

## Supporting Information

# Threonine-based stimuli-responsive nanoparticles with aggregation-induced emission-type fixed cores for detection of amines in aqueous solutions

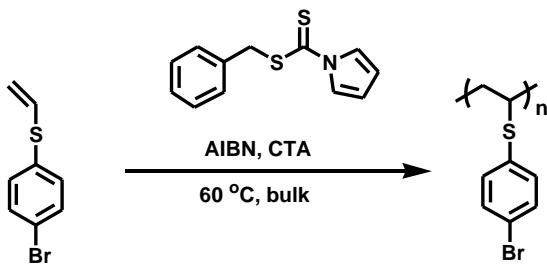
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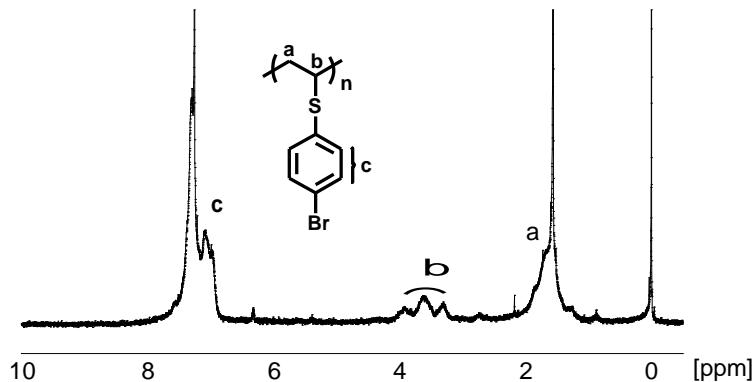
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**Scheme S1.** Synthesis of PBPVS.

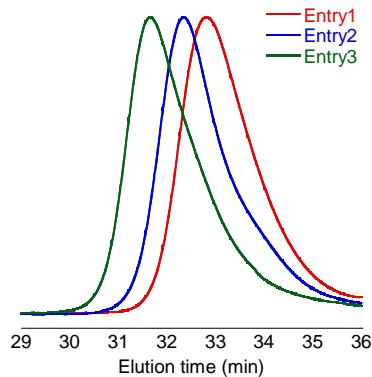


**Figure S1.**  $^1\text{H}$  NMR spectrum of PBPVS in  $\text{CDCl}_3$ .

**Table S1.** Synthesis of PBPVS in bulk at different  $[\text{M}]/[\text{CTA}]_0$  ratios and  $60^\circ\text{C}$  for 24 h <sup>a)</sup>

Entry	$[\text{Monomer}]_0/[\text{CTA}]_0$	Conv. <sup>b)</sup> (%)	Yield <sup>c)</sup> (%)	$M_n$ <sup>d)</sup> (theory)	$M_n$ <sup>b)</sup> ( $^1\text{H}$ NMR)	$M_n$ <sup>e)</sup> (SEC)	$M_w/M_n$ <sup>e)</sup> (SEC)
1	25	36	6	2200	3000	1400	1.41
2	50	55	24	6100	5400	2000	1.39
3	100	51	27	11200	10500	3200	1.33

<sup>a)</sup>  $[\text{CTA}]_0/[\text{AIBN}]_0 = 2$ . <sup>b)</sup> Calculated by  $^1\text{H}$  NMR. <sup>c)</sup> Hexane-insoluble part. <sup>d)</sup> The theoretical molecular weight ( $M_{n,\text{theory}}$ ) = (MW of BPVS)  $\times$   $[\text{BPVS}]_0/[\text{CTA}]_0 \times$  conv. + (MW of CTA). <sup>e)</sup> Measured by SEC using polystyrene standard in DMF (10 mM LiBr).

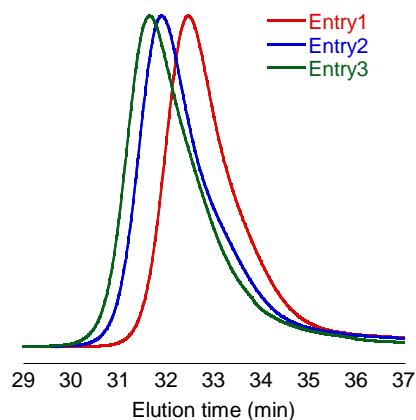


**Figure S2.** SEC curves of PBPVS prepared by RAFT polymerization at different [M]/[CTA] ratios.

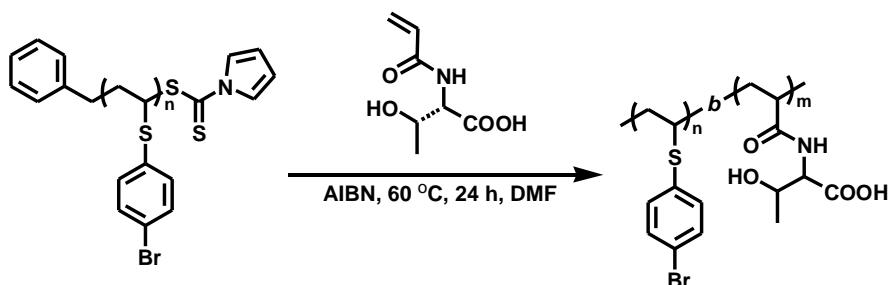
**Table S2.** Synthesis of PBPVS in bulk at 60 °C<sup>a)</sup>

Entry	Time (h)	Conv. <sup>b)</sup> (%)	Yield <sup>c)</sup> (%)	$M_n$ <sup>d)</sup> (theory)	$M_n$ <sup>b)</sup> ( <sup>1</sup> H NMR)	$M_n$ <sup>e)</sup> (SEC)	$M_w/M_n$ <sup>e)</sup> (SEC)
1	6	19	6	4320	4000	1900	1.32
2	12	41	18	9000	6400	2700	1.34
3	24	51	27	11200	10500	3200	1.33

<sup>a)</sup>  $[M]_0/[CTA]_0/[AIBN] = 200/2/1$ . <sup>b)</sup> Calculated by <sup>1</sup>H NMR. <sup>c)</sup> Hexane-insoluble part. <sup>d)</sup> The theoretical molecular weight ( $M_{n,\text{theory}}$ ) = (MW of BPVS)  $\times$   $[BPVS]_0/[CTA]_0 \times$  conv. + (MW of CTA). <sup>e)</sup> Measured by SEC using polystyrene standard in DMF (10 mM LiBr).



**Figure S3.** SEC curves of PBPVS prepared for different polymerization times.

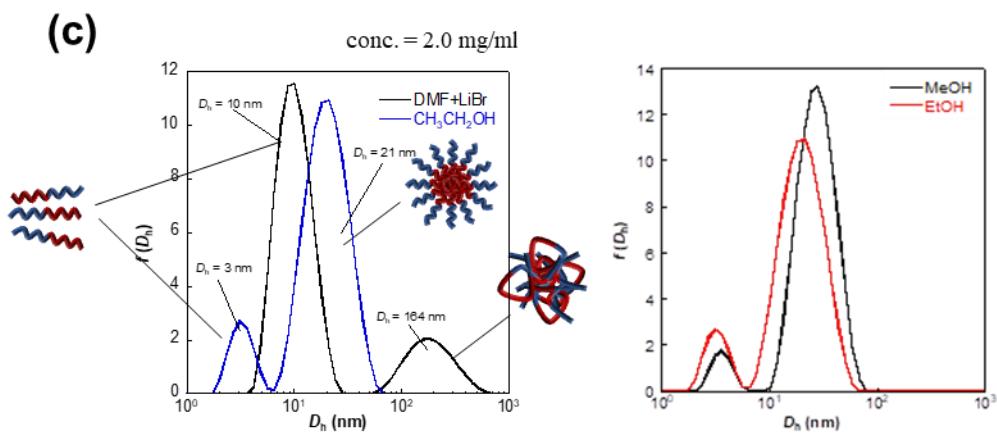
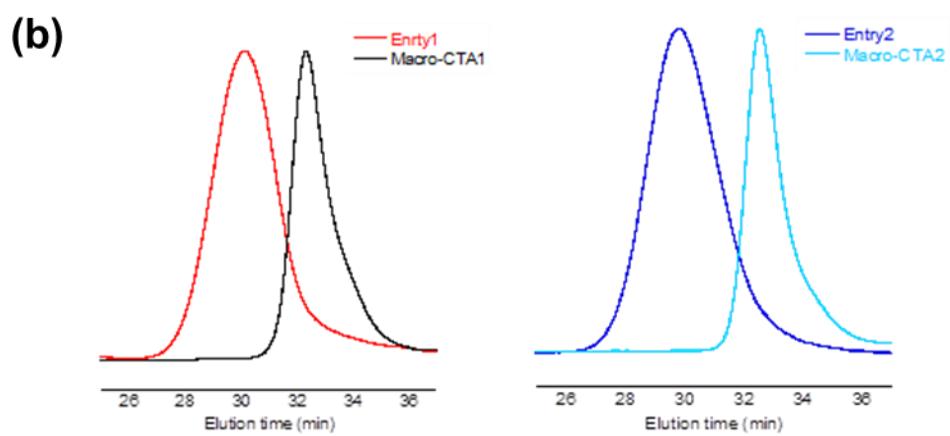
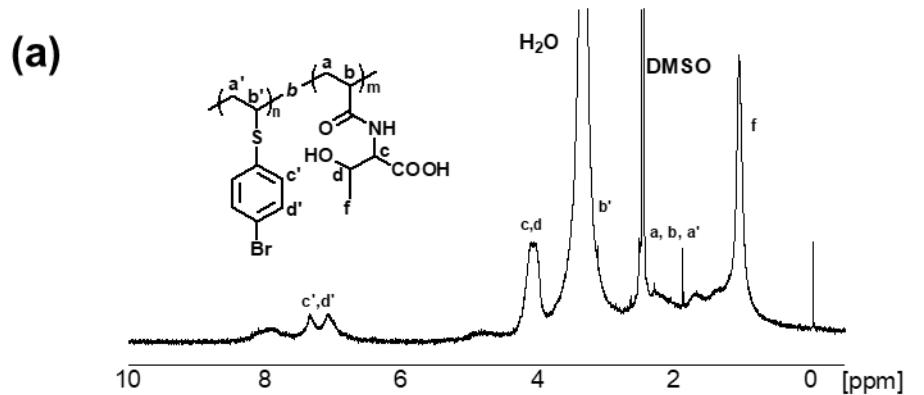


**Scheme S2.** Synthesis of PBPVS-*b*-PAThrOH.

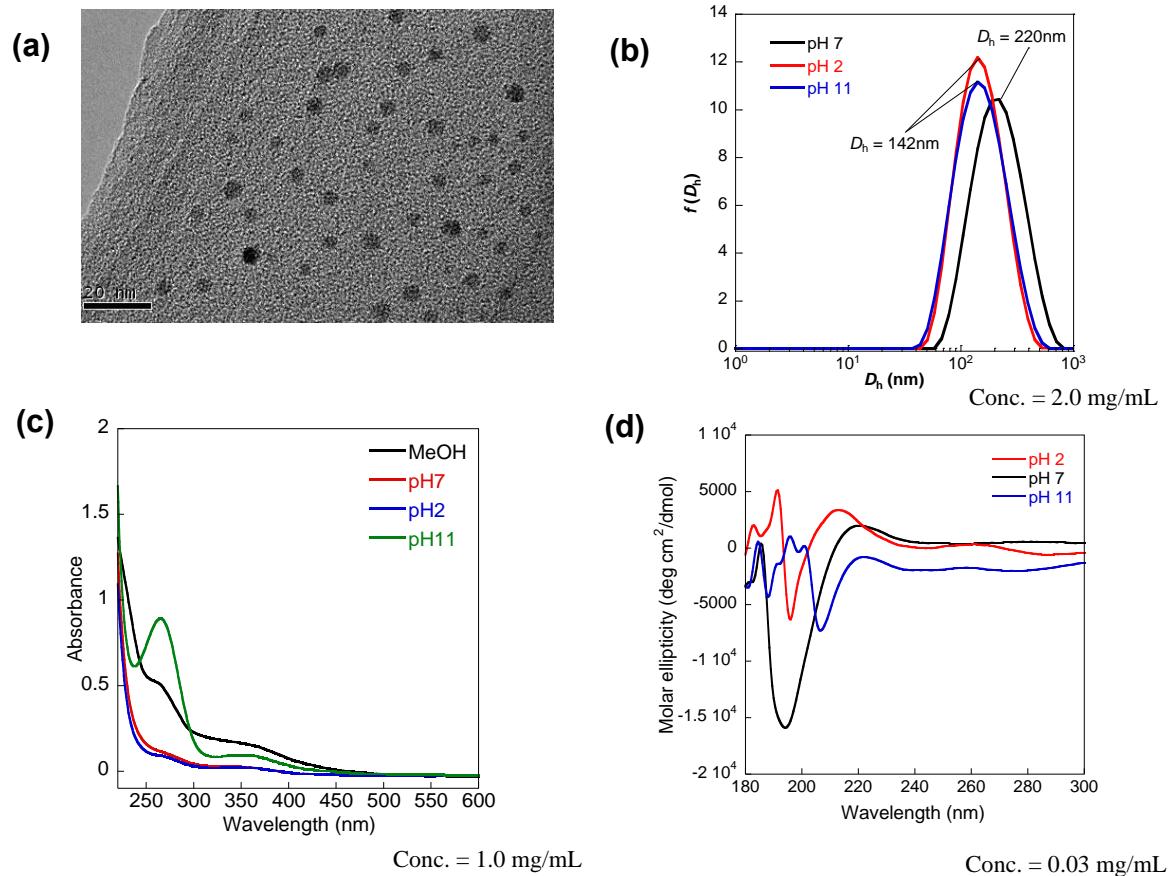
**Table S3.** Synthesis of PBPVS-*b*-PAThrOH in DMF at 60 °C for 24h

Entry	[I] <sub>0</sub> /[Macro- CTA] <sub>0</sub> / [Monomer] <sub>0</sub>	Conv. <sup>a)</sup> (%)	Yield <sup>b)</sup> (%)	<i>M<sub>n</sub></i> <sup>c)</sup> (theory)	<i>M<sub>n</sub></i> <sup>a)</sup> ( <sup>1</sup> H NMR)	<i>M<sub>n</sub></i> <sup>d)</sup> (SEC)	<i>M<sub>w</sub></i> / <i>M<sub>n</sub></i> <sup>d)</sup> (SEC)	<i>n/m</i> <sup>a)</sup>
1 <sup>e)</sup>	1/2/200	89	54	20800	10700	23000	1.42	24/76
2 <sup>f)</sup>	1/2/400	65	54	26000	17000	22500	1.49	12/88

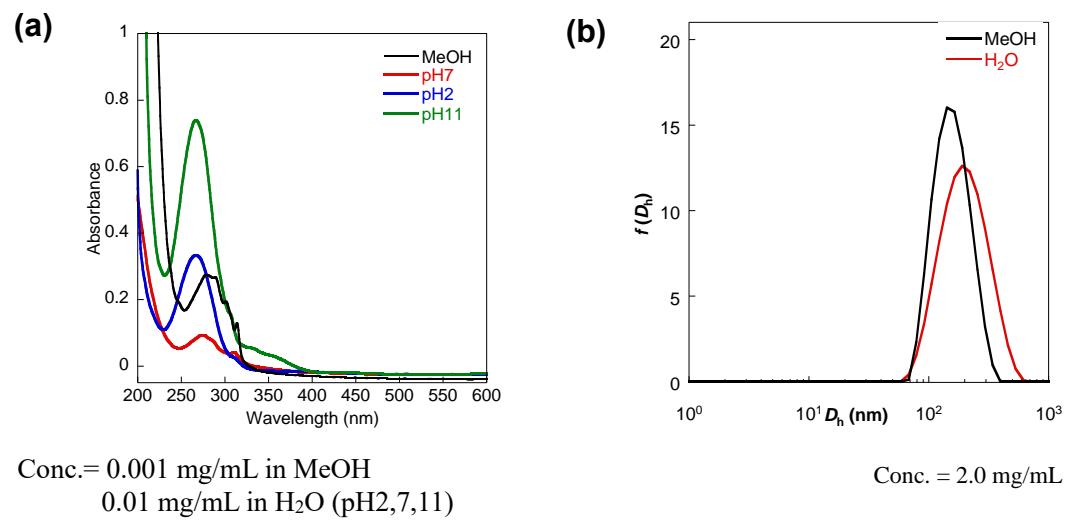
<sup>a)</sup> Calculated by <sup>1</sup>H NMR. <sup>b)</sup> Ethyl acetate insoluble part. <sup>c)</sup> The theoretical molecular weight (*M<sub>n</sub>,theory*) = (MW of AThrOMe) × [AThrOH]<sub>0</sub>/[CTA]<sub>0</sub> × conv. + (*M<sub>n</sub>* of macro-CTA). <sup>d)</sup> Methylated PBPVS-*b*-PAThrOH was measured by SEC using polystyrene standard in DMF (10 mM LiBr). <sup>e)</sup> Macro-CTA (Entry 1) : *M<sub>n</sub>*(SEC) = 2000, *M<sub>n</sub>*(<sup>1</sup>H NMR) = 5400, *M<sub>w</sub>*/*M<sub>n</sub>* = 1.39. <sup>f)</sup> Macro-CTA (Entry 2) : *M<sub>n</sub>*(SEC) = 1700, *M<sub>n</sub>*(<sup>1</sup>H NMR) = 3500, *M<sub>w</sub>*/*M<sub>n</sub>* = 1.37.



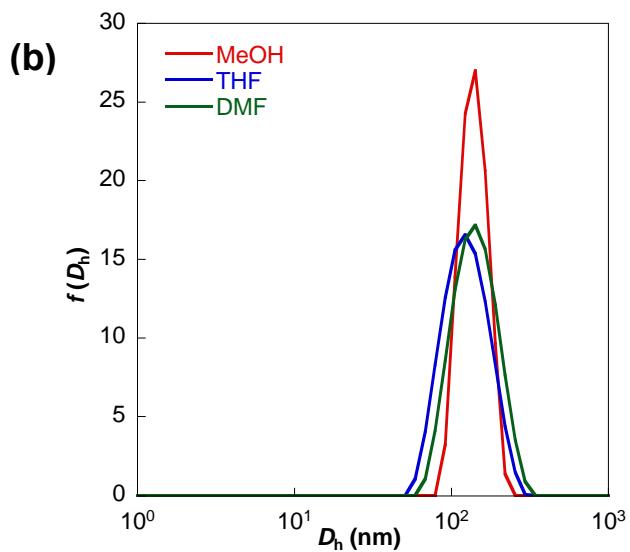
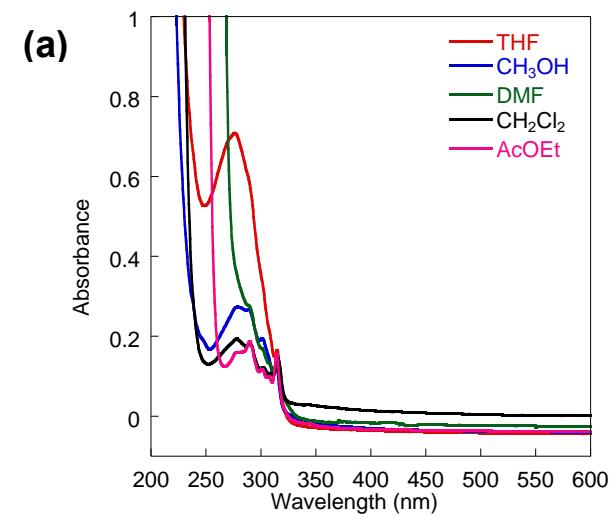
**Figure S4.** (a)  $^1\text{H}$  NMR spectrum in  $\text{DMSO}-d_6$ , (b) SEC curves, and (c) DLS traces of PBPVS-*b*-PAThrOH.



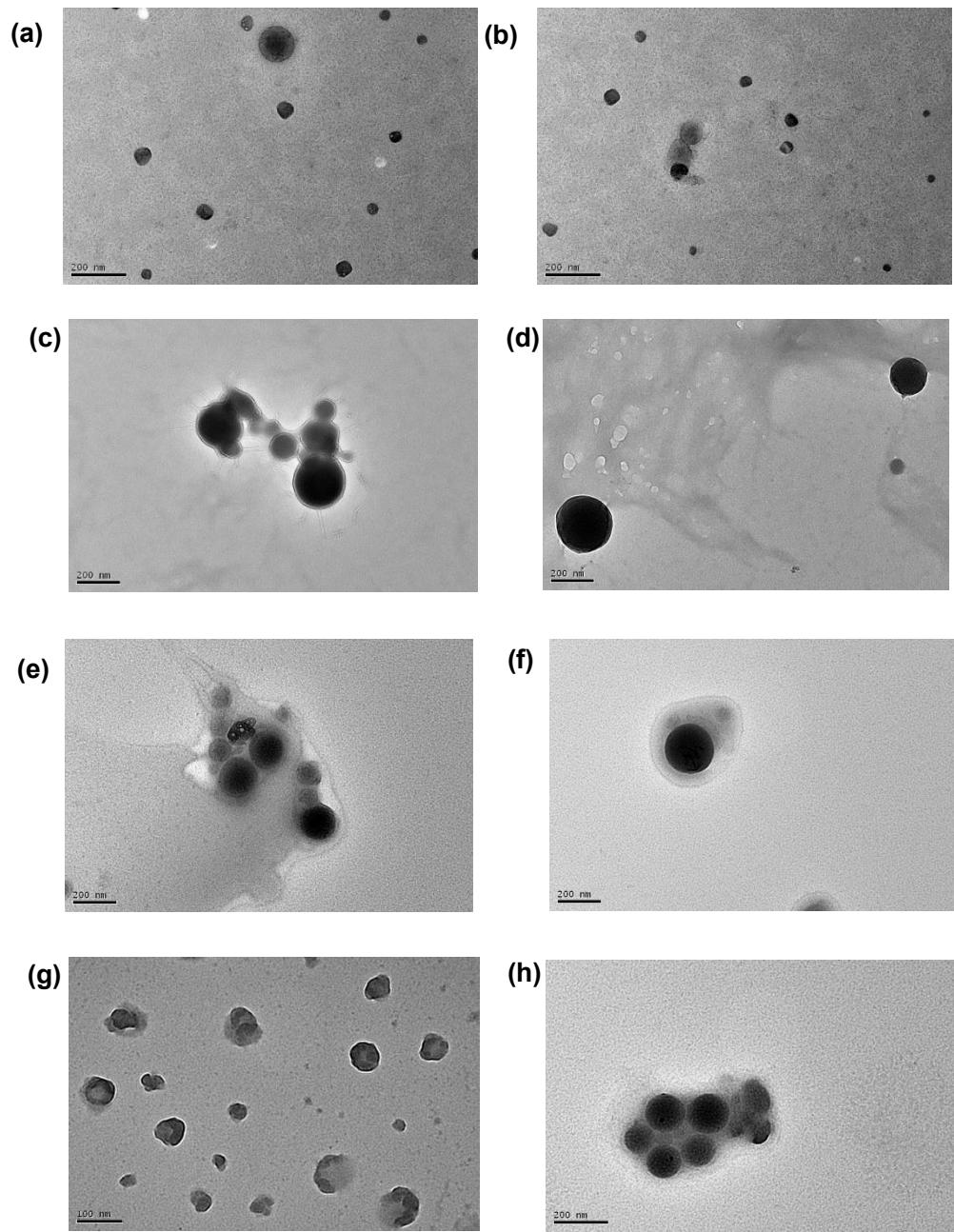
**Figure S5.** (a) TEM image, (b) DLS traces, (c) UV-vis spectra, and (d) CD spectra of NP(dTh) in MeOH and water at different pH values.



**Figure S6.** (a) UV-vis spectra and (b) DLS traces of NP(Fl) in MeOH and water.



**Figure S7.** (a) UV-vis spectra of NP(Fl) in different organic solvents (conc. = 0.001 mg/mL) and (b) DLS traces in different solvents (2.0 mg/mL).



**Figure S8.** TEM images of NP(FI) samples prepared from diluted (a, b) AcOEt, (c, d) DMF, (e, f) CHCl<sub>3</sub>, and (g, h) THF solutions.

**Table S4.** Solubility of block copolymer, NP(dTh), and NP(Fl)

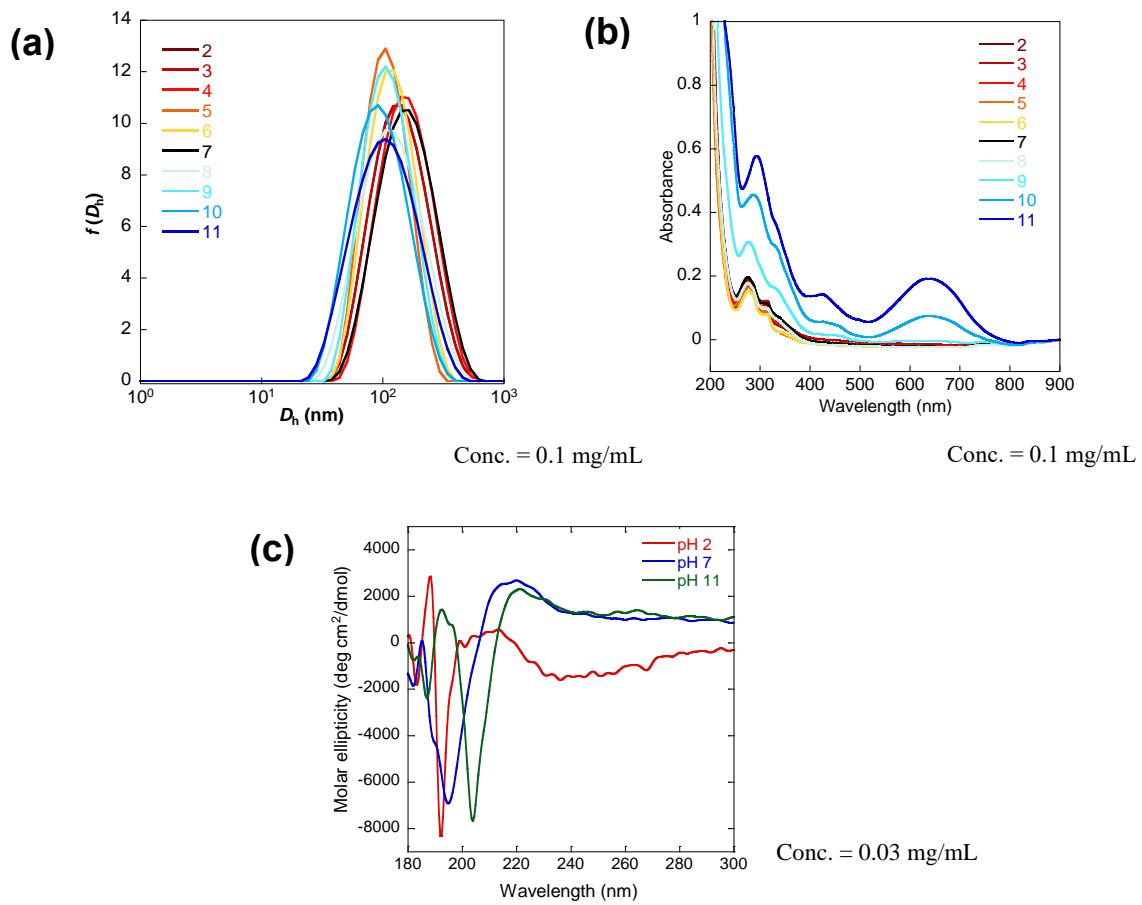
sample	CHCl <sub>3</sub>	CH <sub>2</sub> Cl <sub>2</sub>	THF	CH <sub>3</sub> OH	Ethanol
PBPVS- <i>b</i> -PAThrOH	—	—	—	+	+
NP(dTh)	+ —	+	+	+ —	+ —
NP(Fl)	+	+	+ —	+ —	+ —

sample	Diethyl ether	Ethyl acetate	1,4-dioxane	hexane	Toluene
PBPVS- <i>b</i> -PAThrOH	—	—	—	—	+ —
NP(dTh)	+ —	+ —	+ —	+ —	+
NP(Fl)	—	+ —	+ —	—	+

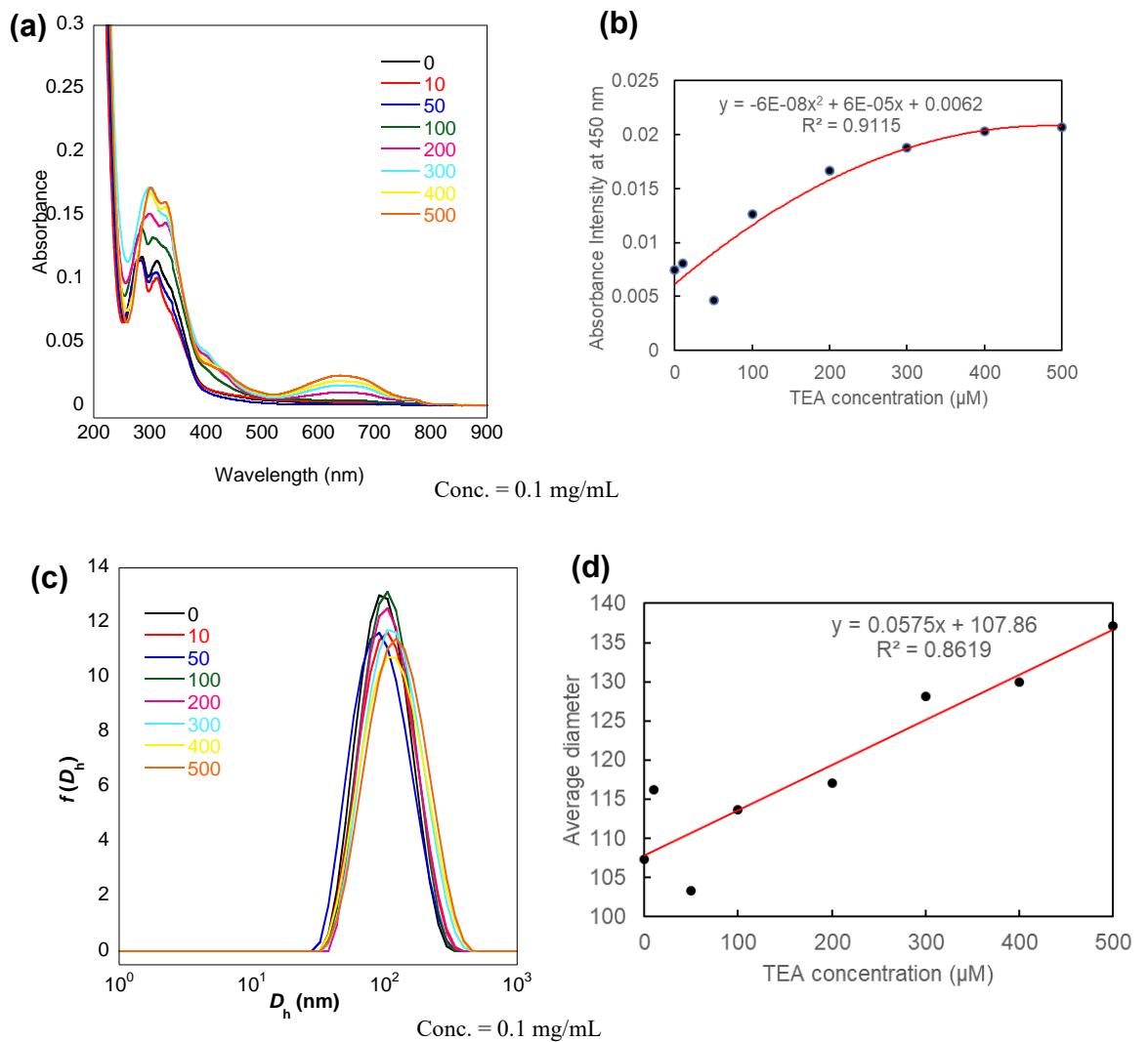
sample	Acetone	2-propanol	DMF	DMSO	H <sub>2</sub> O
PBPVS- <i>b</i> -PAThrOH	—	+ —	+	+	+
NP(dTh)	+ —	+ —	+ —	+ —	+ —
NP(Fl)	—	+	+ —	+	+ —

+ : Soluble at room temperature, + —: partially soluble and/or soluble under diluted conditions,

— : Insoluble at room temperature.



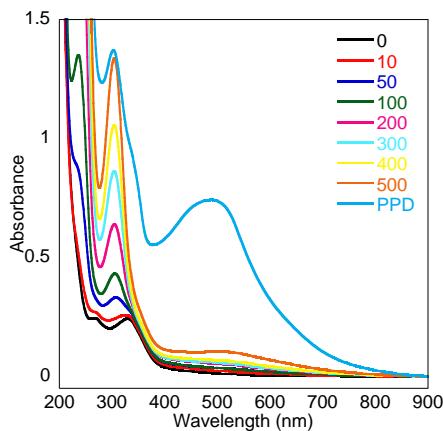
**Figure S9.** (a) DLS traces, (b) UV-vis spectra, and (c) CD spectra of NP(Fl) in H<sub>2</sub>O at different pH values.



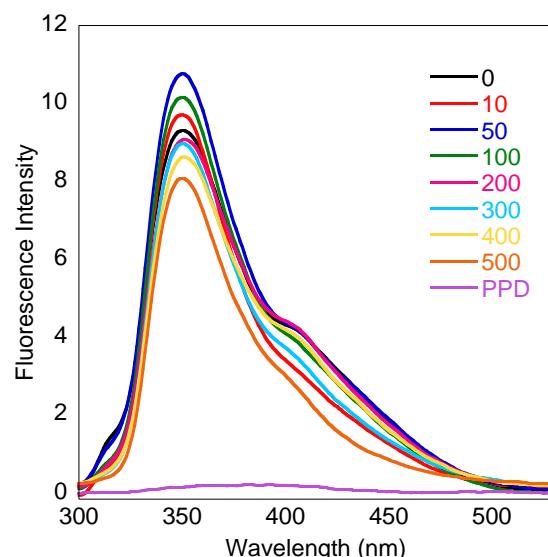
**Figure S10.** (a) UV-vis spectra, (b)  $I_{450}$  plots, (c) DLS traces, and (d) diameter plots of NP(Fl) in  $H_2O$  after addition of TEA.

**Table S5.** Summary of fluorescence quantum yields of NP(Fl) in H<sub>2</sub>O after addition of PPD

PPD ( $\mu\text{M}$ )	0	10	50	100	200	300	400	500
$\Phi$	0.0102	0.00671	0.00423	0.00491	0.00324	0.00275	0.00228	0.00171



**Figure S11.** UV-vis spectra of NP(Fl) in H<sub>2</sub>O after addition of PPD.



**Figure S12.** Fluorescence spectra of NP(Fl) in H<sub>2</sub>O (conc.= 0.1 mg/mL,  $\lambda^{\text{abs}} = 280 \text{ nm}$ ) after addition of PPD.