ESRF	**Experiment title:** High-resolution powder diffraction of a homologous series of 2-oleo disaturated triacylglycerols.	**Experiment number:** CH-510
Beamline: BM16	**Date of experiment:** from: 30 August 1998 7:00 to: 01 September 1998 7:00	**Date of report:** 18 August 1999
Shifts: 6	**Local contact(s):** Eric Dooryhee	*Received at ESRF:* 8/99

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Report:

In this session a series of the β-C_nOC_n type (n=even) triacylglycerols was measured for determination of cell parameters only (see proposal). The expected cell parameters of these long-chain compounds were based upon crystallographic data of other triacylglycerols. A combination of one long (ranging from 50 to 80 Å) and one short cell axis (~5.5 Å) was expected and huge cell volumes. With the measurements at BM16 we succeeded in obtaining accurate 2θ values for all long spacing reflections, even the (h00).

Since the sample of β-LOL (melting point ~15° C) was molten during mounting of the capillary at the goniometer in a cooled environment, the measurement of LOL in the desired β polymorph failed. We succeeded in the measurement of LOL in the β' polymorph, but up to now we could not determine the cell parameters. In a next measurement session we will try to measure LOL when crystallized in the β polymorph.

The cell parameters of the other members of the series: SOS, POP and MOM could be determined from the powder patterns. No further information about the crystal structure could be derived yet

Also some measurements for structure determination from powder diffraction data were made. Among them samples of two crystalline long-chain diols: from one of these the crystal structure was solved and refined. This work is published in *J. Synchrotron Rad.* 6, 1035-1043. The structure of the other one has been solved also, and is now in the refinement stage. Another sample C_4Br_4S has been measured at 50 K, since heavy atomic disorder was expected for this structure. Now, the structure is solved and refined. A publication about this crystal structure is in preparation.

Finally, we measured a compound of $Ca(C_3H_5O_3^-)_2(C_3H_6O_3)_2$ having a tetragonal cell. We solved the structure of this compound but until now we could not refine this structure.