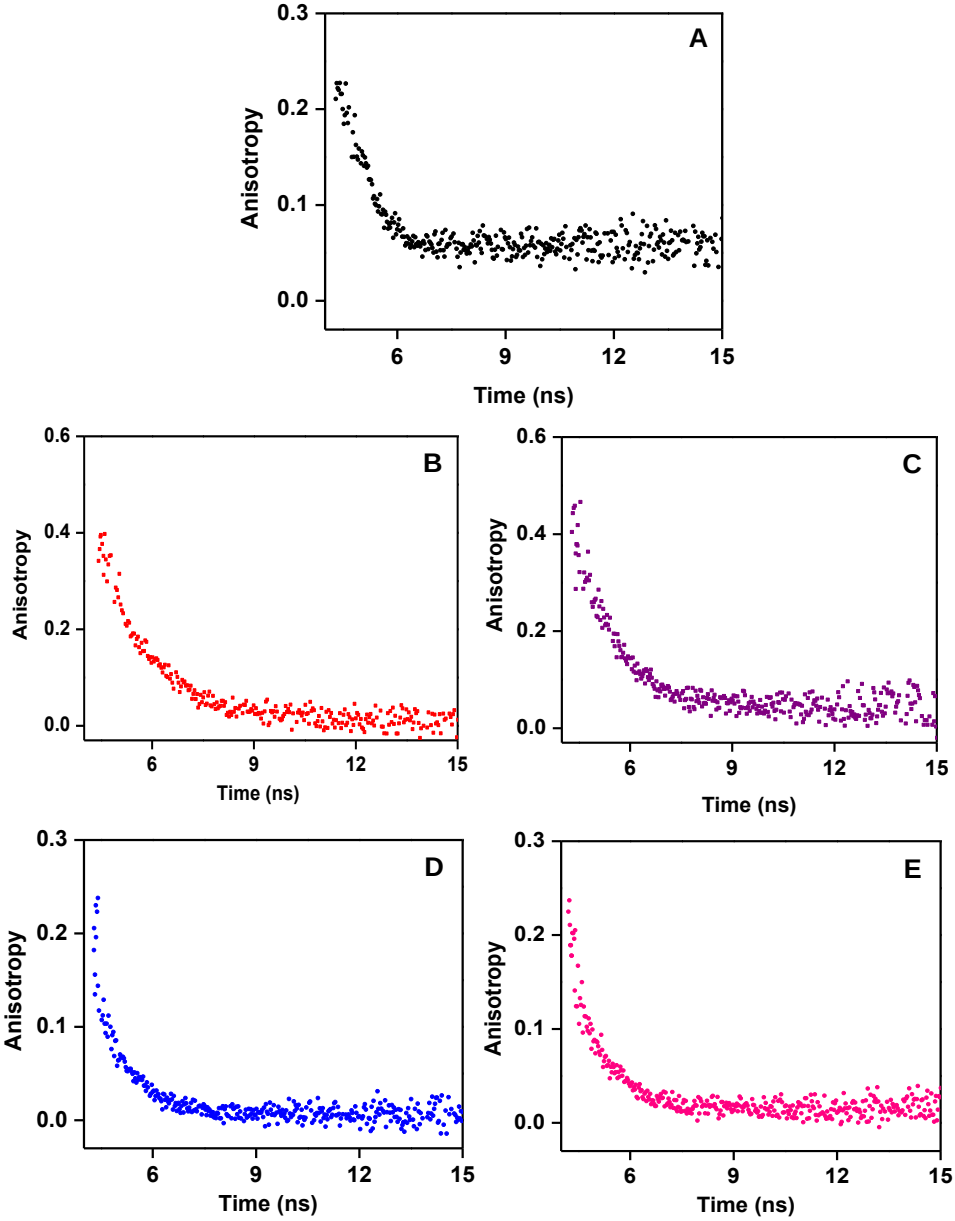

Fig. S10. Fluorescence anisotropic decay curves of SBOH-Z-SBOH (5.0 μM) in (A) absence and (B–E) presence of deviation saturated concentration of different self-assembled systems at pH 10.5: (B), CTAB (5.0 mM); (C), DDAB (3.0 mM); (D), TX-100 (6.0 mM) and (E) DOPC (4.0 mM).

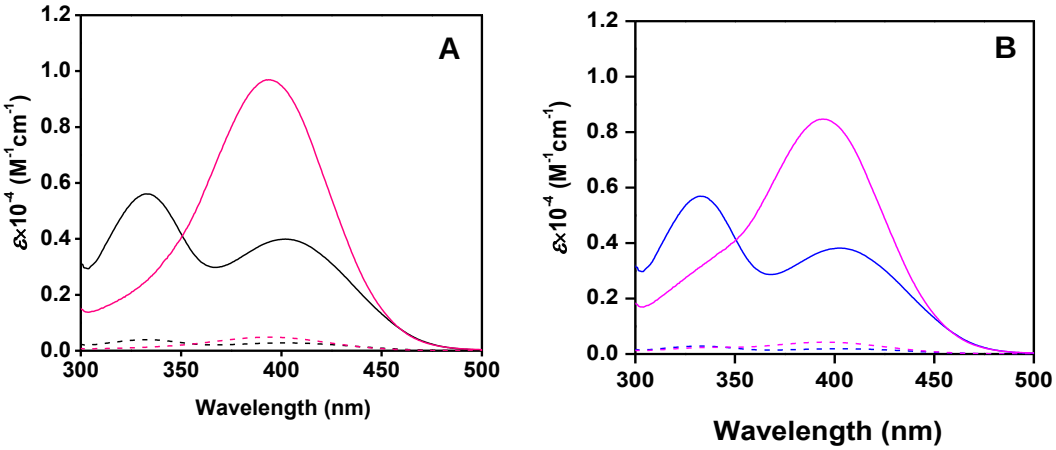

Fig. S11. UV-Vis absorption spectra of SBOH-Z-SBOH (5.0 μM) in presence (solid) of different deviation-saturated concentration of ULVs, and (broken) its filtrated solution: (A) DDAB: red, pH 9.0; black, pH 8.0. (B) DOPC: pink, pH 11.5; blue, pH 10.5. The filtrated solution was obtained using a 100K MW cut-off filter.

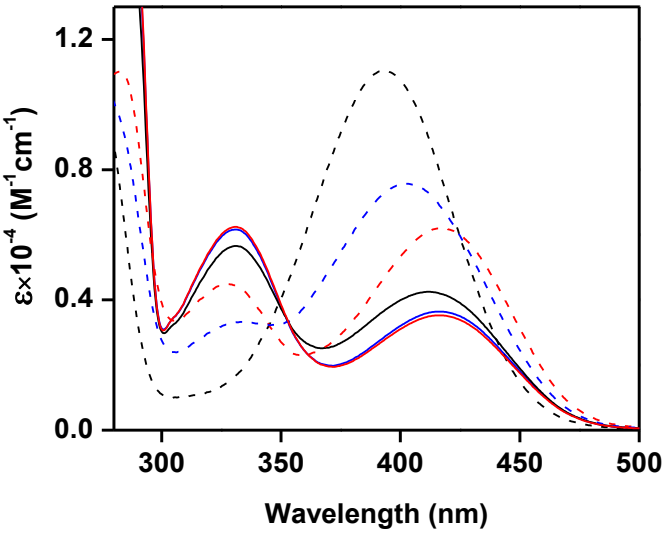

Fig. S12. UV-Vis absorption spectra of SBOH-Z-SBOH (5.0 μM) in the absence (dash) and in presence of SDS (solid) in different pH: black, pH 12.5; blue, pH 9.5; red, pH 7.0.

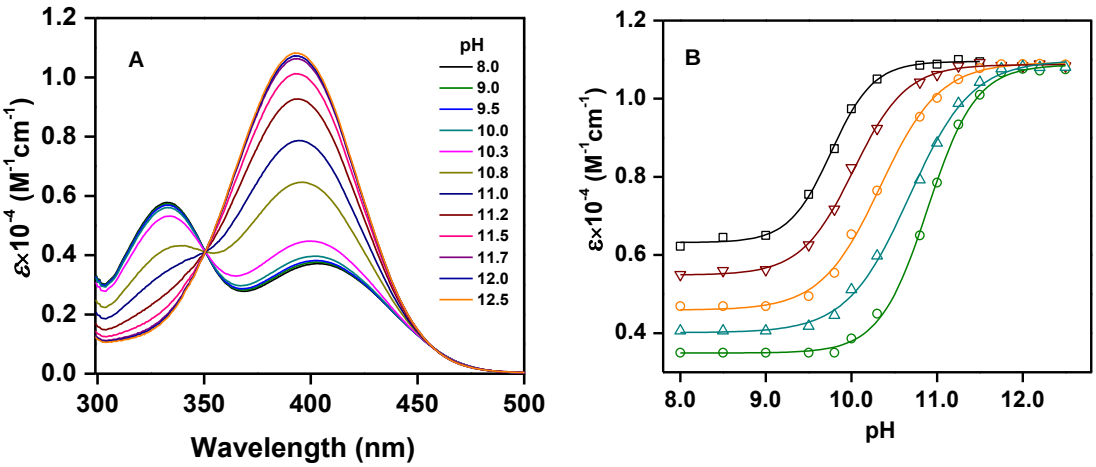

Fig. S13. (A) pH dependent UV-Vis absorption spectra of SBOH-Z-SBOH (5.0 μM) in 53% (w/w) ethanol containing buffer medium. (B) Molar extinction coefficient (ε) at the absorption intensity maxima (395–420 nm) at different pH under different solvent polarity (κ) of ethanol/buffer mixed: black, 78.5; brown, 70.0; orange, 60.0; cyan, 50.0; green, 43.0.

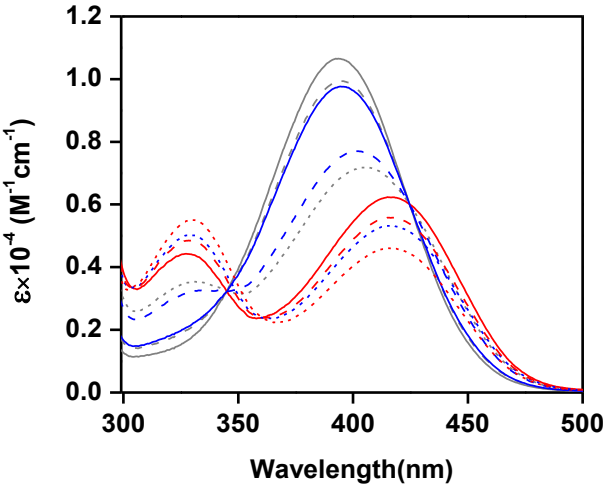

Fig. S14. UV-Vis absorption spectra of SBOH-Z-SBOH (5.0 μM) in buffer of different pH (10.8, gray; 10.0, blue; 8.0, red) and κ (solid, 72.0; short dash, 48.0; broken, 25.0) of the medium.