

Supporting Information

Conformation and Self-Assembly Changes of Isomeric Peptide Amphiphiles Influenced by Switching Tyrosine in the Sequences

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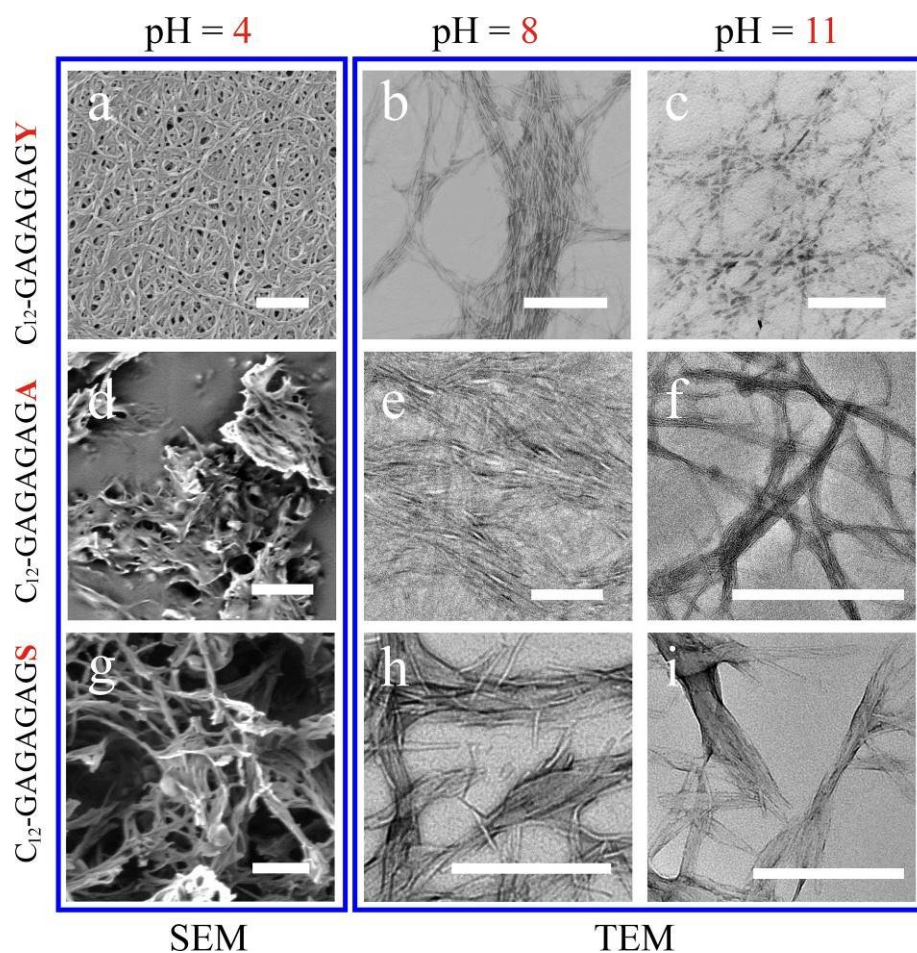


Figure S1. SEM and TEM images of self-assembled C_{12} -GAGAGAGY (a-c, ref. 27 in the text), C_{12} -GAGAGAGA (d-f), and C_{12} -GAGAGAGS (g-i), 1 mg/mL, respectively. As all the PAs formed self-supporting hydrogels or precipitates at pH 4, SEM was employed for a better observation instead of TEM. All bars indicate 500 nm.

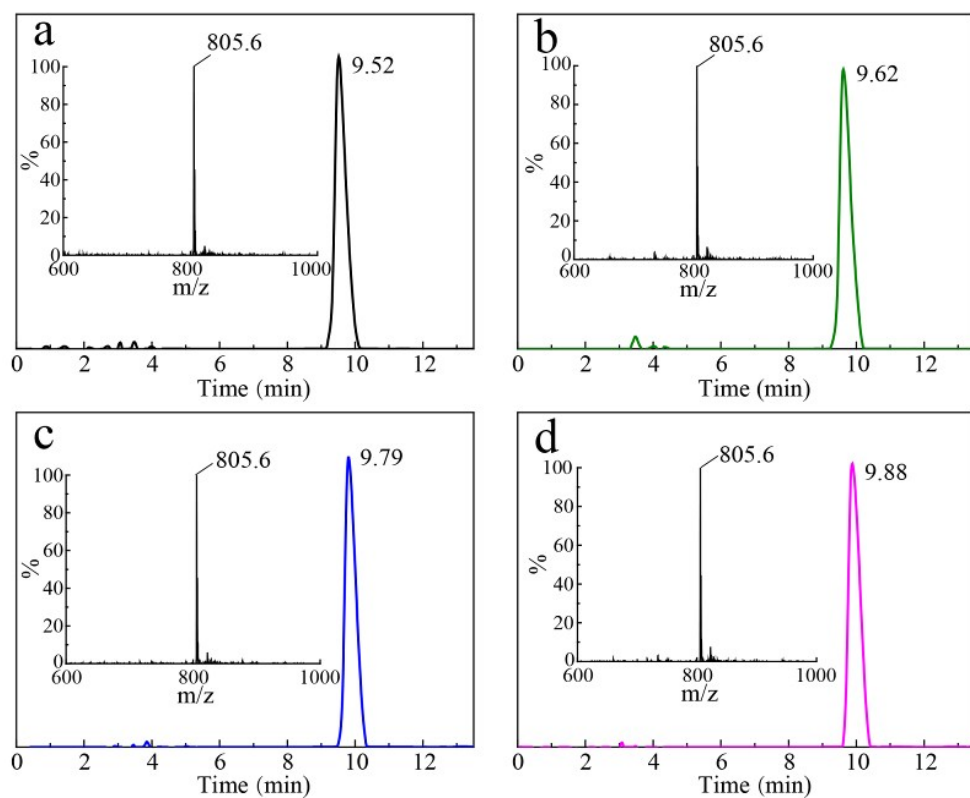


Figure S2. LC/ESI-MS analysis of C_{12} -GAGAGAGY (a), C_{12} -GAGAGYGA (b), C_{12} -GAGYGAGA (c), and C_{12} -GYGAGAG (d), respectively.

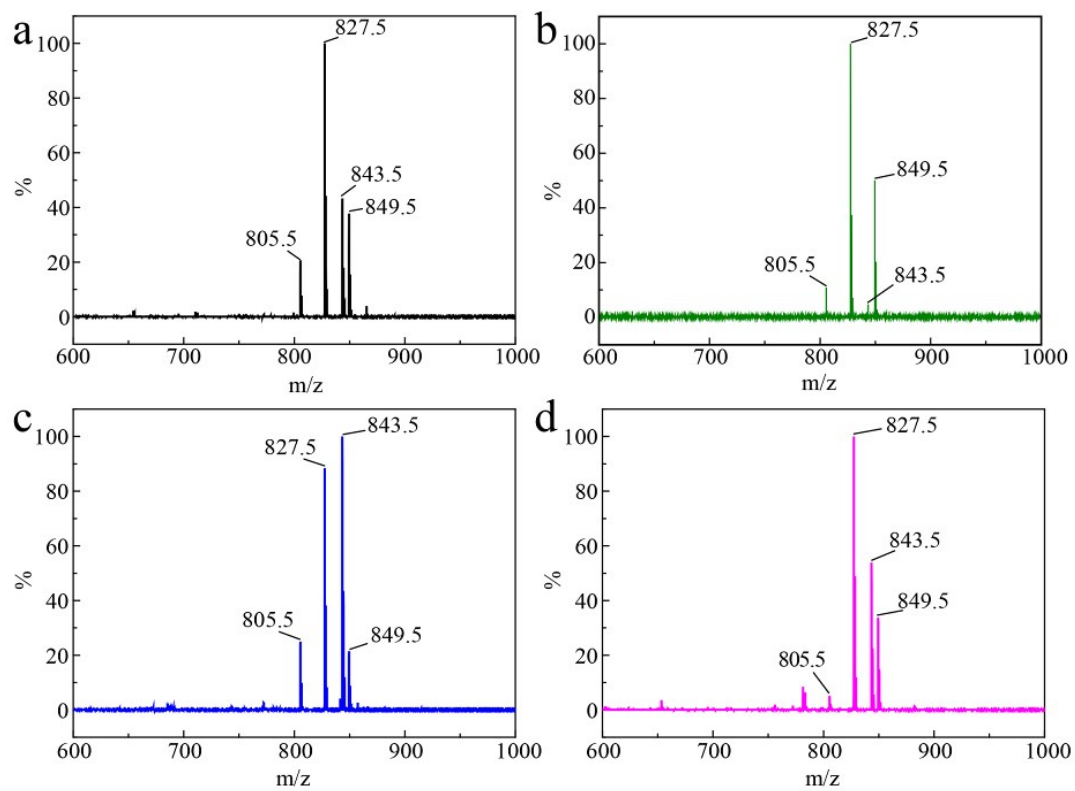


Figure S3. MALDI-TOF mass spectra of C₁₂-GAGAGAGY (a), C₁₂-GAGAGYGA (b), C₁₂-GAGYGA (c), and C₁₂-GYGAGAG (d), respectively.

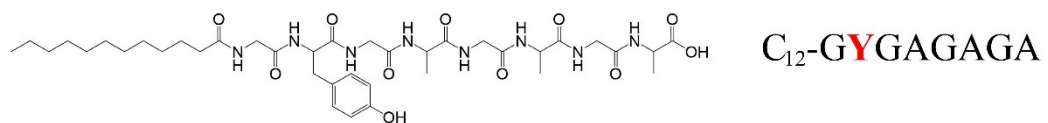
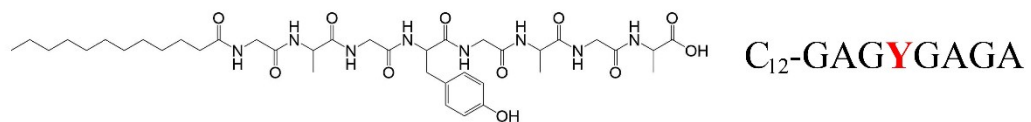
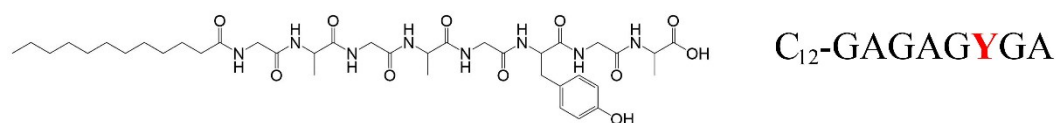
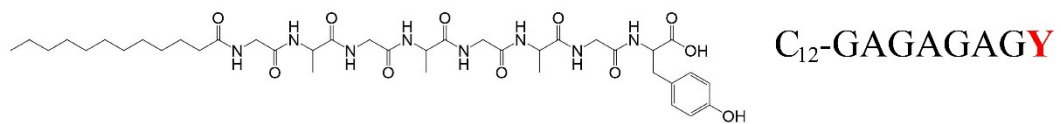


Figure S4. Chemical structure of C₁₂-GAGAGAGY, C₁₂-GAGAGYGA, C₁₂-GAGYGAGA, and C₁₂-GYGAGAGA.

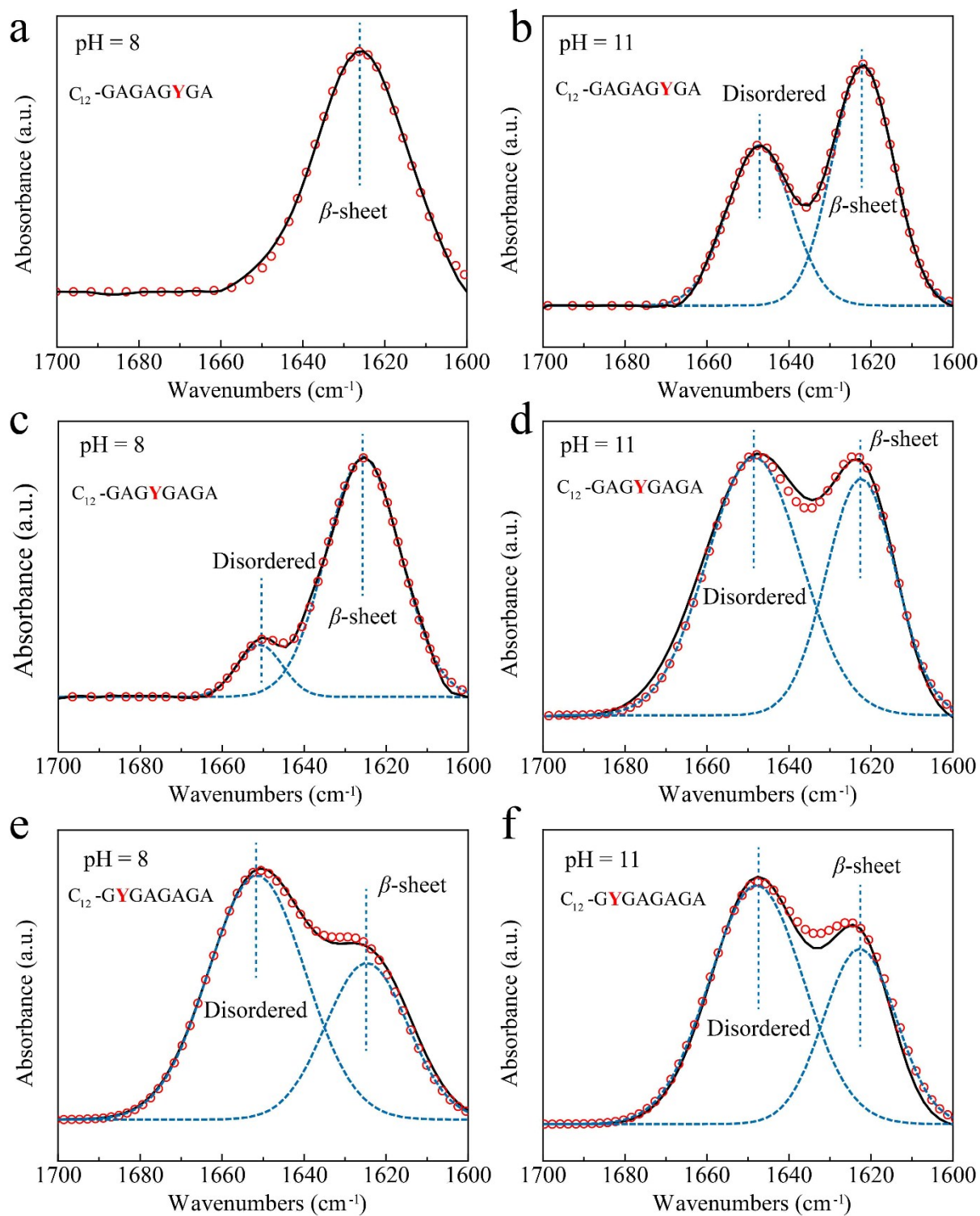


Figure S5. The fitted results of FT-IR spectra of C₁₂-GAGAGYGA (a, b), C₁₂-GAGYGAGA (c, d), and C₁₂-GYGAGAGA (e, f) at pH 8 and 11, respectively. The black full lines, blue dash lines and red circles indicate the original FT-IR spectra, peak splitting and fitting results.

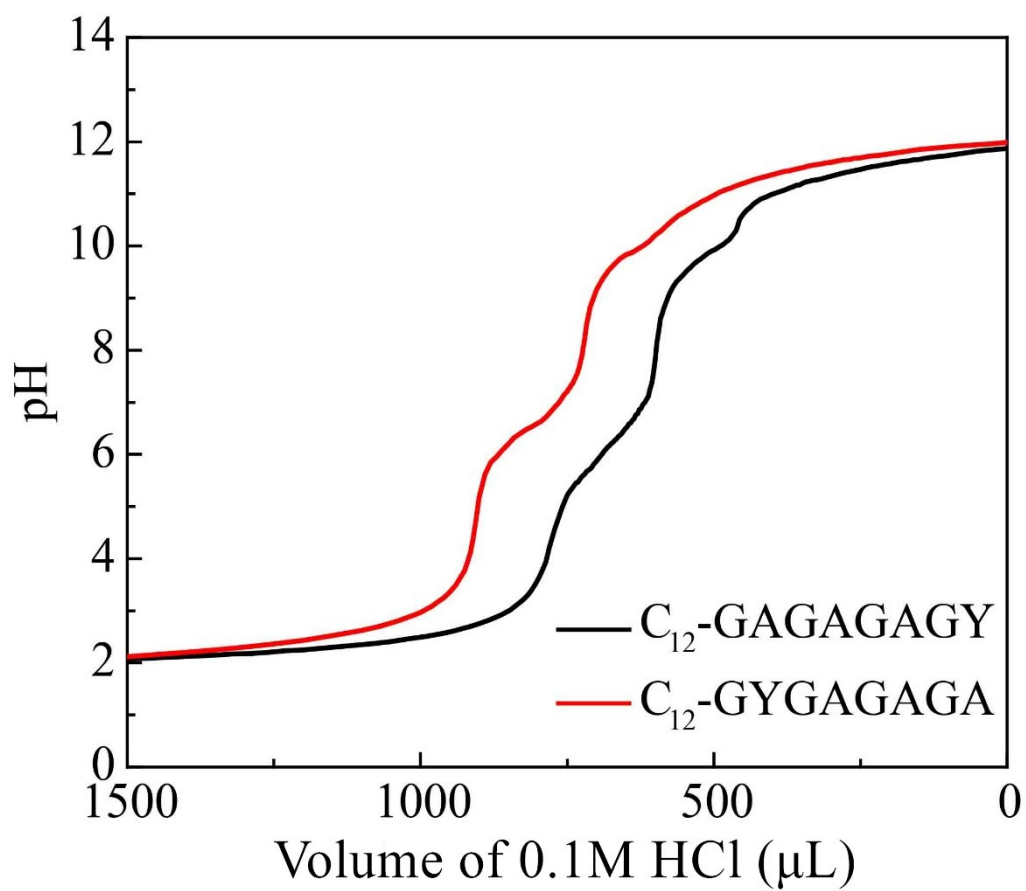


Figure S6. pH titration curves of C₁₂-GAGAGAGY (black) and C₁₂-GYGAGAGA (red), 1 mg/mL, aqueous solution.

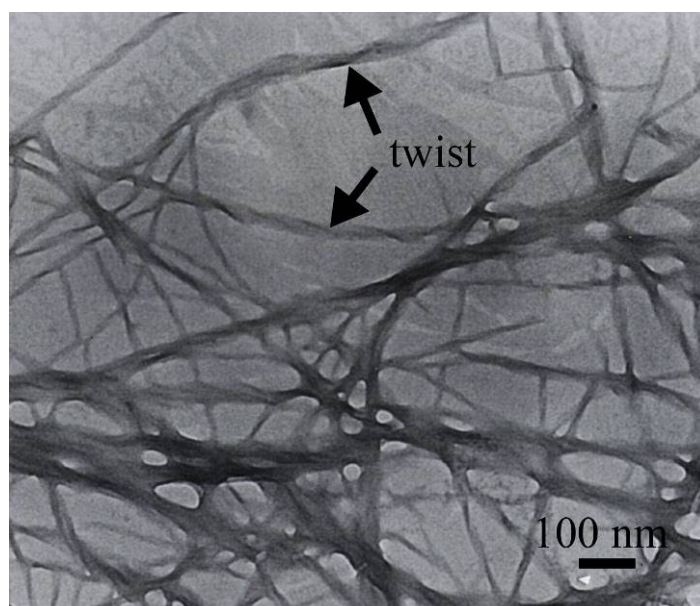


Figure S7. TEM image of twisted nanofibers assembled from C_{12} -GAGAGAGY at pH 8, pointed by the black arrows.

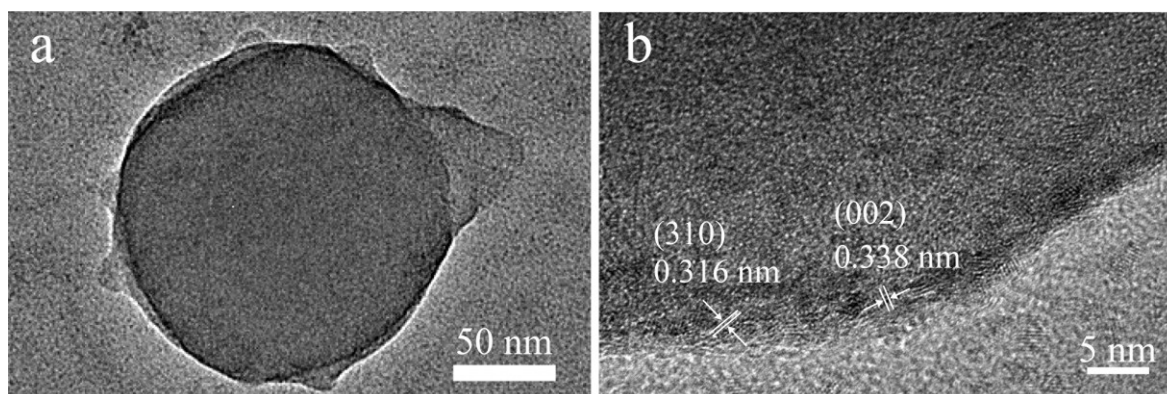


Figure S8. (a) TEM image of a nanosphere assembled from C_{12} -GYGAGAGA. The protuberance structures indicate the rugged surface of this nanosphere. (b) HRTEM image of the same nanosphere, which exhibits a hydrophilic surface confirmed by the lattice spacing ascribed to orthorhombic $C_4H_6O_6U \cdot 2H_2O$.

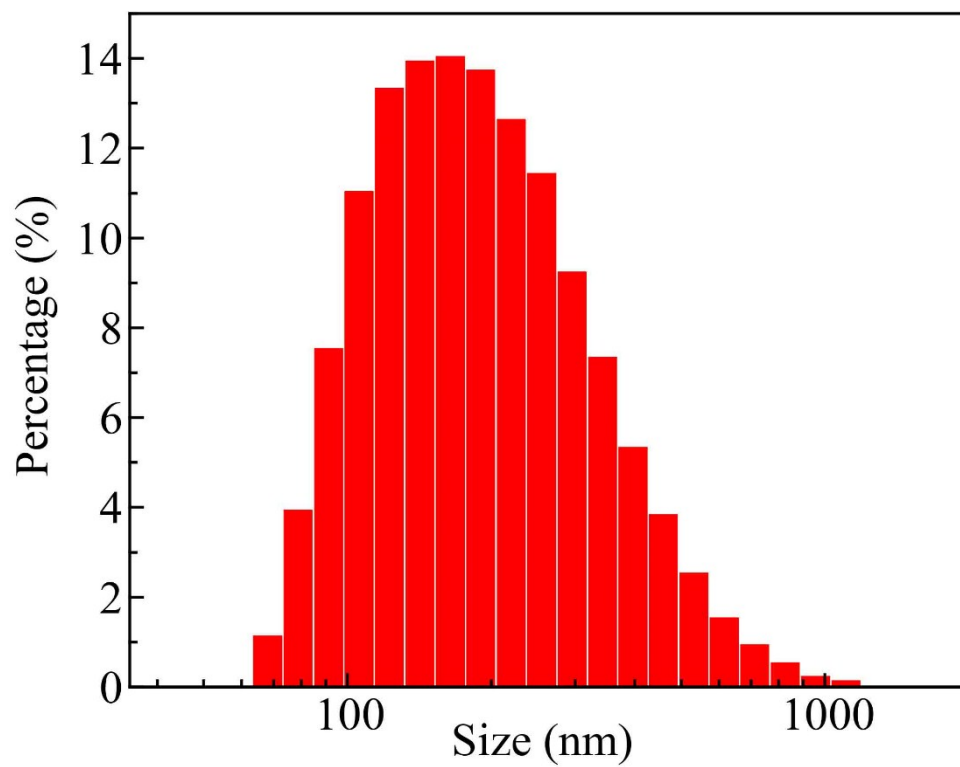


Figure S9. Size distribution of self-assembled C₁₂-GYGAGAGA at pH 11 obtained via the Dynamic Light Scattering (DLS) measurement.

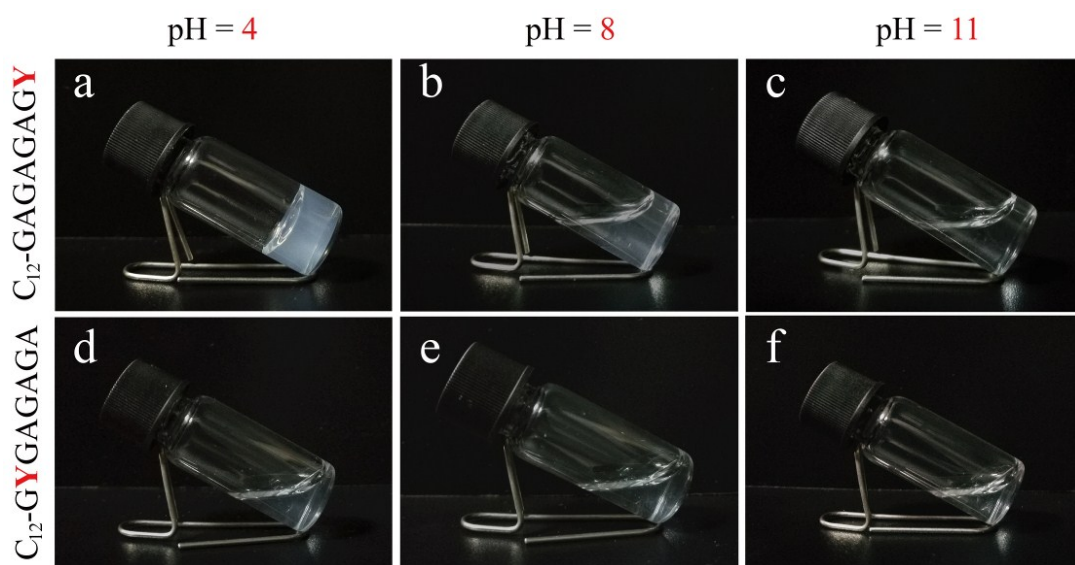


Figure S10 Optical images of C₁₂-GAGAGAGY/H₂O (a-c, reworked from ref. 27 in the text) and C₁₂-GYGAGAGA/H₂O (d-f) systems at pH 4, 8 and 11.

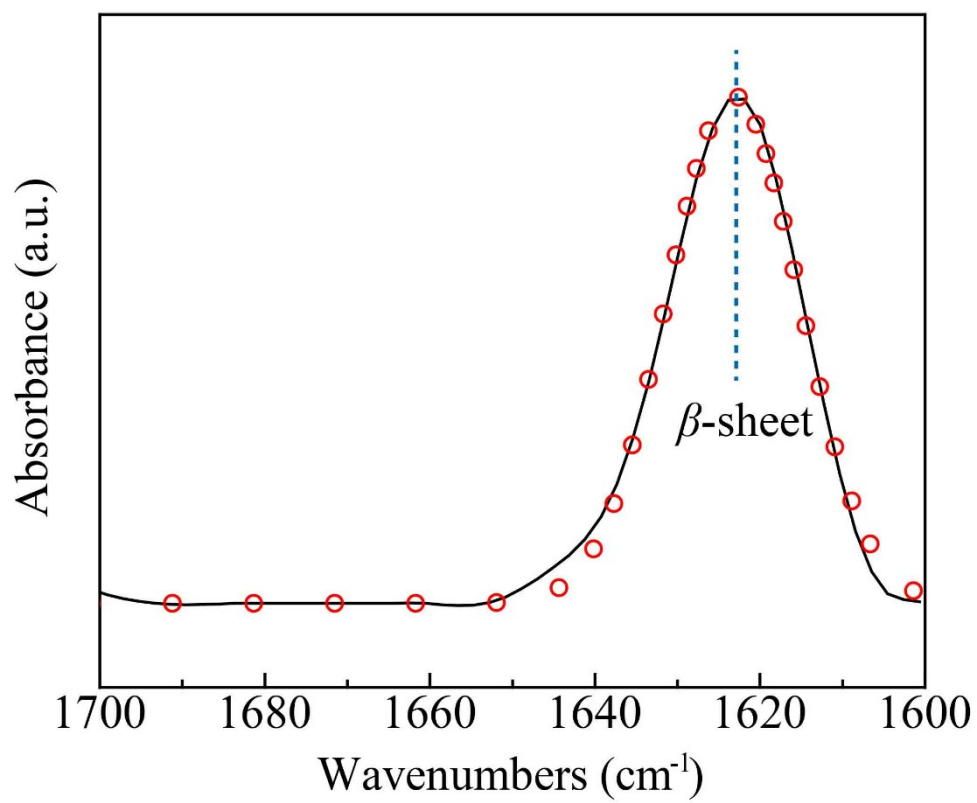


Figure S11. FT-IR spectrum and its fitted result of self-assembled C₁₂-GAGYGAGA at pH 4.

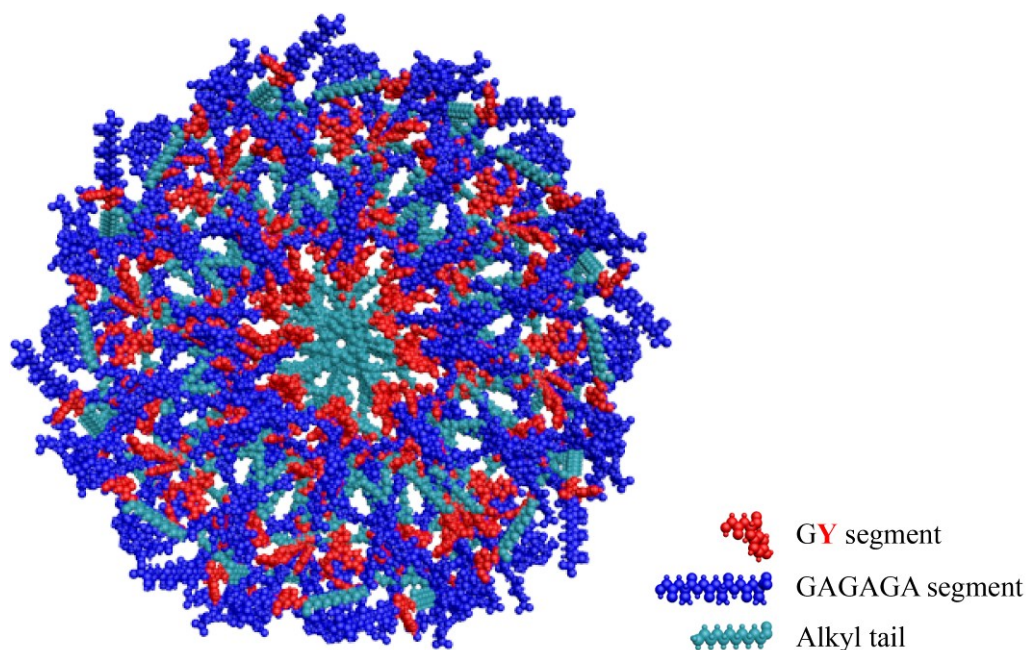


Figure S12. Schematic illustration of the cross section of the nanosphere consisted of C₁₂-GYGAGAGA with a disordered conformation. Red, blue, cyan patterns indicate the GY, GAGAGA and alkyl chain, respectively.

Table S1 Z-Average and particle dispersion index (PDI) results of self-assembled C₁₂-GAGYGAGA (pH 11), C₁₂-GYGAGAGA (pH 11) and C₁₂-GYGAGAGA (pH 8) at different concentrations via the Dynamic Light Scattering (DLS) measurement.

PAs (pH)	1 mg/mL			0.1 mg/mL		
	Z-Average (nm)	PDI	Size Distribution (nm)	Z-Average (nm)	PDI	Size Distribution (nm)
C ₁₂ -GAGY(GA) ₂ pH = 11	290	0.29	70-600	300	0.29	70-600
C ₁₂ -GY(GA) ₃ pH = 11	260	0.30	80-600	260	0.36	80-600
C ₁₂ -GY(GA) ₃ pH = 8	310	0.50	100-650	310	0.44	90-650