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| | **Experiment title:**<br>A SAXS Study of the Effect of Surfactant-Like Peptides on Lipid Membrane Order: From Form Factor to Chain Packing | **Experiment number**:<br>SC-4739 |
| **Beamline**: | **Date of experiment**:<br>from: 25/7/18 to:26/7/18 | **Date of report**:<br>11/01/22 |
| **Shifts:** | **Local contact(s)**:<br>Alessandro Mariani | *Received at ESRF:* |
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**Report:**

As well as the proposed samples, we examined the self-assembly of a novel lipopeptide C16KTTβAH was designed that incorporates the KTT tripeptide sequence from "Matrixyl" lipopeptides along with the bioactive βAH (β-alanine-histidine) carnosine dipeptide motif, attached to a C16 hexadecyl lipid chain. We show that this peptide amphiphile self-assembles above a critical aggregation concentration into β-sheet nanotape structures in water, PBS and cell culture media. Nanotape bundle structures were imaged in PBS, the bundling resulting from nanotape associations due to charge screening in the buffer. In addition, hydrogelation was observed and the gel modulus was measured in different aqueous media conditions, revealing tunable hydrogel modulus depending on concentration and nature of the aqueous phase. Stiff hydrogels were observed by direct dissolution in PBS and it was also possible to prepare hydrogels with unprecedented high modulus from low concentration solutions by injection of dilute aqueous solutions into PBS. These hydrogels have exceptional stiffness compared to previously reported β-sheet peptide-based materials. In addition, macroscopic soft threads can be drawn from concentrated aqueous solutions of the lipopeptides which contain aligned nematic structures. SAXS measurements on ID02 were complemented by those on Diamond B21.

Figure 1 contains data from measurements to probe the assembly of $C_{16}$KTTβAH in water. The SAXS intensity profiles shown in Figure 1 measured at two concentrations above the *cac*, reveal form factors shapes which were fitted using a model for lipopeptide bilayers[1, 2] (based on a model for lipid bilayers[3]), consistent with the nanotape structures observed by TEM. The TEM image for a sample dried from a 1 wt% solution shown in Figure 1b shows nanotape (or nanofibril bundle) structures, consistent with cryo-TEM. Fibre XRD was performed to determine the secondary structure of the peptide and the XRD

intensity profile shown in Figure 1c confirms a β-sheet structure, since peaks are observed corresponding to a "cross-β" XRD pattern[4, 5] with spacings $d$ = 4.7 Å (β-strand spacing) and 8.9 Å (β-sheet spacing).

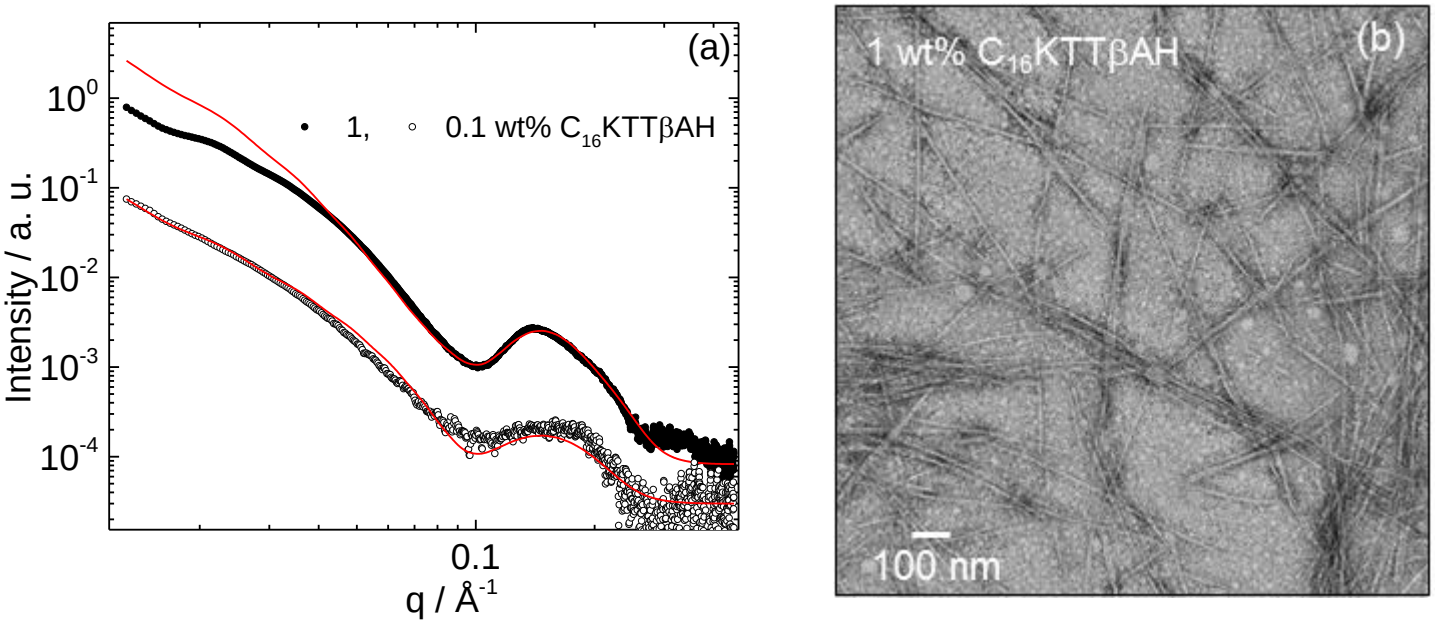


**Figure 1**. Self-Assembly of $C_{16}$KTTβAH in water: (a) SAXS data, (b) TEM image. The full lines in (a) correspond to the fitting of the SAXS data

This work has been published.[6] Another paper also acknowledges SC-4739, although the measured SAXS data was not included in the final publication.[7]

## 5. References


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