ESRF

ESRF	**Experiment title:** SAXS study of bile salt micellar aggregates	**Experiment number**: SC-1233
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Report:

Data on micellar aggregates of dihydroxy (sodium and calcium taurodeoxycholate, NaTDC, CaTDC, and glycodeoxycholate, NaGDC, CaGDC) and trihydroxy (sodium taurocholate, NaTC, and glycocholate, NaGC) bile salts have been collected. The dependence of their size and shape on the concentration and ionic strength has been studied.

Due to the limited number of shifts accorded, the number of samples studied has been reduced. The bile salt concentrations and the ionic strength conditions have been reduced. The study of NaTC and the study in function of pH and temperature have been cancelled.

The main goal of the experiments was a study at low bile salt concentration, with the aim to reduce the interference contribution. The results obtained are very good.

1) In the case of NaGDC, the data collected at low bile salt concentration (20, 40 mM) present a good S/N ratio. At low bile salt concentration, the interaction effect is strongly reduced respect to the systems previously studied in our laboratory (with a Compact Kratky camera) at 100 mM. From the data analysis, pair distribution functions (p(r)), absolute I(0) intensities, aggregation numbers and gyration radii for the particle and for the cross section have been determined. A cylindrical growth has been observed in the 300 - 600 mM NaCl concentration range. Experimental p(r)'s are in very good agreement with a cylindrical model proposed in our laboratory. A manuscript is in preparation.

2) Three solutions with NaGDC in presence of $CaCl_2$ have been collected. For the same ionic strength (NaCl or $CaCl_2$), the presence of Ca^{2+} ions induces a strong aggregation, giving rise to cylindrical aggregates. Dimensions and aggregation numbers have been determined and a good agreement with p(r) calculated for a cylindrical model. An extensive study on the Ca salts is necessary.

3) Data collected on NaGC (a trihydroxy bile salt) - NaCl systems show that the dihydroxy bile salts (NaGDC and NaTDC) present bigger aggregates than the NaGC. At low NaCl concentration, NaGC show stronger interference effects which necessitate a particular attention in the data interpretation. The analysis, integrated with transport properties studies (QELS and PGSE-NMR measurements) is in progress.

4) The data for a limited number of samples containing a dihydroxy and a trihydroxy bile salt (NaGDC/NaGC and NaTDC/NaTC) have been collected. The trihydroxy salt inhibits the growth of the bile salt forming bigger size aggregates (dihydroxy salt), giving rise to a growth poisoning. The SAXS results confirm the QELS results obtained in our laboratory.
The setup of the camera allowed us to collect data in the 0.018-0.30 $Å^{-1}$ k range. The data can be analysed for particles with a maximum dimension of 170 Å. In some case, dimensions bigger than 170 Å have been observed. In this case, data collection at lower k, with a higher sample-detector distance would be necessary.

The results will be compared with QELS and PGSE-NMR data collected in our laboratory. This will allow to integrate the SAXS results with transport properties experiments, and to get an agreement between the geometry of a colloidal particle, obtained from SAXS measurements, and that obtained from transport properties. This strategy has been applied with success in our laboratory [1,2].

1) Galantini L., Pavel N. V. J. Chem. Phys. 118, 2865 (2003).

2) Galantini L., Giglio E., Leonelli A., Pavel N. V. J. Phys. Chem. B 108, 3078 (2004).