Electronic supporting information for:

Solution Structure of Linear Battacin Lipopeptides – the Effect of Lengthening Fatty Acid Chain

Shinji Kihara[a,b], Gayan Heruka De Zoysa[a,b], Rayomand Shahlori[a,b], Praveen G. Vadakkedath[a,b],

Timothy M. Ryan[b,c], Jitendra P. Mata[d], Vijayalekshmi Sarojini[a,b], and Duncan J. McGillivray[a,b]*

[a] School of Chemical Sciences, The University of Auckland, Auckland 1010, New Zealand

[b] The MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington 6140, New Zealand

[c] Australian Synchrotron, Clayton 3168, Victoria, Australia

[d] ACNS, Australian Nuclear Science and Technology Organisation (ANSTO), Lucas Heights, NSW 2234, Australia
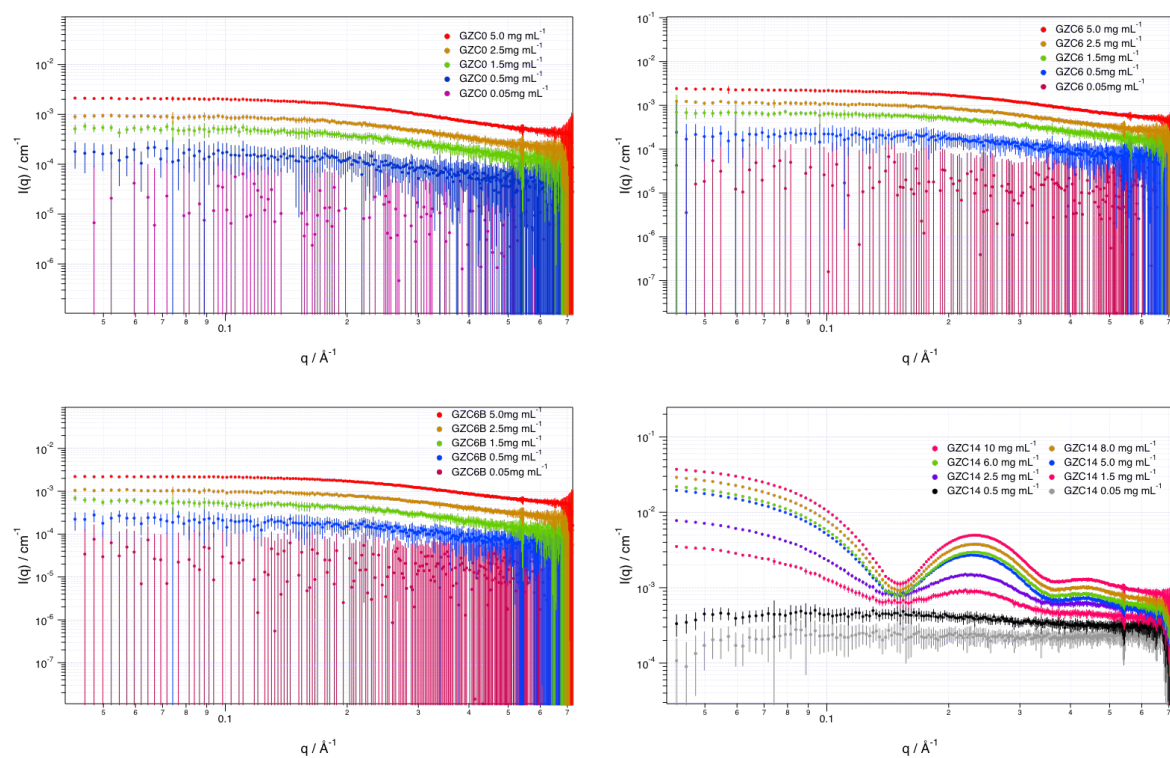
Small angle X-ray Scattering (SAXS)

Figure S1. SAXS plots of linear battacin lipopeptides with various concentrations.
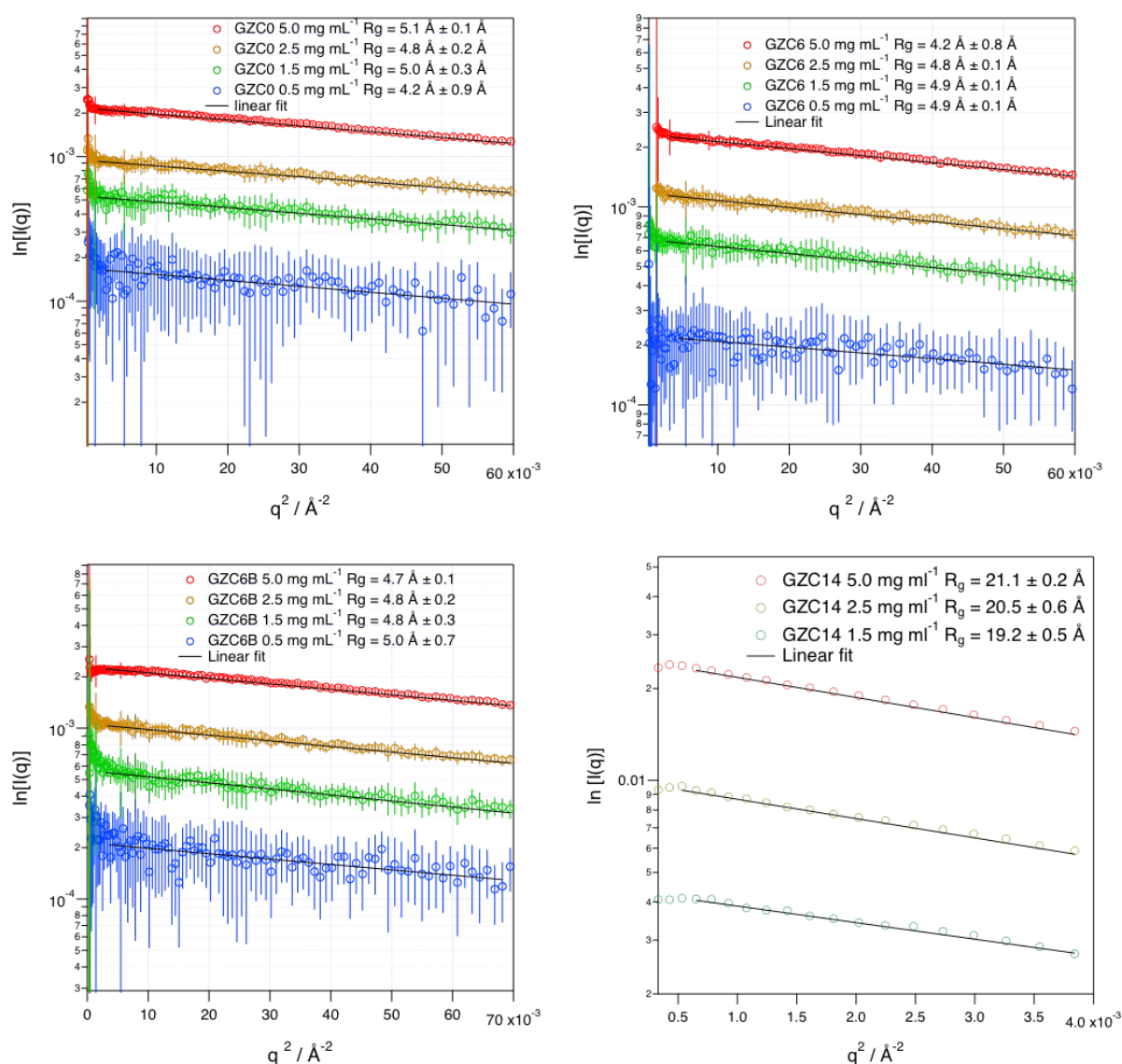
Figure S2. Guinier plots of linear battacin lipopeptides at various concentrations.

The R_g values for all the battacin lipopeptides did not change drastically, except for the GZC14 due to the self-assembly above 1.5 mg mL^{-1}. No additional features in the scattering plots were observed with varying concentrations. Also, the molecular weight was calculated based on the absolute scale analysis with the calculated partial specific volume and contrast. The values did not deviate by an order of magnitude from their theoretical values.

Table S1. Summary of R_g values resolved by Guinier analysis.

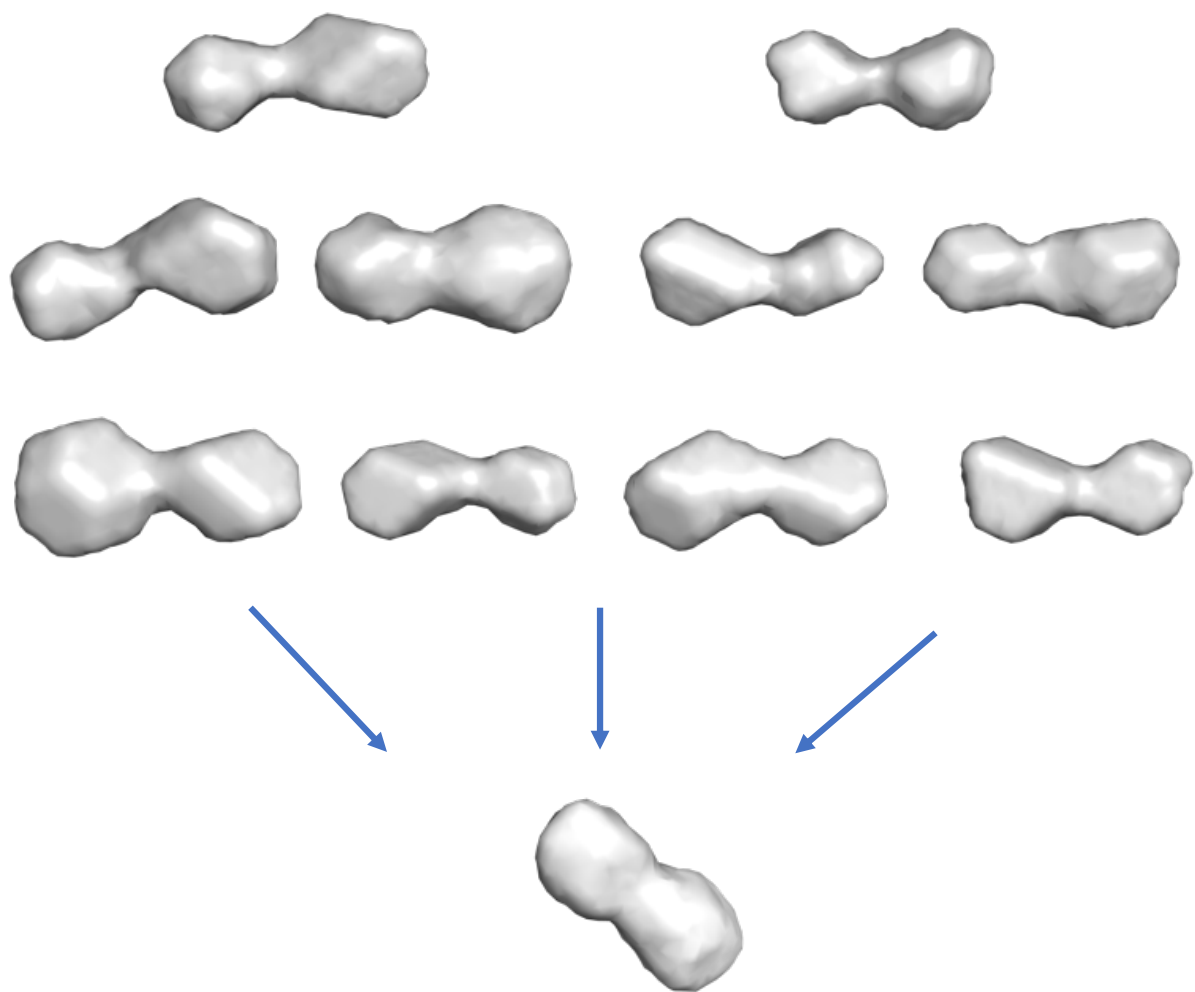| Concentration	R_g / Å			
	GZC0	GZC6	GZC6B	GZC14
0.5 mg mL^{-1}	4.2 ± 0.9	4.9 ± 0.8	5.0 ± 0.7	Insufficient signals
1.5 mg mL^{-1}	5.0 ± 0.3	4.9 ± 0.1	4.8 ± 0.3	19.2 ± 0.5
2.5 mg mL^{-1}	4.8 ± 0.2	4.8 ± 0.1	4.8 ± 0.2	20.5 ± 0.6
5.0 mg mL^{-1}	5.1 ± 0.1	4.2 ± 0.1	4.7 ± 0.1	21.1 ± 0.2

Figure S3. Representation of ten candidate *ab initio* models used, and the final model at the bottom (for GZC0).

Peptide number calculation

The volume of each aggregate $= \frac{4}{3}\pi r^3$

Where $r = 12.5$ Å $+ 9.1$ Å from the fitting parameters in Table 3.

Volume of an aggregate $= 42200$ Å^3

We then can estimate the volume of each GZC14 molecule within the aggregate from SLD.

$$SLD = \frac{\sum_i b_i}{V}$$

where b_i is bound coherent scattering length.[1]
SLD values used or fitted ware used for this calculation

The combined volume of peptide and fatty acid chain is 272 Å^3. The number of GZC14 molecules that constitute one aggregate is approximately 155.
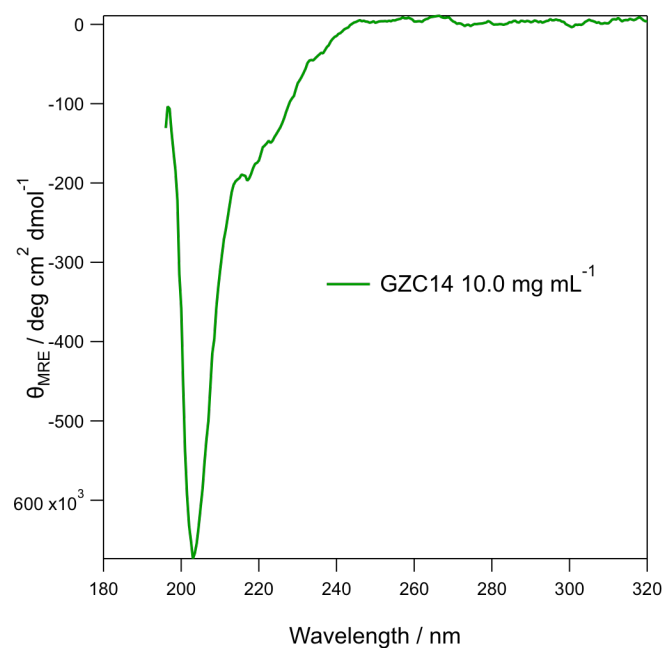
Figure S4. CD spectra of GAZC14 at 10.0 mg mL^{-1}.

Reference

1.   Sears, V. F., Neutron scattering lengths and cross sections. *Neutron news* **1992,** *3* (3), 26-37.