Supplementary Information

Surfactant-like peptide gels are based on cross- β amyloid fibrils

Abhinaba Das,^a Ordy Gnewou,^a Xiaobing Zuo,^b Fengbin Wang,^{c,*} and Vincent P. Conticello^{a,*}

^a Department of Chemistry, Emory University, Atlanta, GA, 30322, USA.

^b X-ray Science Division, Argonne National Laboratory, Lemont, IL, 60439, USA

^c Biochemistry and Molecular Genetics Department, Heersink School of Medicine, University of Alabama at Birmingham, Birmingham, AL, 35233, USA

*Correspondence: vcontic@emory.edu and jerrywang@uab.edu



Fig. S1 Analytical HPLC (a) and ESI-MS (b) data for peptide **L2**, Ac-KLIIIK-NH₂. Peptide purity was estimated at 98.6%. Calculated monoisotopic mass for Ac-KLIIIK-NH₂, 767.6 Da; experimental mass from mass spectrum, 767.6 Da.



Fig. S2 Analytical HPLC (a) and ESI-MS (b) data for peptide **L5**, Ac-KIIILK-NH₂. Peptide purity was estimated at 98.1%. Calculated monoisotopic mass for Ac-KIIILK-NH₂, 767.6 Da; experimental mass from mass spectrum, 767.6 Da.



Fig S3. Inversion test for hydrogel formation from solutions of peptides L2 (left) and L5 (right) incubated for seven days at ambient temperature (32 mM in ddH₂O).



Fig. S4 Circular dichroism (CD) spectropolarimetry of bola-like peptides; Ac-KLIIIK-NH₂ (**L2**) and Ac-KIIILK-NH₂ (**L5**). Samples were incubated in ddH₂O for 2 weeks and diluted to a concentration of 25 mM.



Fig. S5 Modified Guinier analysis for sheet-like forms applied to the experimental SAXS scattering data for the L2 (32 mM) in ddH_2O .



Fig. S6 Synchrotron wide-angle X-ray scattering (WAXS) measurements for peptide assemblies in aqueous solution (32 mM). The line indicates the position of the momentum transfer (*q*) associated with a Bragg distance (*d*) of ~4.7 Å, which corresponds to the hydrogen-bonding distance between strands in a cross- β fibril.



Fig. S7 Averaged power spectra (**a**) and representative class average (**b**) derived from cryo-EM analysis of Ac-KIIILK-NH₂ (**L5**) filaments. The positions of the indexed layer lines and associated Bessel orders are highlighted in the power spectrum.



Fig. S8 "Gold-standard" map:map Fourier Shell Correlation (FSC) calculation for the **L5** nanotube using a 0.143 criterion.

Parameter	Ac-KI ₃ LK-NH ₂ (L5)
Data collection and processing	
Voltage (kV)	300
Electron exposure (e-/ Å ²)	48.0
Pixel size (Å)	1.08
Particle images (n)	702,524
Helical symmetry	
Point group	C5
Helical rise (Å)	4.94
Helical twist (°)	-1.77
Map resolution (Å)	
Reconstruction software	CryoSPARC
Model:map FSC (0.5)	3.1
Map:map FSC (0.143)	2.7
Refinement and Model validation	
Map sharpening method	DeepEMhancer
RSCC	0.86
Bond lengths rmsd (Å)	0.013
Bond angles rmsd (°)	1.759
Clashscore	0.18
Ramachandran Favored (%)	98.9
Ramachandran Outlier (%)	0
MolProbity score	0.57
Deposition ID	
PDB (model)	9CZ3
EMDB (Map)	46060

Table S1 Cryo-EM and refinement statistics for the Ac-KI₃LK-NH₂ (L5) nanotubes.