ESRF	**Experiment title:** Structural study of properties of unilamellar DMPC vesicles incorporating the saponin escin, cholesterol and ibuprofen and combinations of those.	**Experiment number**: SC-4393
Beamline: ID02	**Date of experiment**: from: 31.08.2016 to: 02.09.2016	**Date of report**: 08.09.2016
Shifts: 3	**Local contact(s)**: Rajeev Dattani	*Received at ESRF:* *6*

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Report:

The experiment adresses the influence of the additives choelsterol, ibuprofen and the saponin escin on the structure of DMPC lipid -vesicles.

The experiment was performed with some experimental changes with respect to the orginally proposed experiment. The measurements were not performed in an automated sample changer but in a Linkam stage with a flow-through Kapton capillary with 1 mm diameter to ensure good thermalization and optimal background subtraction for the weakly scattering samples. This sample environment was brought by the user and installed on the sample table with the technical staff of ID02. The form factors were measured via SAXS at 2 sample-detector distances using the RayonX Detector at 10 m and 1 m so that a q-range from 0.001 - 6 nm^{-1} was covered. Simultaneous WAXS experiments were performed using also a RayonX detector to investigate the lateral structure of the lipid bilayers.

During the allocated beam time 3 sets of samples were measured, thus including DMPC vesicles as a function of the saponin escin (0-30 mol%), DMPC vesicles + 10 mol% cholesterol as a function of escin content (0-30 mol%) and DMPC vesicles + 10 mol% ibuprofen as a function of escin content (0-30 mol%) . The experiment was performed first at one dector distance at all temperatures (10-50°C in 5 °C steps) for all samples, and afterwards at the second detector distance at all temperautres for all samples. The WAXS experiment was performed simultaneously to the SAXS at low q (10 m). The WAXS detector

was removed for the SAXS experiments at high q. Each series of samples included 7-10 samples. In total, 25 samples were measured at 9 different temperatures.
The obtained data was averged and integrated. The WAXS data was additionally treated for polarization effects.
Figures 1-6 show exemplarly small-angle scattering curves obtained at 1 m for 6 different samples at an escin content of 10 and 30 mol% for pure DMPC vesicles and DMPC vesicles with 10 mol% cholesterol and 10 mol% ibuprofen.

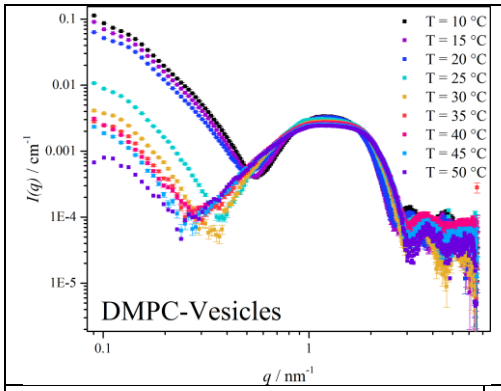

Fig.1: SAXS: DMPC vesicles from 10-50 °C at 1m

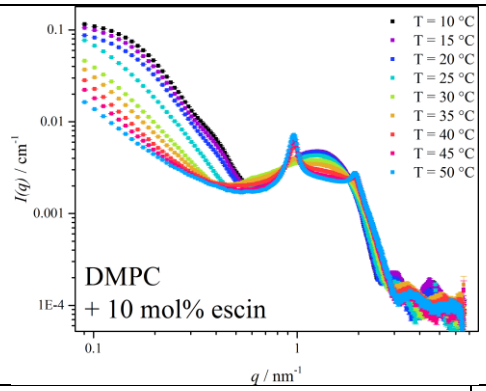

Fig.2: SAXS: DMPC vesicles + 10 mol% escin from 10-50 °C at 1m

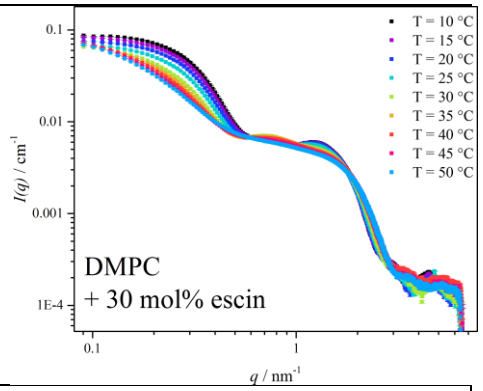

Fig.3: SAXS: DMPC vesicles + 30 mol% escin from 10-50 °C at 1m

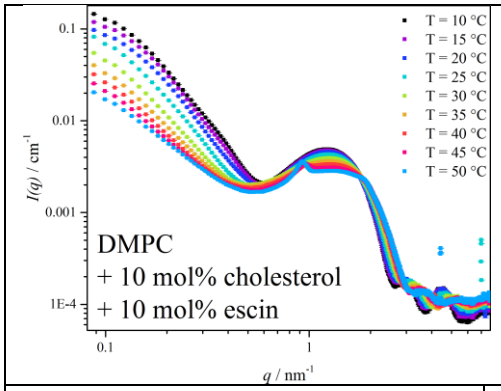

Fig.4: SAXS: DMPC vesicles + 10 mol% escin and 10 mol% cholesterol from 10-50 °C at 1m

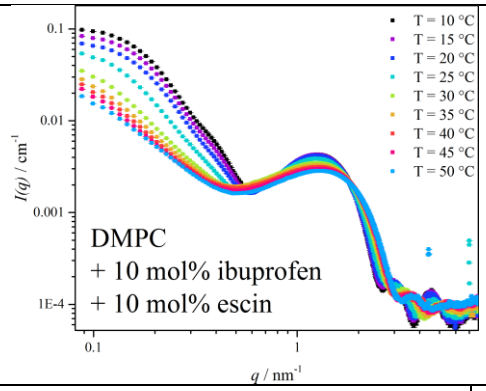

Fig.5: SAXS: DMPC vesicles + 30 mol% escin and 10 mol% ibuprofen from 10-50 °C at 1m

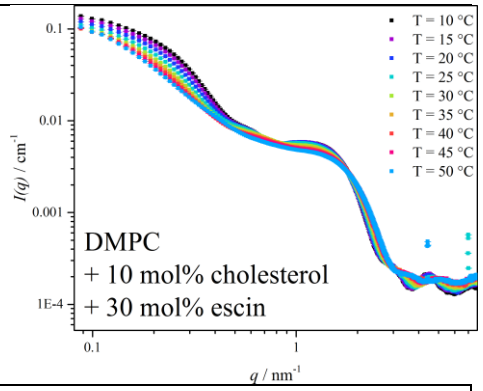

Fig.6: SAXS:DMPC vesicles + 30 mol%escin and 10mol% cholesterol from 10-50°Cat 1m

Major structural changes can be observed as a function of temperature for each sample, and incorporated species. These structural changes were found to be reversible with temprature. The data analysis ist still ongoing.
Further model dependent and model independent analysis, as mentioned in the related proposal, of the SAXS data will reveal insights on the obtained structures as function of temperature and incoporated molecules. Moreover, the role of the escin molecule in terms of the structure formation will be revealed.
The WAXS and the SAXS data at low q require further data reduction and cannot be presented here for now.
Due to data collection in a flow-through sample environment for excellent background subtraction and careful temperature regulation, the overal aim of the proposed experiment, to study the temperature dependent structures of combinations of cholesterol, ibuprofen and escin until ISCOM formation, was only partially realized during the allocated beam time.