ESRF	**Experiment title:** High-resolution powder diffraction of a homologous series of 2-oleo disaturated triacylglycerols of the type	**Experiment number**: CH-943
Beamline: BM16	**Date of experiment**: from: 25-01-2001 to: 28-01-2001	**Date of report**: 31-08-2001
Shifts: 9	**Local contact(s)**: Andy Fitch	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Eva Dova*, Mihaela Pop*, Kees Goubitz*, Rene Peschar, Henk Schenk
Laboratory for Crystallography
Institute for Molecular Chemistry (IMC)
Universiteit van Amsterdam
Nieuwe Achtergracht 166
1018 WV Amsterdam
The Netherlands

Report:

In this session complete high-resolution powder diffraction patterns were collected of the following compounds, referred to here by their acronyms: POS (one of the compounds mentioned in the experiment title), POP, OPP, 15.15.17, 2M, PRR, RJ028, CII, CIII and CAPIII. Also partial data sets were collected of 13.15.13 (beam time finished) and 4M.

The wavelength in all experiments was 0.80008 Å. All samples, except for CII and CIII , were prepared in capillaries that were rotated during exposure. In most instances data collection was carried out in the interval interval 0-48.0º 2θ with 0.5 º 2θ min^{-1}, a sampling time of 100 ms and a final binning of the pattern at 0.005º 2θ. In case of RJ028 and PRR a slightly higher 2θ upper limit (50 and 52 º 2θ respectively) was used. Except for CII, CIII and CAPIII, data collection was carried with the purpose to index the pattern and to undertake crystal structure determination. Therefore, a scan protocol was used in which the exposure time increased as function of 2θ.

The first four compounds (POS, POP, OPP and 15.15.17) are different types of triacylglycerols and POS and POP in particular are main constituents of fats and oils. The patterns of POS (= β-1-palmityl,2-oleoyl,3-stearylglycerol collected at T = 287 K, POP (= β-2-oleoyl,1,3-dipalmitylglycerol) collected at T = 275 K, OPP (β-1-oleoyl,2,3-dipalmitylglycerol) collected at T = 287 K and the pattern of 15.15.17 (= 1,2-

pentadecanoin,3-heptadecanoinglycerol) collected at T = 275 K have all been indexed using a local program. It is now attempted to determine their crystal structures.

The compound 2M is a β-type cyclodextrin complexed with mefenamic acid. The pattern has been indexed and the crystal structure determination has been successful. The Rietveld refinement is now at the final stages and a publication is in preparation.

The compounds CII and CIII, both being types of chocolate made according to different recepies, were carved into a capillary shape (~ 3x4 mm) suitable for data collection. Although being co-crystallized mixtures of various triacylglycerols and other ingredients, the diffraction patterns are of good quality and they are now being analyzed.

The patterns of the organic compounds PRR and RJ028 have been indexed and structure determination is in progress.