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Production of esters by biocatalysed transesterification in supercritical CO2 and Hexane

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The development of sustainable processes that use renewable raw materials and minimize chemical and energetic waste has attracted considerable attention and represents a great challenge to both academic researchers and industrial experts.
The use of enzymes to catalyse chemical transformations can constitute a more sustainable alternative to some traditional chemical processes and more than 100 biotransformations are already operated at an industrial scale [1]. Lipases usually operate in mild conditions and can catalyse both hydrolytic and synthetic reactions, depending on the surrounding medium. The hydrolysis of esters can be performed in water, but the reverse production reactions are not favoured in this medium, and are usually performed in organic solvents.
Supercritical CO2 can constitute a more sustainable alternative to organic solvents as a reaction medium, provided that it does not have a direct adverse effect on the enzyme's active site or significantly reduce its activity.
Decyl acetate was chosen as a model compound and its production by a transesterification reaction catalysed by Novozym 435 (immobilized Candida Antarctica Lipase B) was studied in both hexane and supercritical CO2. A comparative analysis between these two alternatives was performed, focusing on the differences on the enzyme's catalytic activity, solubilities of the substrates and mass transfer rates; which significantly affect the outcome of the reaction process and its productivity and provide information on when such solvents can be used.
[1] Straathof, A.J.J., Panke, S., Schmid, A. The production of fine chemicals by biotransformations. Current Opinion in Biotechnology, 2002, 13(6), 548-556.