



	Experiment title: Crystal structure determination of metastable and stable trans fatty acids containing triacylglycerols using high	Experiment number: CH-1635
Beamline: BM01B	Date of experiment: From: 27-02-2004 to: 01-03-2004	Date of report: 18-08-2004
Shifts: 6	Local contact(s): Wouter van Beek	<i>Received at ESRF:</i>
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Report:

The technical settings at the start of the experiments were $\lambda = 0.79936 \text{ \AA}$, beam width = 2.5 mm, beam height = 1.0-1.5 mm

For data collection a general strategy was adopted, consisting of scanning a set of overlapping 2θ intervals (0.53-35, 9-35, 19-35, 26-35 and 31-35 $^{\circ}2\theta$). All combined scans were binned at 0.005 $^{\circ}2\theta$

Data collection was carried out trans fatty acid (elaidic acid) containing triglycerides and several other types of triglycerides, with β , β' , γ and δ denoting the basic type of polymorph and the subscripts '1' and '2' denoting a lower-melting and higher melting phase, respectively:

- 1) *trans*-9-monounsaturated triglycerides 1,2-distearoyl-3-elaidoylglycerol (sub- α -SSE, β_2 -SSE), 1,3-distearoyl-2-elaidoylglycerol (β -SES), 1,2-dipalmitoyl-3-elaidoylglycerol (β -PPE), and 1,3-dipalmitoyl-2-elaidoylglycerol (β' -PEP)
- 2) the *cis*-9-*cis*-12-unsaturated triglyceride 1,3-distearoyl-2-lineoylglycerol (γ -SlinS)
- 3) the *cis*-9-monounsaturated triglyceride 1,3-dimyristoyl-2-oleoylglycerol (β -MOM)
- 4) cocoa butters from Bahia (Brazil) and Ivory Coast, both in the β -VI phase
- 5) The compounds L11, Imazetapir and synthetic

A preliminary analysis revealed some remarkable results. In case of PPE a novel β phase was observed. For SES the d-spacings do not correspond with those known from literature. Structure analysis of most compounds is in progress.