Experiment title: SAXS study of bile salt micellar aggregates		**Experiment number**: CH-1791
Beamline: BM26B	**Date of experiment**: from: 11-OCT-04 to: 13-OCT-04	**Date of report**: 28/08/2005
Shifts: 6	**Local contact(s)**: Dr. Florian Meneau	*Received at ESRF:*

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Report:

This project is a continuation of the project SC1233. Data on micellar aggregates of dihydroxy (calcium taurodeoxycholate CaTDC, and glycodeoxycholate, NaGDC, CaGDC) 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 (bile salt concentrations and the ionic strength conditions) has been reduced. The study of the trihydroxy bile salts (sodium and calcium taurocholate and glycocholate) 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 good.

1) In the case of NaGDC, the data collected at low bile salt concentration (20, 40, 60 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) Several solutions with NaTDC 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. The dimensions have been determined but a good agreement with p(r) calculated for cylindrical models has not been found. At low q values a persistent attractive interaction effect (or a contribution due to large aggregates) is present. Data analysis is in progress.

Two setups of the camera allowed us to collect data in the 0.018-0.30 $Å^{-1}$ q range. A strong background contribution has been observed at low q values, working with cells equipped with windows of mica. The data can be analysed for particles with a maximum dimension of 170 Å. In some case, unexpected dimensions bigger than 170 Å have been observed.
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 [1-3].

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).

3) Cozzolino S., Galantini L., Leggio C., Pavel N. V.: J. Phys. Chem. B 109, 6111, (2005).