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Optimization of reaction parameters by factorial design for the enzymatic synthesis of natural aroma esters

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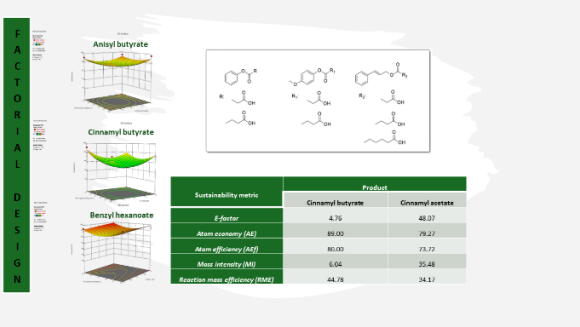
In recent years an increase in the public's demand for bio-products has been observed. This has prompted increased efforts by the food and agricultural industries to develop alternative methods for preparing food ingredients with significantly reduced environmental impact in order to satisfy the general public's needs.

The current work shows the synthesis of seven aroma esters (anisyl propionate and butyrate, cinnamyl propionate and butyrate, benzyl propionate, butyrate and hexanoate) by direct esterification of carboxylic acids with the corresponding alcohols mediated by lipase B from *Candida antarctica* encapsulated in a sol-gel matrix in a solvent-free system using vacuum to remove the resultant water. The reaction parameters were optimized for each reaction system by factorial design experiments considering four factors (acid excess, temperature, applied vacuum and reaction time) on two levels. This study presents an alternative to the currently applied method for obtaining aroma esters which is extraction from natural sources.



By applying factorial design method (central composite) for optimization of each reaction the conversions were significantly increased (for example, from an isolation yield of 49.4% to 94.3% for cinnamyl butyrate). A semi-preparative experiment was further set-up for cinnamyl butyrate preparation and green chemistry metrics were determined for the above-mentioned synthesis. A mass intensity of 6.04 and a *E*-factor of 4.76 demonstrated that the newly developed enzymatic process is suitable for industrial application based on the green chemistry principles.

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