

Determination of the Equilibrium Constant for the Acidolysis of Triolein and Caprylic Acid Catalyzed by a 1,3 Specific Lipase

E. Hita, M.J. Jiménez, L. Esteban, P.A. González, A. Rodríguez, L. Martín, A. Robles
Department of Chemical Engineering. University of Almería. Spain

The acidolysis reaction between triolein (TO, LGL) and caprylic acid (M), catalyzed by the 1,3 specific lipase Lipozyme IM, is a good reaction model for obtaining structured triacylglycerols (TAGs) with the MLM structure. The equilibrium data of this acidolysis reaction were determined, with the aim of determining the equilibrium constants. The influence of M/TO molar ratio (m_0), and of initial TO concentration on equilibrium was studied. The equilibrium data were fitted to a model that take into account the four possible reactions that occurs for the exchange of an odd fatty acid (M) by a native fatty acid (L) which are located at positions 1 and 3. These reactions are:



where, in the TAGs LGL, MGL, LGM and MGM only the fatty acids at positions 1 and 3 that participate in the exchange are indicated; G represents the 2-monoacylglycerol which remains unaltered. If considering that positions 1 and 3 are equivalent and that equilibrium constants for the first and second exchanges are equal, all the equilibrium constants, K, are equal and it can be determined by equation:

$$K_{ap} = K \frac{\gamma_M}{\gamma_L} = \frac{(3F_{Me})^2}{(2 - 3F_{Me})(m_0 - 3F_{Me})}$$

which allows to calculate the apparent equilibrium constant, K_{ap} , from the molar fraction of M in the TAG at the equilibrium (F_{Me}) and from the free fatty acid/TAG molar ratio (m_0). γ_M and γ_L are the activity coefficients for odd and native fatty acids, respectively.

The result obtained suggest that the equilibrium composition does not depend on the initial TO concentration, which would indicate that this variable, at the range tested, has low influence on γ_M and γ_L . K_{ap} was determined using the previous equation and it was well correlated with m_0 , which allows to observe as the equilibrium is displaced toward the product formation when m_0 increased. The equilibrium compositions of the most abundant native fatty acids (palmitic, oleic and linoleic acids) were also correlated with m_0 and F_{Me} ; this has allowed to calculate the apparent equilibrium constants of these fatty acids for each molar ratio and to estimate the percentage of each fatty acid at position 2 and at positions 1 and 3. It has been observed that this fatty acid distribution is similar to the statistic distribution of fatty acids at the three positions of TAGs.