

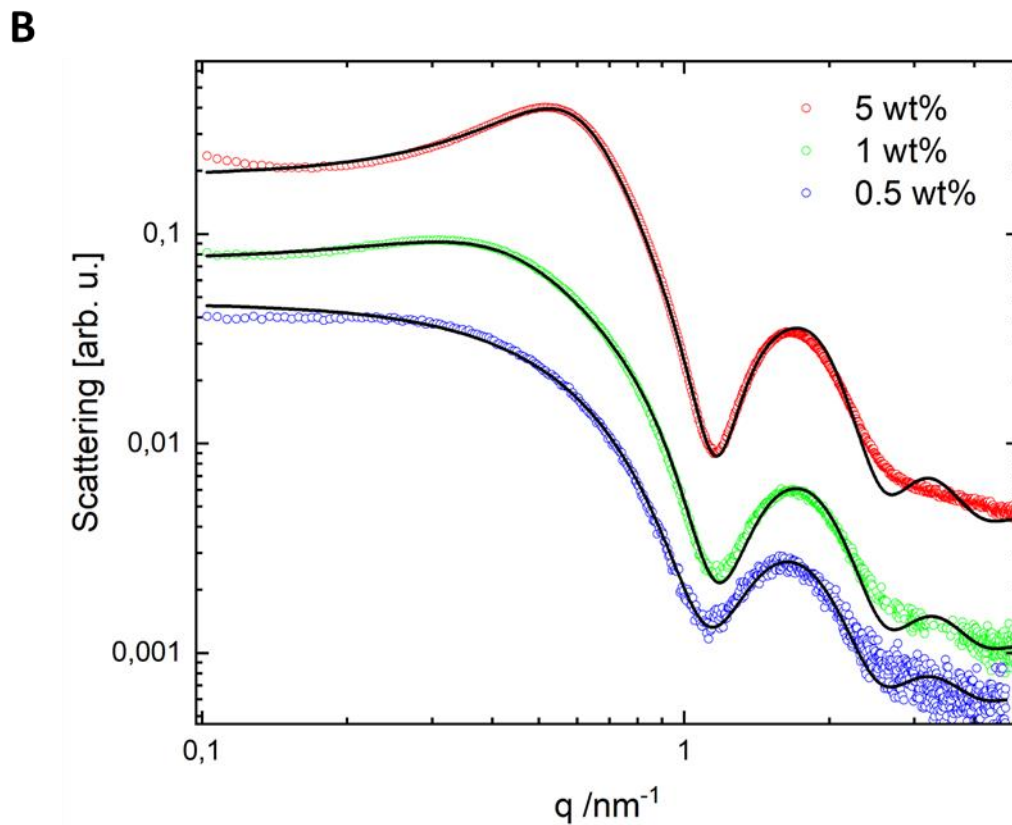
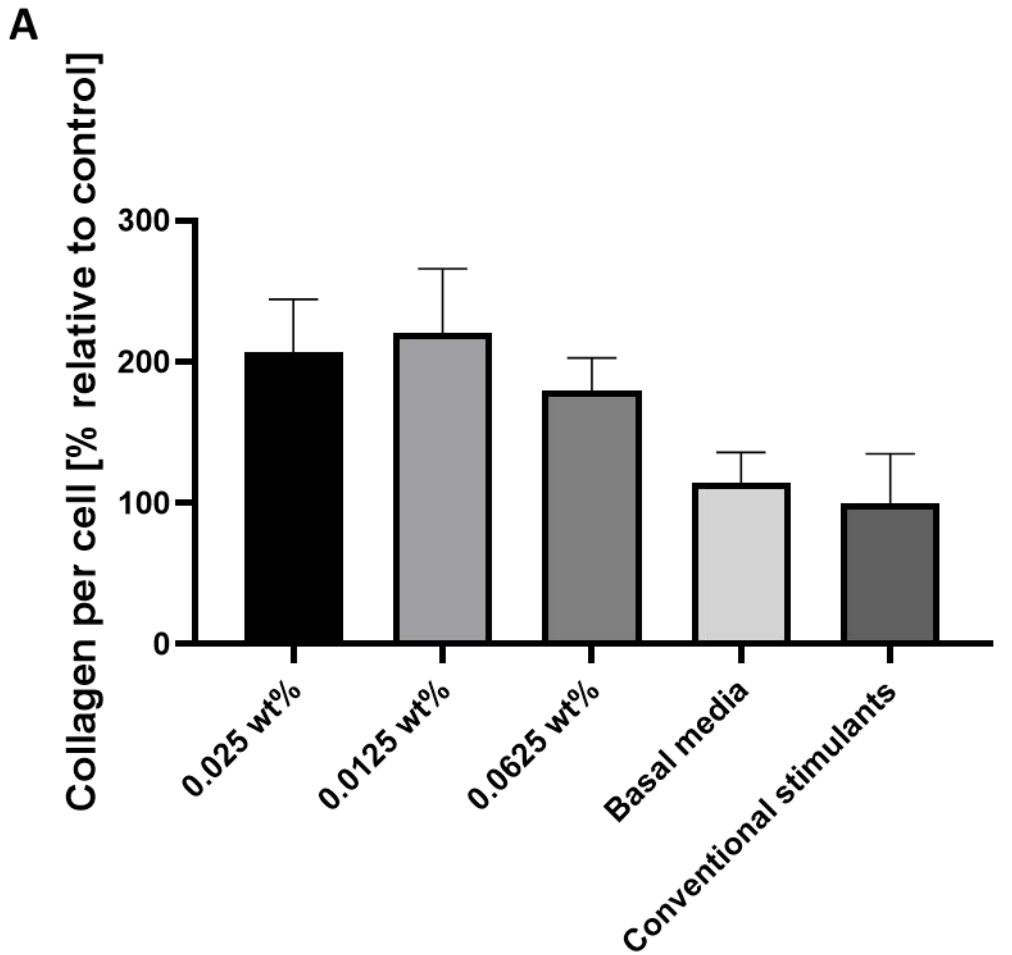


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|  | <b>Experiment title:</b><br>SAXS Studies of the Nanoscale Structure of SARS-CoV-2 Spike Peptides and their Interactions with Lipid Membranes and DNA | <b>Experiment number:</b><br>MX-2422 |
| <b>Beamline:</b>   | <b>Date of experiment:</b><br>from: 02/11/22 to: 04/11/22  | <b>Date of report:</b><br>28/11/22   |
| <b>Shifts:</b>   | <b>Local contact(s):</b><br>Mark Tully   | <i>Received at ESRF:</i>             |
| <b>Names and affiliations of applicants</b> (* indicates experimentalists):<br><br>Prof. Ian W. Hamley*, Lucas Rodrigues de Mello*, Prof. Emerson Rodrigo da Silva |  |                                      |

### Report:

Due to severe health problems, Prof. Emerson was unable to ship the SARS-CoV spike peptides and lipid membranes from Brazil.

Due to these exceptional circumstances, we shifted the aim of this run to examine the self-assembly of peptide amphiphiles (PAs) related to the sequence KTTKS, along with other peptides. A conjugate PA farnesyl-mercapto(diethylene glycol)-KTTKS (FMdEG-KTTKS) was designed with the aim to enhance the KTTKS collagen-stimulating sequence and also achieve better cytocompatibility. By cellular assays, we determined that this molecule stimulates fibroblasts to produce > 200% (Figure 1A) more collagen per cell than conventional stimulants. Also, it has been observed that this PA self-assembles at higher concentrations and the SAXS data obtained at ESRF indicates the presence of micelles. The data was fitted using the models for core-shell sphere form factor (with an additional hard sphere structure factor for the 1 wt% and 5 wt% samples), and both the original curves and fits are shown in Figure 1B.



**Figure 1.** A - Collagen production obtained by the absorbance at 540 nm after incubating the cells with Sirius red, a dye with affinity for collagen. HDFa cells were incubated with different concentrations of the PA and compared with controls incubated only in media without additives of conventional additives found in literature with the action of enhancing collagen production (insulin, ascorbic acid and TGF- $\beta$ ). B - SAXS curves of FMdEG-KTTKS at 5 wt% (red), 1 wt% (green) and 0.5 wt% (blue).

The data obtained in this run has been already analyzed and will be incorporated in the paper, which we intend to submit to a peer reviewed journal shortly.<sup>1</sup>

Several other peptide samples were also studied using the BioSAXS set-up and the data will be useful in the preparation of further papers.

## **References**

(1) Castelletto, V.; de Mello, L. R.; da Silva, E. R.; Seitsonen, J.; Hamley, I. W., *in preparation* **2022**.