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Solid-state dynamic properties contribute to development of gas  
sorption and storage materials with microporous coordination  
polymers. Organic crystals function as dynamic materials due to their  
flexibility and diversity. We study on steroidal bile acid derivatives  
which serve as host components and form dynamic inclusion crystals  
for intercalation and enantioresolution of guest molecules. So far,  
we reported that cholamide has various types of flexible bilayers  
where secondary aliphatic alcohols are accommodated. Among them,  
2,2-dimethyl-3-hexanol induces a rare bilayer structure which is  
responsible for high enantioselectivity. Here we present intercalation  
and enantioresolution of 2,2-dimethyl-3-hexanol by using inclusion  
crystals of cholamide with 1,4-dioxane. It was found that guest  
exchanges took place with retention of the crystalline state in  
appearance. The crystal structures were determined before and after  
the intercalation by means of powder X-ray diffraction, indicating  
that the intercalation accompanied layer inversion on the lipophilic  
sides of the bilayers. Moreover, it was found that the resulting crystals  
include (S)-2,2-dimethyl-3-hexanol in over 95% ee yield.

Keywords: inclusion compounds, dipeptides, molecular  
recognition

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Structure and polymorphism of trans mono-unsaturated triacylglycerols  
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Trans fats are in a natural way in small quantities present in  
animal foods. Moreover, unsaturated plant fats are often partially  
hydrogenated to raise melting temperatures for preparation of foods,  
and then, as a minor side reaction, a small part of the cis-bonds will  
change into trans-configuration. Like saturated fats, fats with trans  
acid residues will have negative effects for human health (1).  
The presence of the elaidoyl chain, one of the major trans fatty-acid  
chains, is suspected of increasing health risks because it resembles the  
steaoyl chain. When incorporated in biological membranes elaidoyl  
chains will be influencing the physical-chemical properties of the  
membranes. Thus insight in the influence of the differences between  
the fatty-acid composition of trans and saturated triacylglycerols  
(TAGs) on the conformation and packing, on polymorphic stability,  
and on phase-transition behavior, will be useful. By combining  
X-ray powder diffraction (XRPD) techniques a better understanding of  
trans mono-unsaturated TAGs and their related saturated ones  
can be obtained. Synchrotron and advanced laboratory time- and  
temperature-resolved XRPD reveal the stability and phase-transition  
behavior of the important polymorphs like the β and β'. These results  
can be related to the underlying crystal structure packing that can  
be obtained from XRPD data using direct-space search techniques.  
Our recent results will be discussed including novel meta-stable β'  
polymorphs and the structure of one them, methyl-end plane packing  
analysis in relation to observed melting points for various subgroups  
of TAGs, and the difference in β' to β phase-transition behaviour of  
symmetric versus asymmetric TAGs.  
(1) The EFSA Journal, 2004, 81, 1-49

Keywords: trans mono-unsaturated triacylglycerols, time- 
temperature-resolved diffraction, powder structures

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Enantioselective inclusion of methyl phenyl sulfoxides  
by (S)-alkylglycyl-(S)-phenylglycine  
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As dipeptide host molecules, (S)-alkylglycyl-(S)-phenylglycines  
were examined in terms of enantioselective inclusion for racemic methyl  
phenyl sulfoxides. Among them, (S)-leucyl-(S)-phenylglycines  
(LeuPhg) and (S)-isoleucyl-(S)-phenylglycines (IlePhg)  
mainly included S-form of methyl phenyl sulfoxides with high  
enantioselectivity. By single crystal X-ray analyses of these inclusion  
compounds, it was elucidated that the dipeptide molecules self-  
assembled to form layer structures and included the sulfoxides between  
these layers by hydrogen bonding between the proton of ‘NH2’ and the  
oxygen of the sulfoxide. In the cavity, C-terminal phenyl group of the  
dipeptide interacts  
with the phenyl group of sulfoxides. In addition to these host-guest  
interactions, the two homochiral sulfoxides belonging in upper and  
lower layers make a pair having 2-fold rotation axis or 2-fold screw  
axis along the channel cavity. In other words, the self-recognition of  
sulfoxides made a homochiral pair to achieve high enantioselectivity.

Keywords: inclusion compound, chiral recognition, intercalation