Supporting Information

Diverse Nanostructures and Antimicrobial Activity of Lipopeptides Bearing Lysine-Rich Tripeptide Sequences

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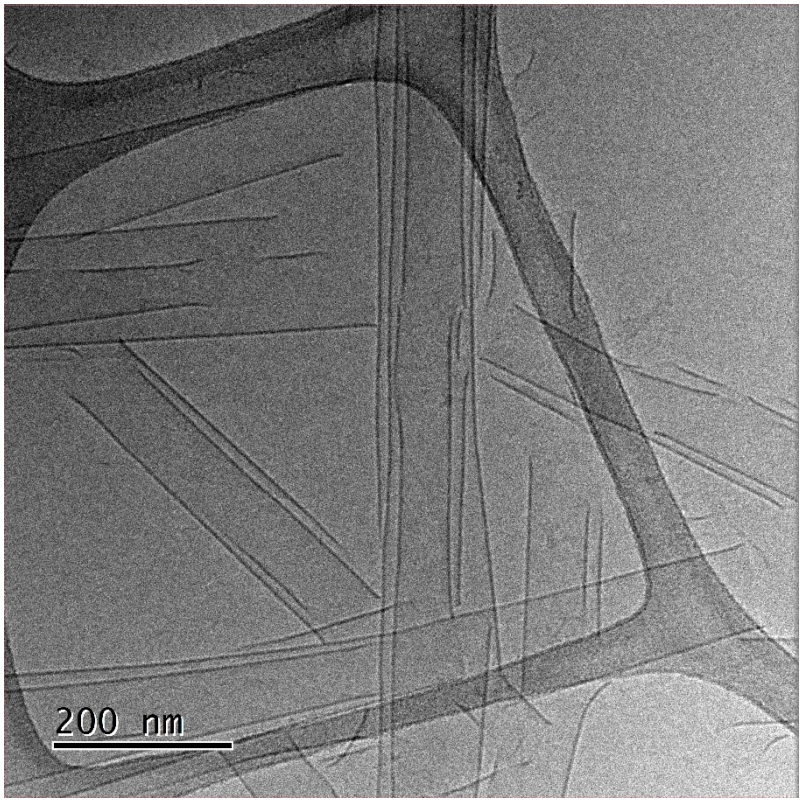
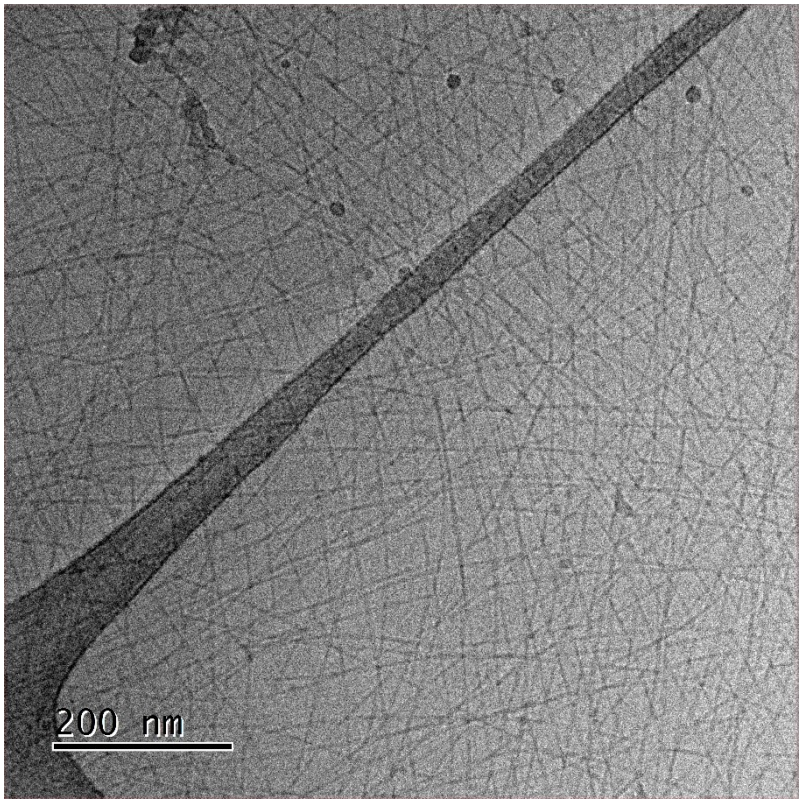
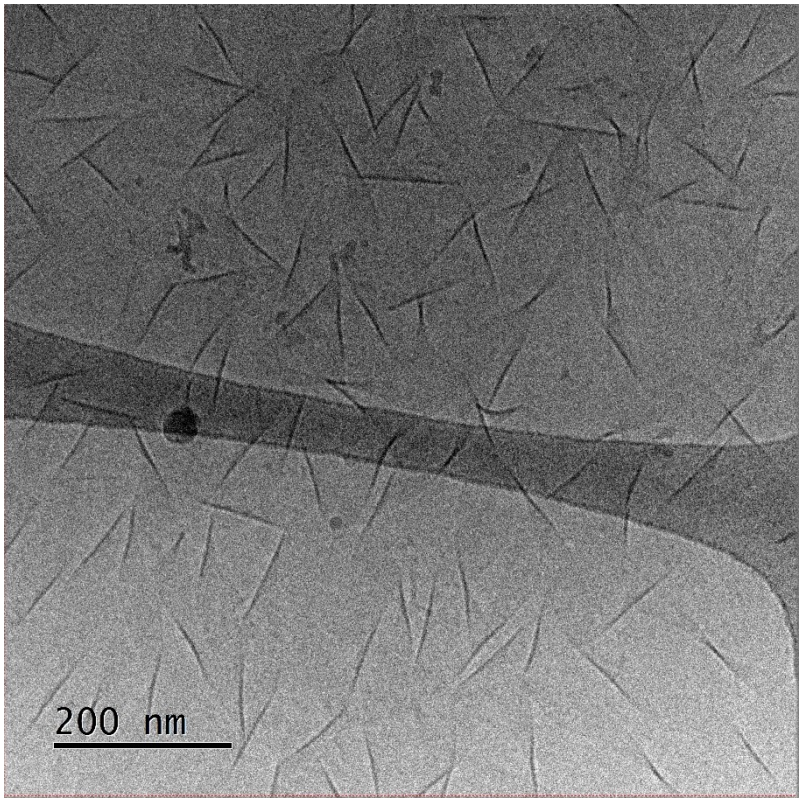
(a)



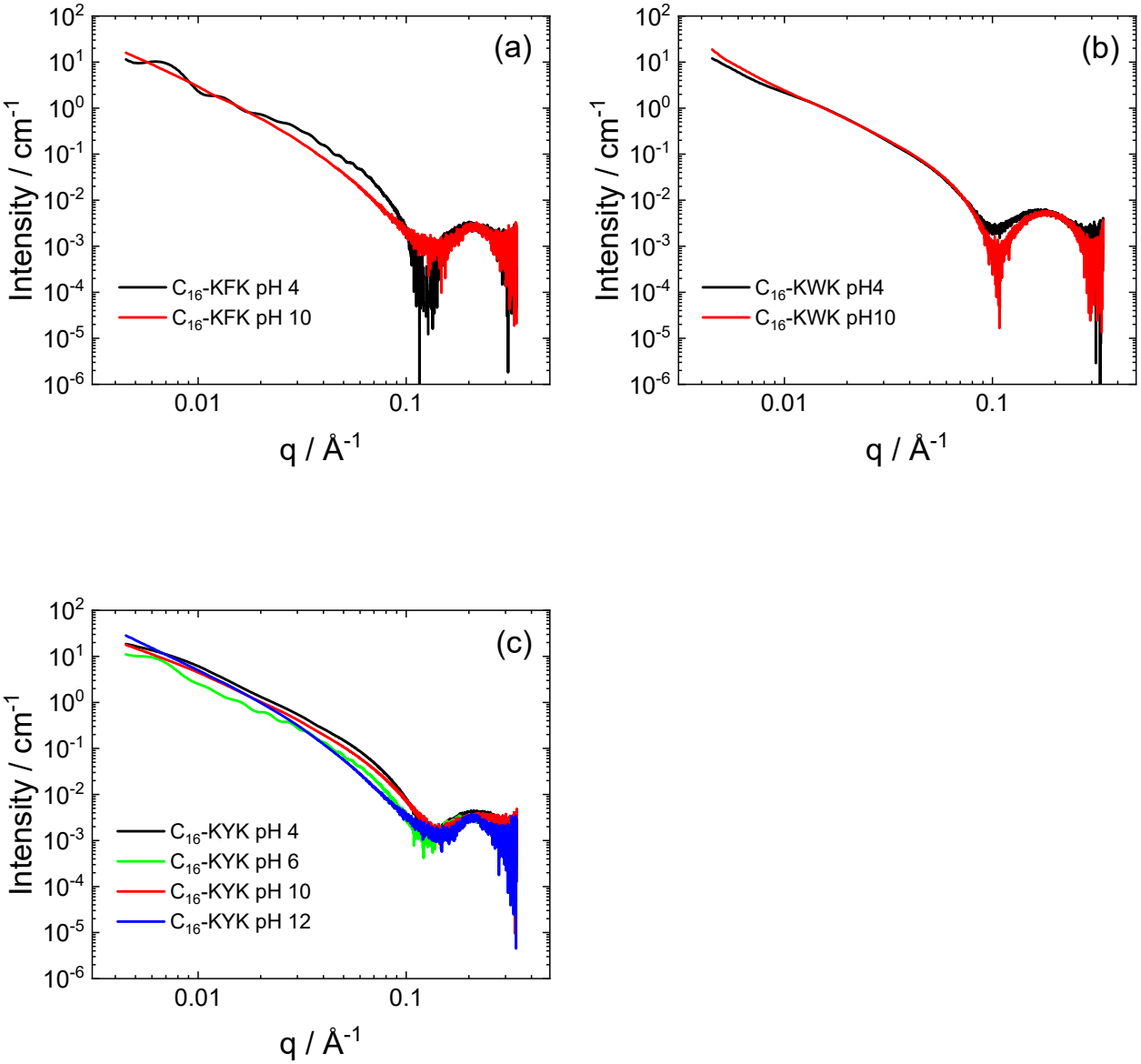
(b)



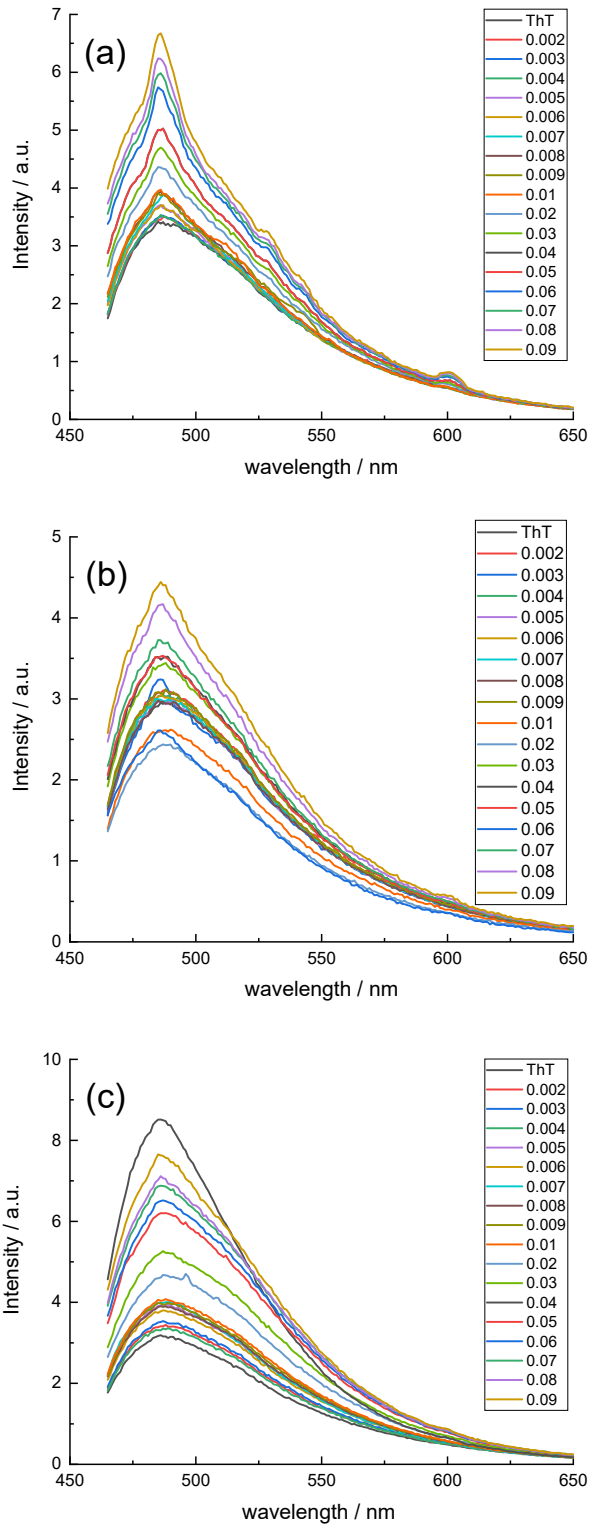
(c)



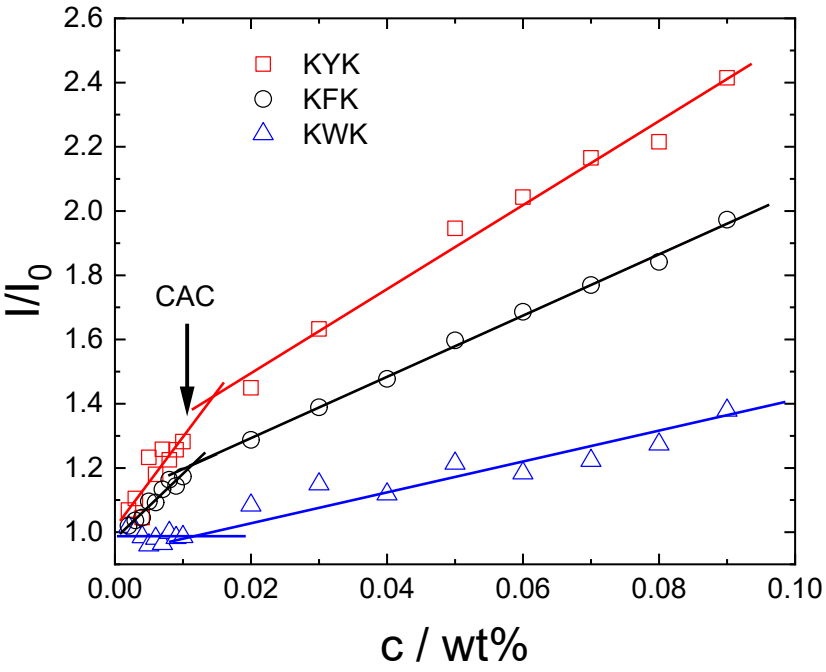
SI Fig.S1. Additional cryo-TEM images for 1 wt% native pH samples: (a) C_{16}-KFK, (b) C_{16}-KWK, (c) C_{16}-KYK.



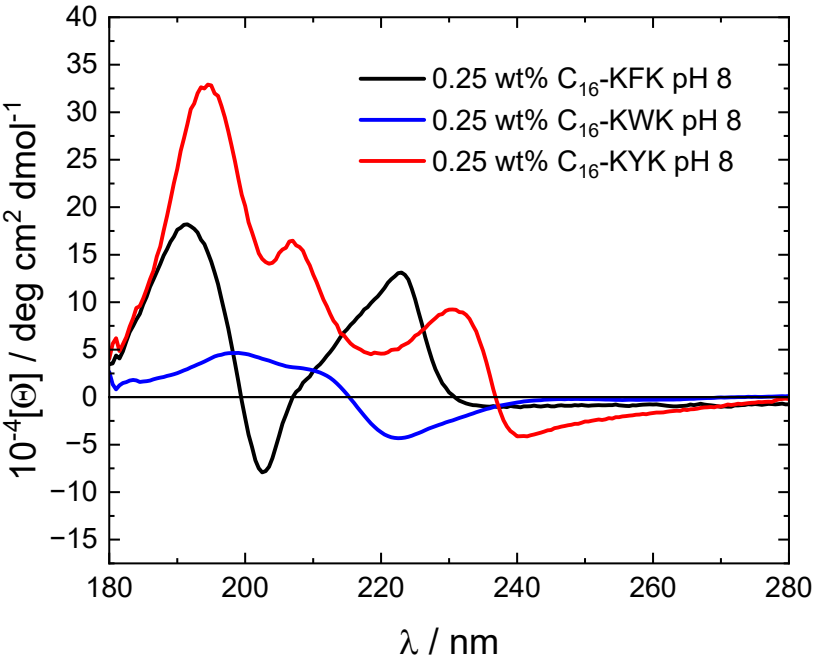
SI Fig.S2. SAXS data at other pH values (a) C_{16}-KFK, (b) C_{16}-KWK, (c) C_{16}-KYK.



SI Fig.S3. ThT emission fluorescence spectra at concentrations (wt%) indicated, at native pH. (a) C_{16}-KFK, (b) C_{16}-KWK, (c) C_{16}-KYK.



SI Fig.S4. ThT fluorescence peak intensity (I/I_0, where I_0 is the peak intensity for the ThT only solution) assay to determine critical aggregation concentration (CAC) of the three lipopeptides, as indicated, at pH 8.



SI Fig.S5. CD spectra for 0.25 wt% samples, as indicated at pH = 8.

Table S1. Parameters extracted from the fitting of the SAXS data for 1 wt% solutions at pH 8.[a]

	C_{16}-KFK *Bilayer+ Long cylindrical shell (for nanotube)*	**C_{16}-KWK** *Bilayer*	**C_{16}-KYK** *Bilayer*
w_1	0.99	N/A	N/A
$r_H \pm \Delta r_H$ [Å]	26.0 ± 2.4	27.0 ± 4.0	24.0 ± 2.0
ρ_H	7.12×10^{-7}	7.08×10^{-7}	6.42×10^{-7}
σ_H [Å]	4.0	5.7	6.4
ρ_C	1.08×10^{-6}	-1.69×10^{-7}	-9.82×10^{-8}
σ_C [Å]	6.3	10.0	10.0
D [Å] [b]	400	700	700
w_2	0.01	N/A	N/A
R [Å]	376 ± 10		
s [Å]	38.0		
ρ_{core}	-1.38×10^{-7}		
ρ_{shell}	7.51×10^{-7}		
ρ_{solv} [b]	1.00×10^{-8}		
L [b]	500		
C	1.4×10^{-3}	8×10^{-4}	6×10^{-4}

[a] Data fitted using the software SASfit.[1, 2]

[b] Fixed Parameter

[c] Additional overall scale factor applied to fit data

Key: Gaussian bilayer: layer thickness r_H (Gaussian polydispersity Δr_H), scattering contrast of outer (headgroup) layers ρ_H, and core (lipid chain) layer ρ_C, Gaussian widths σ_C and σ_H of core and headgroup layers respectively, D diameter (width) of layer system (when $D >> t$ as here, it acts as a scaling parameter for the form factor). **Long cylindrical shell:** R core radius (Gaussian polydispersity Δt), s shell thickness, scattering contrasts of core ρ_{core}, shell ρ_{shell} and solvent ρ_{solv}, L length. **Background:** constant background, C. Weightings for two-component form factors, w_1, w_2.

Table S2. Calculated pKa values at pH 8 from H++.[3, 4]

Moiety	**WKK**	**KWK**	**YKK**	**KYK**
N terminus	6.7	6.7	6.7	6.8
Tyr			9.2	9.5
Lys-N	10.1	10.4	10.6	10.3
Lys-C	11.5	11.6	11.9	11.7
C terminus	1.9	1.8	1.8	1.9

Lys-N denotes N-terminal side lysine and Lys-C the C-terminal one.

References

1. I. Bressler, J. Kohlbrecher and A. F. Thünemann, *Journal of Applied Crystallography*, 2015, **48**, 1587-1598.
2. J. Kohlbrecher and I. Bressler, *Journal of Applied Crystallography*, 2022, **55**, 1677-1688.
3. J. C. Gordon, J. B. Myers, T. Folta, V. Shoja, L. S. Heath and A. Onufriev, *Nucleic Acids Res.*, 2005, **33**, W368-W371.
4. R. Anandakrishnan, B. Aguilar and A. V. Onufriev, *Nucleic Acids Res.*, 2012, **40**, W537-W541.