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Figure S1 ¹H NMR spectrum of G3.5-Ad (DMSO-d₆).



Figure S2 ¹H NMR spectrum of β-CD-Br (DMSO-d₆).



Figure S3 1 H NMR spectrum of β -CD-g-PNIPAAm (DMSO-d₆).



Figure S4. ¹H NMR spectrum of β -CD-g-PNIPAAm/G3.5-Ad (D₂O).



Figure S5. The intermediate state of the transformation from nanospheres to nanorods.



Figure S6. The intermediate state of the transformation from nanosheets to nanospheres upon addition of G3.5-Ad.



Figure S7. The fluorescence spectra of samples at room temperature. The concentration of samples is 5 mg mL⁻¹. G3.0 PAMAM, β -CD-g-PNIPAAm and β -CD-g-PNIPAAm/G3.5-Ad supramolecular were dissolved in distilled water, and G3.5-Ad was dissolved in methanol. The excitation wavelength is 388 nm.



Figure S8. The fluorescence spectra of β -CD-g-PNIPAAm/G3.5-Ad aqueous solutions with different pH value. The concentration of samples is 5 mg mL⁻¹ and the excitation wavelength is 388 nm.

pKa of β-CD-g-PNIPAAm/G3.5-Ad supramolecular

As shown in Figure S4, pH decreased rapidly and then decreased slowly with the addition of HCl solution. Tertiary amine groups ionized gradually as the pH decreased, and when pH is below 3.7, tertiary amine segments ionized mostly completely, and the pH decreased slowly in the range from 3.7 to 3.0 with the increasing amount of HCl added in the solution. Thus it can be seen, the pKa of β -CD-g-PNIPAAm/G3.5-Ad is about 3.7.



Figure S9. The pH as a function of the volume of HCl (0.05 mol/L) added in 20 mL β -CD-g-PNIPAAm/G3.5-Ad solution (0.5 mg/mL) at room temperature.



Figure S10. Cytotoxicity tests of β -CD-g-PNIPAAm/G3.5-Ad supramolecular. The

data are presented as mean \pm SD (n = 5).