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# Studies on the lipase bioesterification of *Coffea* kaurane diterpenes, cafestol and kahweol

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**Abstract** Coffee oil is very important in the functional and sensory properties of coffee beverage, as it carries the aromas and gives creaminess by emulsification. It is also used as emollient in cosmetics. Coffee oil, also known as the "lipid fraction", corresponds from 7 to 17 % of the bean, and the main components are triacylglycerides (75-85 %), followed by diterpene esters (up to 20 %) with different fatty acids as *n*-$C_{14:0}$, $C_{16:0}$, $C_{16:1}$, $C_{17:0}$, $C_{18:0}$, $C_{18:1}$, $C_{18:2}$, $C_{18:3}$, $C_{20:0}$, $C_{20:1}$, $C_{22:0}$, $C_{24:0}$. Besides, a small amount in the free diterpenes as dialcohol occurs (< 0.4 %), esters of steroids (3.2 %) and their free form (2.2 %), tocopherols (0.05 %), phosphatides (0.3 %) and tryptamine derivatives (≤ 1 %) [1]. These diterpenes are alcohol based pentacyclic diterpene with a furokaurane skeleton whose main compounds are cafestol and kahweol, the last one present only in the Arabica bean (*C. arabica* L., Rubiaceae) and that differs from cafestol due to the presence of a double bond between $C_1$-$C_2$. In this study, we describe the lipase-catalyzed esterification of cafestol and kahweol with different fatty acid sources. Type of solvent, temperature, stirring, amount of enzyme and acyl donor, common parameters that affect esterification by lipases, were optimized by a Central Composite Rotatory Design, using palmitic acid as acyl donor. The highest yields were obtained with toluene as solvent, substrate molar ratio of 1: 5 (alcohol: fatty acid), an enzyme load of 73.3 mg $mL^{-1}$, 70 °C and 240 rpm for 3 days, giving kahweol palmitate in 86.6 % of conversion and cafestol palmitate in 85.7 %. These conditions were then used to produce the esters from *n*- $C_{14:0}$, $C_{18:0}$, $C_{18:1}$, $C_{18:2}$, $C_{18:3}$, $C_{20:0}$ fatty acids [2]. Toluene, used as solvent in this lipase catalysed esterification, seems to decrease the steric hindrance of the enzyme active site and facilitates fatty acid incorporation into the furokaurane diterpenes from *Coffea*.

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[2] Novaes, F. J. M., Sutili, F. K., Souza, R. O. M. A., Aquino Neto, F. R., Rezende, C. M. Cafestol and Kahweol diterpene esters synthesis catalyzed by Lipase. 2015, submitted.