Identification of 1,3- and 1,2-diacylglycerols by NMR Analysis

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Acylglycerols are a class of lipids commonly found in fats and oils, and they consist of a glycerol molecule esterified with one, two, or three fatty acid chains. Acyl group migration refers to the process in which fatty acid chains within monoacylglycerols or diacylglycerols rearrange their positions on the glycerol backbone.

As a part of our project new hybrid molecules in which stigmasterol was linked with 1,3-acylglycerols of palmitic and oleic acid were synthesized. In the synthetic pathway, we carried out the reduction of the carbonyl group of 1,3-dioleoyloxypropanone (1) using sodium borohydride (Scheme 1).



Scheme 1. Reduction of carbonyl group of 1,3-dioleoyloxypropanone (1).

Apart from the expected 1,3-dioleoylglycerol (2), we observed also formation of second compound, which turned out to be 1,2-dioleoylglycerol (3), the product of an oleoyl group migration from external to internal position. Thanks to the difference in their retardation factors (R_f), both regioisomers were separated, purified by flash chromatography and identified by NMR analysis.

Acyl migration occurs commonly during the synthesis of acylglycerols by biotechnological and chemical methods. In this communication the detailed spectroscopic analysis of 1,3-dioleoylglycerol (2) and its 1,2-isomer (3) was presented to facilitate their identification and differentiation for future research on the structured acylglycerols.

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