	Experiment title: A BioSAXS Study of the Interaction between lipid membranes and antimicrobial peptides	**Experiment number**: MX-2345
Beamline:	**Date of experiment**: from: 17/6/21 to:18/6/21	**Date of report**: 11/01/22
Shifts:	**Local contact(s)**: Mark Tully	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

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Report:

Due to COVID-19 restrictions, the experiments were carried out with no users on site by Dr Mark Tully on BM29. The BioSAXS measurements were performed with the standard EMBL BioSAXS robot setup.

Due to changed laboratory arrangements caused by COVID-19 restrictions, the proposed samples were not run. Instead the self-assembly of related lipopeptides was examined, in particular PRWG-$(CH_2)_{17}(CH_3)$ and PRWG-$[(CH_2)_{17}(CH3)]_2$ as part of a study on their influence on acetylcholinesterase inhibition by organopesticides performed by Dr Barbara Gerbelli during her FAPESP (Brazil) funded visit to the Hamley group at Reading.

In addition, we investigated the conformation and aggregation of peptide RSAIEDLLFDKV, which is a sequence common to many animal and human coronavirus spike proteins. This sequence is part of a native α-helical S2 glycoprotein domain, close to and partly spanning the fusion sequence, and is also not predicted to form amyloid by aggregation propensity algorithms. This peptide aggregates into β-sheet amyloid nanotape structures close to the calculated pI =4.2, but forms disordered monomers at high and low pH. The β-sheet conformation revealed by FTIR and circular dichroism (CD) spectroscopy leads to peptide nanotape structures, imaged using transmission electron microscopy (TEM) and probed by small-angle X-ray scattering (SAXS). Fig.1 shows representative BioSAXS data obtained at different pH values along with model form factor fits. At pH 4-6 the data was fitted to form factors corresponding to peptide bilayer nanotapes while at higher and lower pH, form factors of monomers were used (with an additional structure factor term for pH 3).

This work has been published in the high impact factor journal ACS Nano (the highest IF research article journal of the American Chemical Society).[1]

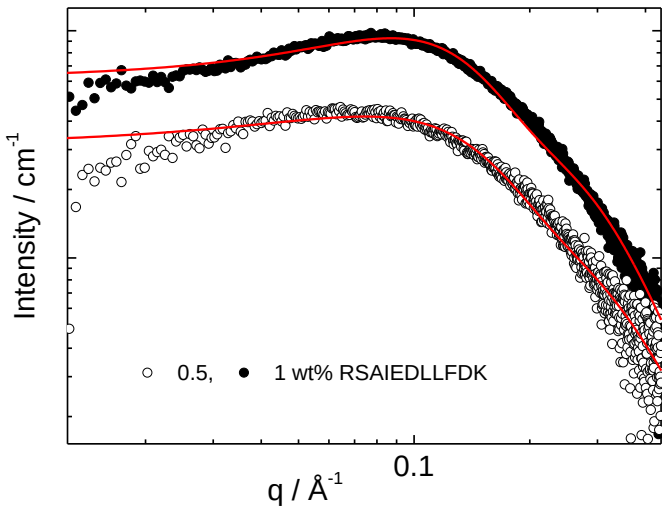

Figure 1. SAXS (open symbols: measured, red lines: fitted form factor profiles) for solutions of coronavirus spike peptide in water at native pH 3, at the concentrations indicated.

As well as the exciting work on the coronavirus spike protein peptide (the first study to our knowledge to show amyloid formation by such peptides), the work on the two lipopeptides is currently being written up.

5. References

1. V. Castelletto and I. W. Hamley, *ACS Nano*, 2021, *in press.*