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ORIGINAL ARTICLE

Optimization of cocoa butter analog synthesis variables using neural networks and genetic algorithm

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Abstract Cocoa butter analog was prepared from camel hump fat and tristearin by enzymatic interesterification in supercritical carbon dioxide (SC-CO_2) using immobilized *Thermomyces lanuginosus* lipase (Lipozyme TL IM) as a biocatalyst. Optimal process conditions were determined using neural networks and genetic algorithm optimization. Response surfaces methodology was used to design the experiments to collect data for the neural network modelling. A general regression neural network model was developed to predict the response of triacylglycerol (TAG) distribution of cocoa butter analog from the process pressure, temperature, tristearin/camel hump fat ratio, water content, and incubation time. A genetic algorithm was used to search for a combination of the process variables for production of most similar cocoa butter analog to the corresponding cocoa butter. The combinations of the process variables during genetic algorithm optimization were evaluated using the neural network model. The pressure of 10 MPa; temperature of 40 °C; SSS/CHF ratio of 0.6:1; water content of 13 % (w/w); and incubation time of 4.5 h were found to be the optimum conditions to achieve the most similar cocoa butter analog to the corresponding cocoa butter.

Keywords Enzymatic interesterification · Camel hump fat · Supercritical carbon dioxide (SC-CO_2) · Neural networks · Genetic algorithm

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Introduction

Cocoa butter, which amounts to 25–36 % in finished chocolate, is responsible for the smooth texture, contractibility, flavor release, and gloss of the product (Liu et al. 1997). Cocoa butter is composed predominantly (>70 %) of three symmetrical TAGs, 1,3-dipalmitoyl-2-oleoylglycerol(POP), 1(3)-palmitoyl-3(1)stearoyl-2-oleoylglycerol (POS), and 1,3-distearoyl-2-oleoylglycerol (SOS). Numerous factors, however, including the degree of uncertainty in supply, variability in quality, and price premium compared to other fats have driven oil industry for alternatives (Hartmann et al. 2001). Producing fats with highly desirable physicochemical properties, such as cocoa butter alternatives by enzymatic interesterification in organic solvents, has become a popular area of biotechnological research (Mojovic et al. 1993; Silroy et al. 2011). However, organic solvent systems are suffering from some major drawbacks such as final solvent removal, which is usually costly and time and energy consuming. The use of supercritical fluid as a solvent and reaction medium for lipids has grown rapidly in recent years. In addition, the solubility of most organics in supercritical fluids is higher than that in gaseous phase and is comparable with liquid solvents. Among supercritical fluids, SC-CO_2 is especially advantageous due to low toxicity, viscosity, cost, surface tension (Kumar et al. 2011). The solvent properties of supercritical carbon dioxide can be readily modified by adjusting pressure or temperature; the diffusivity of solutes in carbon dioxide is higher than in organic solvents. Carbon dioxide can easily be removed from the reaction products to minimize the need for costly downstream clean-up. When carbon dioxide is used in lieu of organic solvents, it has the additional benefit of being an environmentally benign process (Jackson and King 1997; Liu et al. 2007).

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