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## **Supplementary Information**

Self-Complementary Hydrogen-Bond Interaction of Guanosine: a Hub for Constructing Supra-Amphiphilic Polymers with Controlled Molecular Structure and Aggregate Morphology

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Figure S1. <sup>1</sup>H NMR spectrum of G-Br.



Figure S2. <sup>1</sup>H NMR spectrum of G-PNIPAM.



Figure S3. FT-IR spectra of G and G-PNIPAM.



Figure S4. <sup>1</sup>H NMR spectrum of G-N<sub>3</sub>.



**Figure S5.** <sup>1</sup>H NMR spectrum of PCL-alkyne.



Figure S6. <sup>1</sup>H NMR spectrum of G-PCL.



Figure S7. FT-IR spectra of G-N<sub>3</sub>, PCL-alkyne and G-PCL.



**Figure S8.** (a) SEC traces of G-PCL and PCL-alkyne using THF as the eluent. MALDI-TOF-MS traces of (b) G-PNIPAM and (c) G-PCL.



Figure S9. <sup>1</sup>H NMR spectrum of G-OAc.



Figure S10. FT-IR spectra of G-OAc (a) in solid state and (b) CHCl<sub>3</sub>.



Figure S11. Circular dichroism (CD) spectrum of G-OAc at 0.04 mg/mL in CHCl<sub>3</sub>.

Sample	m <sub>G-PNIPAM</sub> : m <sub>G-PCL</sub> <sup>a</sup>	m <sub>G-PNIPAM</sub> : m <sub>G-PCL</sub> <sup>b</sup>
P1	9.0:1.0	9.3:0.7
P2	7.0:3.0	7.8:2.2
Р3	4.0:6.0	4.4:5.6

<b>Table S1</b> . Theoretical and actual weight mixing ratios of G-PNIPAM versus G
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<sup>a</sup> Mixing weight ratios of G-PNIPAM versus G-PCL as designed.

<sup>b</sup> Mixing weight ratios of G-PNIPAM versus G-PCL that is determined by <sup>1</sup>H-NMR measurement after dialysis.



**Figure S12.** (a) <sup>1</sup>H NMR spectrum of PNIPAM-NH<sub>2</sub>, and (b) Digital photograph of the mixture solution containing PNIPAM-NH<sub>2</sub> and G-PCL (weight ratio: 7.0:3.0).

## Shape Evolutionary Mechanism of Self-Assembly in SAPs

As reported,<sup>10, 11</sup> the morphology of polymer assemblies or aggregates can be indicated by the hydrophilic-hydrophobic blocks ratio. Generally, the hydrophilic volume fraction (*f*) parameter was used to reflect the change of SAPs to some extent. As equation  $(1)^{10, 11}$ :

$$f = \frac{\sum V_{philic}}{\sum V_{total}} = \frac{\sum \frac{M_{philic}}{\rho_{philic}}}{\sum \frac{M_{philic}}{\rho_{philic}} + \sum \frac{M_{phobic}}{\rho_{phobic}}} \times 100\%$$
(1)

The  $M_i$  is different block molar mass in the total molecular weight of the block copolymer, and  $\rho_i$  is the density of different blocks, 1.269 g/cm<sup>-3</sup> for PNIPAM,<sup>12</sup> and 1.130 g/cm<sup>-3</sup> for PCL.<sup>13</sup> When f > 50%, spherical micelles were expected to form, worm-like micelles when 40% < f < 50%, vesicles or other lamellar structures for f < 40%.<sup>10, 11</sup>

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