

Supporting Information

Self-assembly of a Catalytically Active Lipopeptide and its Incorporation into Cubosomes

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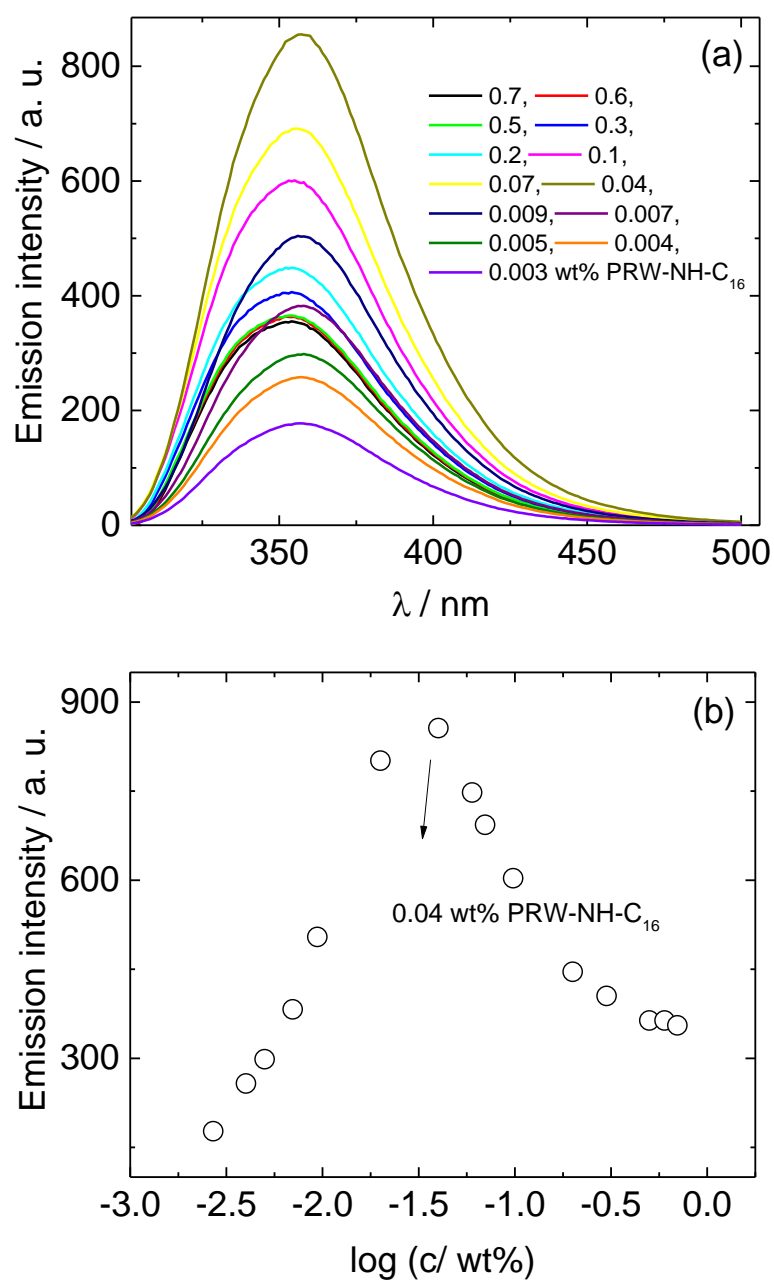


Figure S1. (a) Tryptophan fluorescence for PRW-NH-C₁₆, (b) dependence of the maxima in the fluorescence intensity in (a) with concentration.

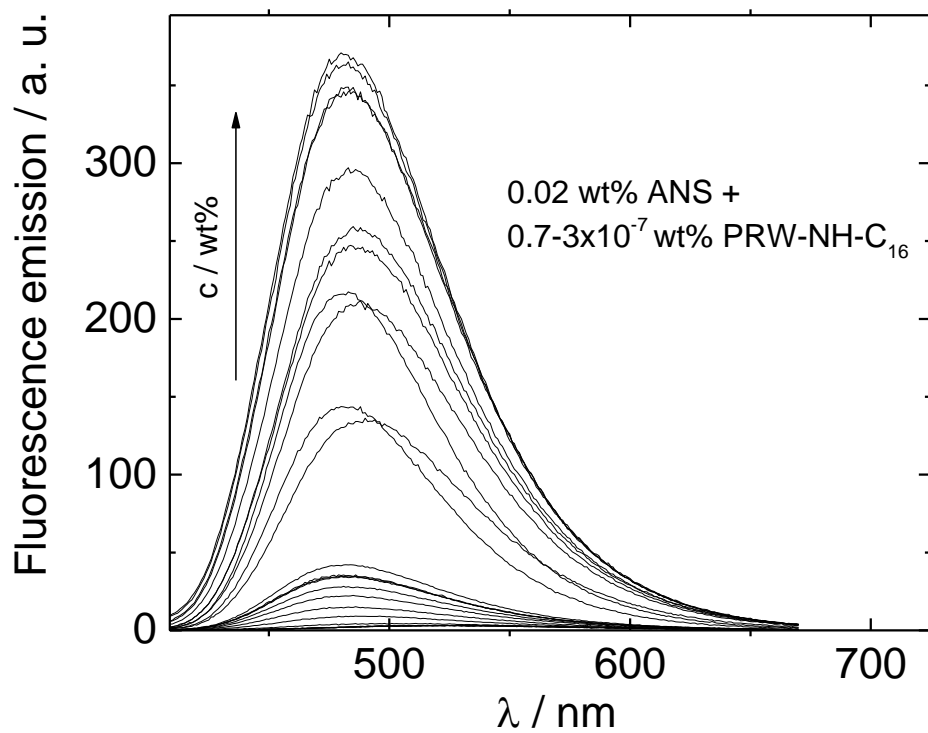


Figure S2. ANS fluorescence spectra for PRW-NH-C₁₆.

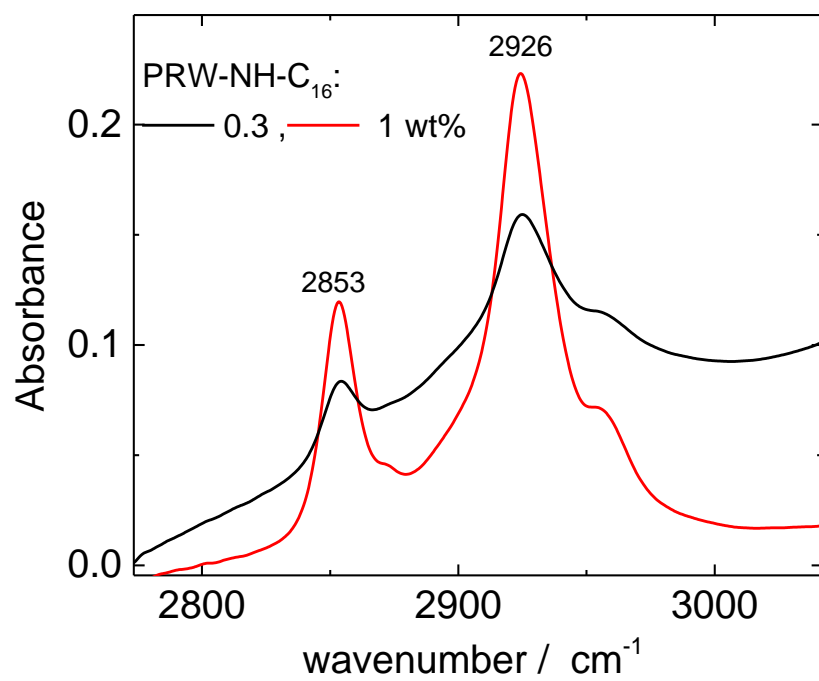


Figure S3. FTIR spectra in the region of CH₂ stretch modes.

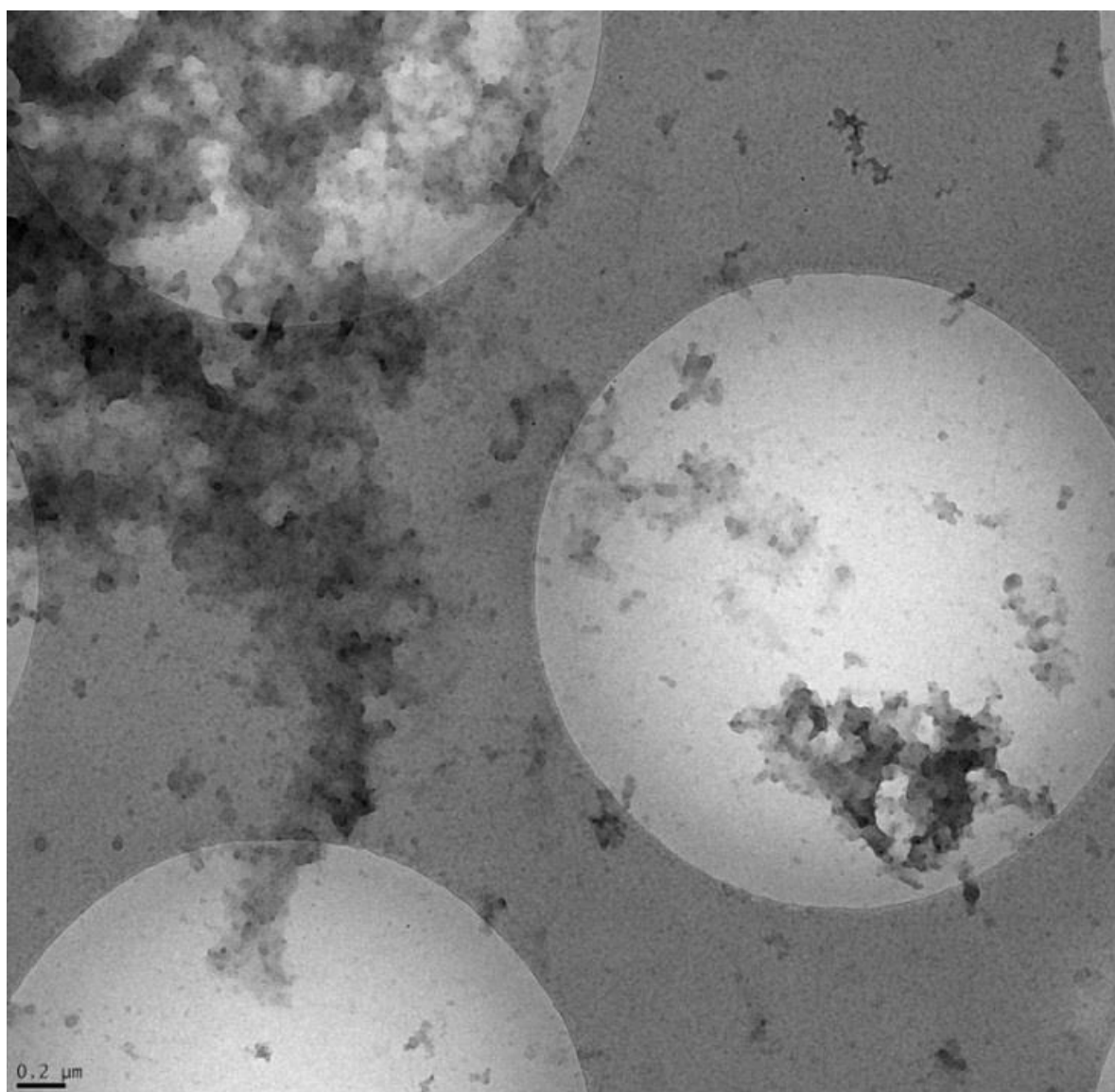
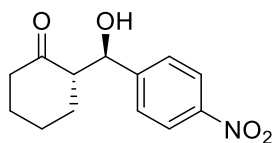
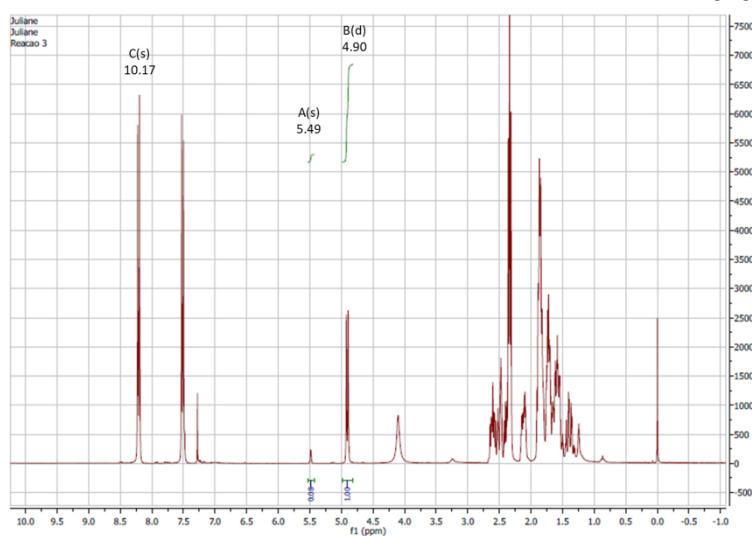


Figure S4. Additional cryo-TEM image from a 1 wt% solution of PRW-NH-C₁₆.

(S)-2-((R)-Hydroxy(4-nitrophenyl)methyl)cyclohexan-1-one



(a)



(b)

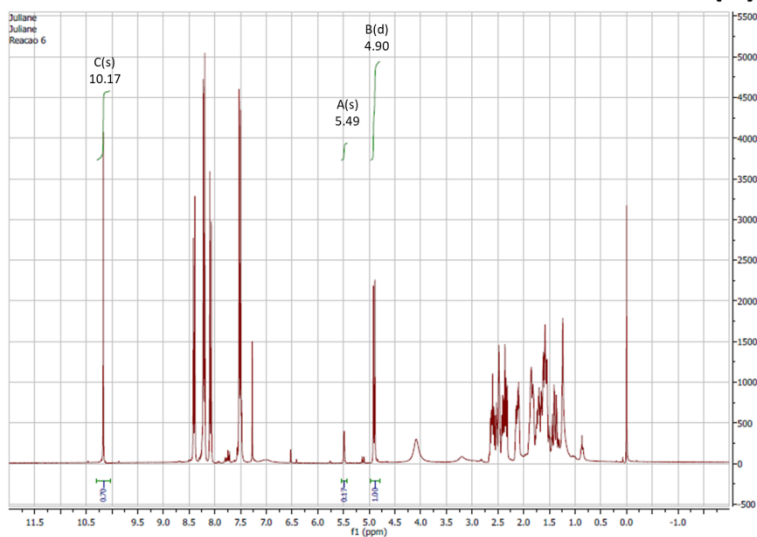
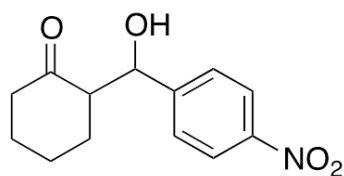


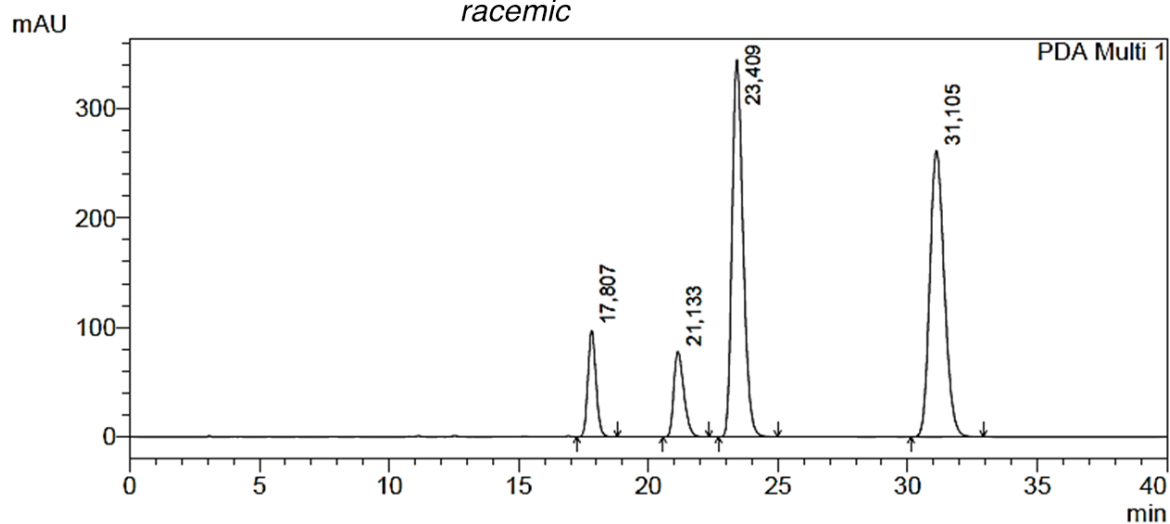
Figure S5. ^1H NMR spectra of crude aldol product for Entries (a) 1 and (b) 4.

^1H NMR (300 MHz, CDCl_3): δ 8.22-8.18 (m, 2H, ArH), 7.51-7.47 (m, 2H, ArH), 5.49 (br s, 1H, *CHOH* of *syn* diastereoisomer), 4.90 (d, $J = 7.5$ Hz, 1H, *CHOH* of *anti* diastereoisomer), 2.66-2.30 (m, 1H, *CHCHOH*), 2.66-2.30 (m, 2H, $\text{CH}_2\text{C}(\text{O})$), 2.16-1.24 (m, 6H, cHex-H).

^{13}C NMR (75 MHz, CDCl_3): δ 214.9, 148.5, 147.7, 128.0, 123.7, 74.1, 57.3, 42.8, 30.9, 27.8, 24.8.



racemic

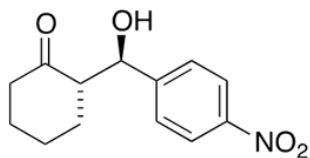


1 PDA Multi 1/254nm,4nm

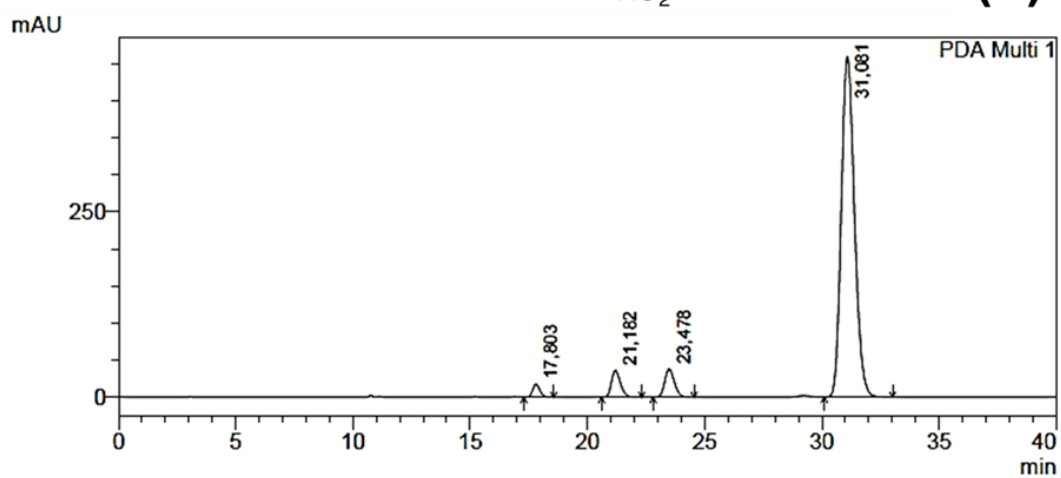
PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	17,807	2098997	96930	8,560	12,422
2	21,133	2101762	77810	8,571	9,972
3	23,409	10148757	344448	41,387	44,144
4	31,105	10172017	261098	41,482	33,462
Total		24521532	780286	100,000	100,000

Figure S6. HPLC chromatogram for racemic aldol product. Conditions: Chiralpak AD-H, hexane/2-propanol (90/10); 1.0 mL·min⁻¹, λ = 254 nm.



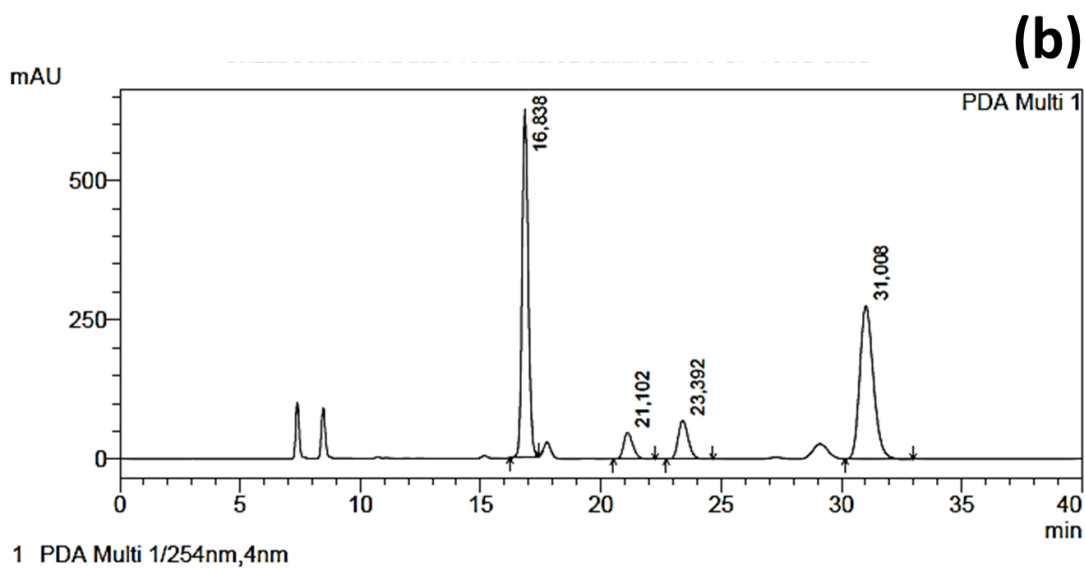
(a)



1 PDA Multi 1/254nm,4nm

PeakTable

PDA Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	17,803	382644	17761	1,882	3,228
2	21,182	966113	35992	4,752	6,542
3	23,478	1094478	37766	5,384	6,865
4	31,081	17886323	458635	87,982	83,365
Total		20329558	550153	100,000	100,000



PeakTable

PDA Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	16.838	10943283	624097	43.746	61.455
2	21.102	1278264	47562	5.110	4.683
3	23.392	2024442	69619	8.093	6.855
4	31.008	10769242	274250	43.051	27.006
Total		25015231	1015528	100.000	100.000

Figure S7. Representative HPLC chromatograms for racemic aldol product and chiral aldol product for entries (a) 1 and (b) 4. Conditions: Chiralpak AD-H, hexane/2-propanol (90/10); 1.0 mL·min⁻¹, $\lambda = 254$ nm. The *anti*:*syn* ratio is obtained from the relative areas of peaks 4 and 3: $[A(\text{peak 4}) - A(\text{peak 3})]/[A(\text{peak 4}) + A(\text{peak 3})]$.

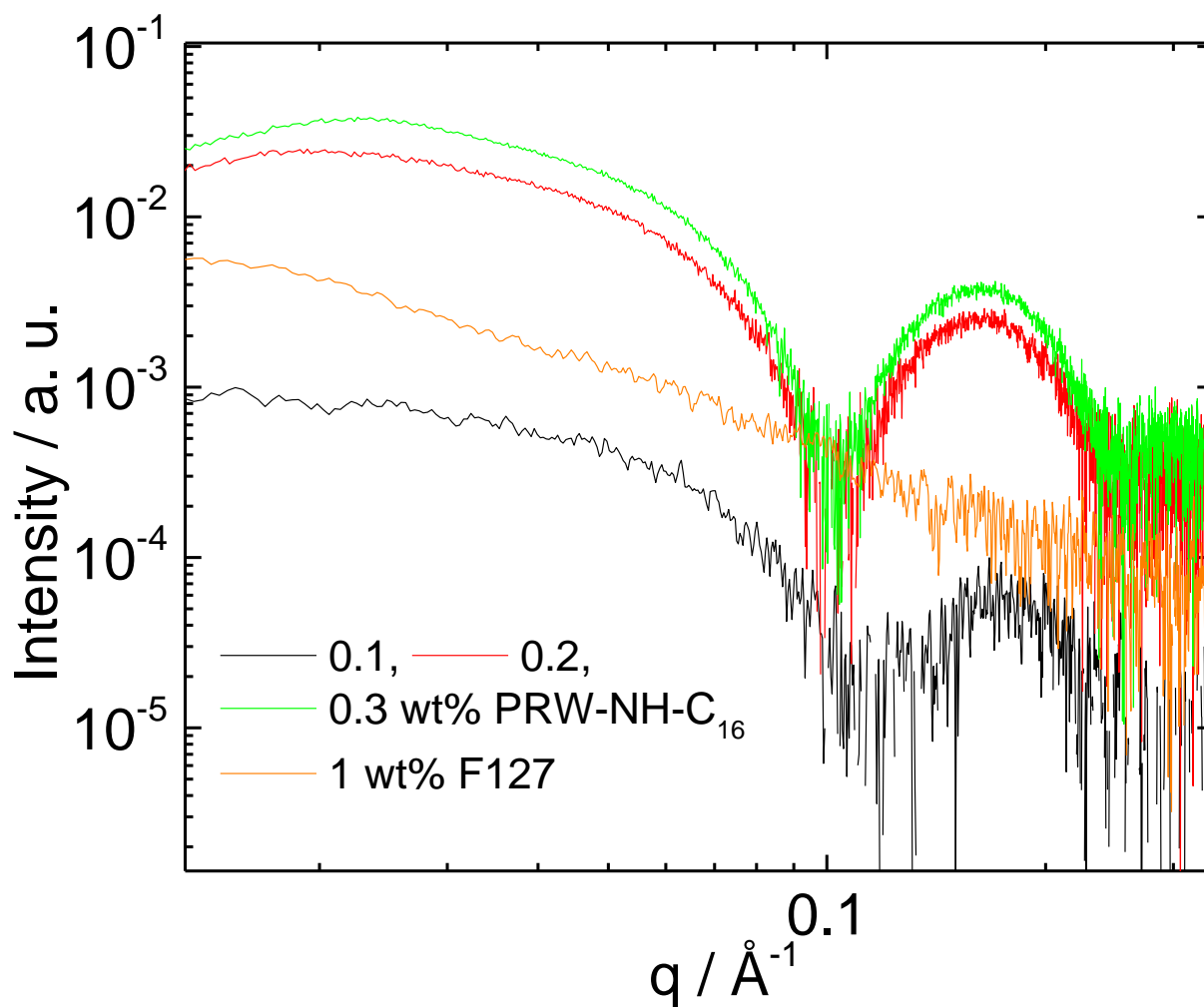


Figure S8. Controls (peptide or F127 only) for the SAXS data in Fig. 3.

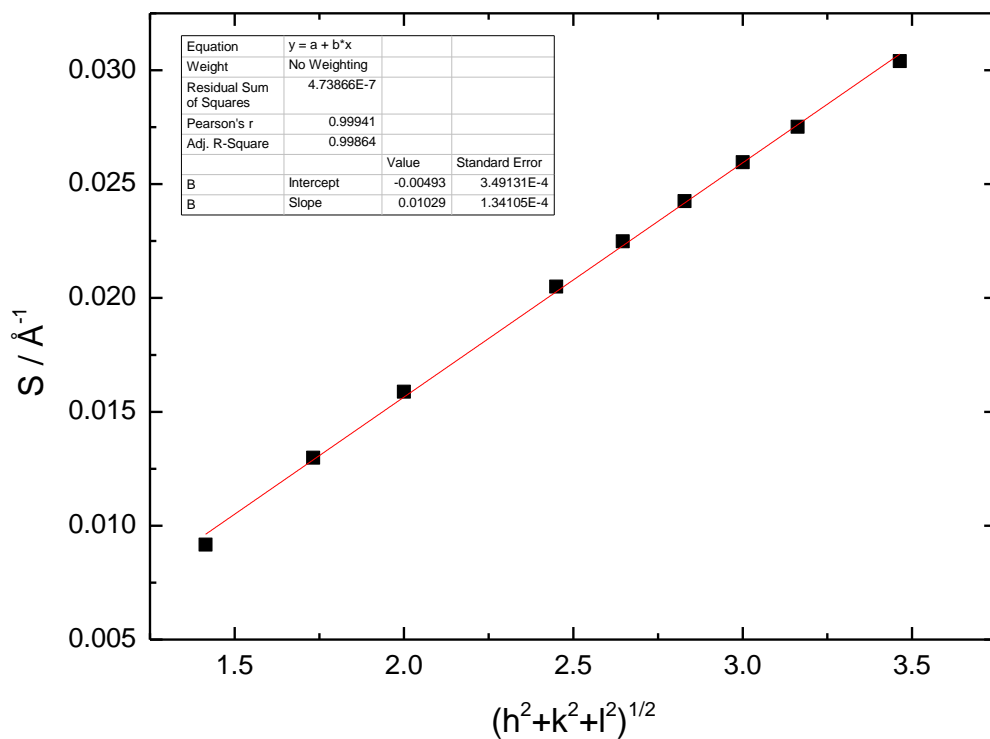


Figure S9. Indexation of SAXS reflections observed for the cubosomes (in the absence of lipopeptide) from the SAXS profile shown in Fig.3a. The lattice constant a is determined as the reciprocal of the gradient.

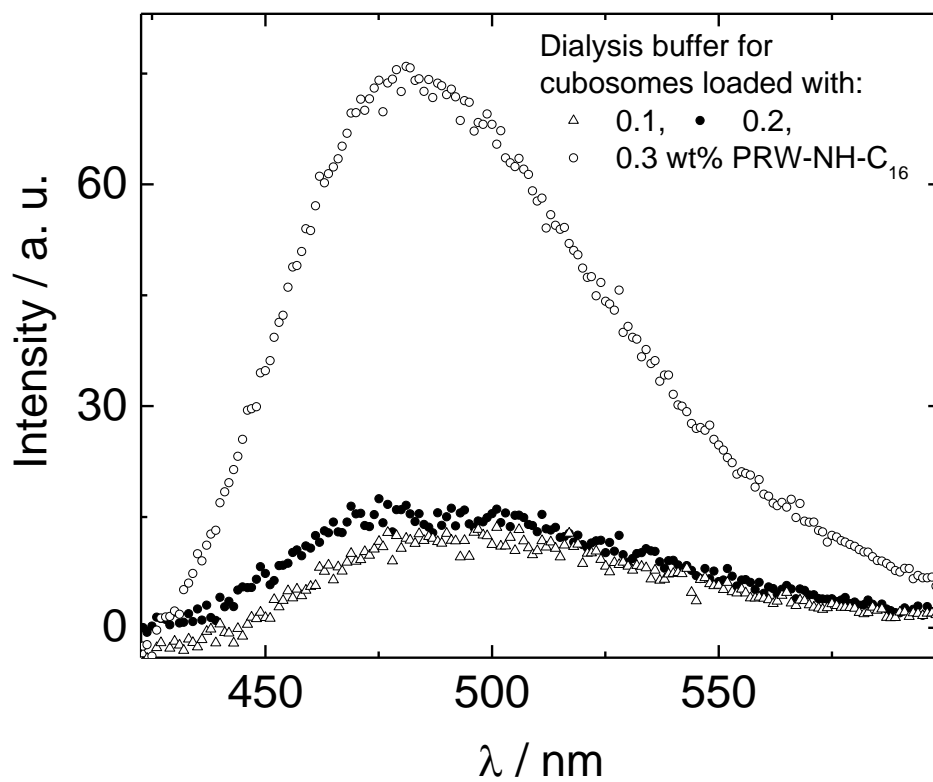


Figure S10. FLC assay on the dialysis buffer of cubosomes made of 10 wt% monoolein+1 wt% F127 and loaded with 0.1, 0.2 or 0.3 wt% PRW-NH-C₁₆.

