Application of artificial neural network for yield prediction of lipase-catalyzed synthesis of dioctyl adipate.

ABSTRACT

In this study, an artificial neural network (ANN) trained by backpropagation algorithm, Levenberg–Marquadart, was applied to predict the yield of enzymatic synthesis of dioctyl adipate. Immobilized Candida antarctica lipase B was used as a biocatalyst for the reaction. Temperature, time, amount of enzyme, and substrate molar ratio were the four input variables. After evaluating various ANN configurations, the best network was composed of seven hidden nodes using a hyperbolic tangent sigmoid transfer function. The correlation coefficient (R 2) and mean absolute error (MAE) values between the actual and predicted responses were determined as 0.9998 and 0.0966 for training set and 0.9241 and 1.9439 for validating dataset. A simulation test with a testing dataset showed that the MAE was low and R 2 was close to 1. These results imply the good generalization of the developed model and its capability to predict the reaction yield. Comparison of the performance of radial basis network with the developed models showed that radial basis function was more accurate but its performance was poor when tested with unseen data. In further part of the study, the feed forward back propagation model was used for prediction of the ester yield within the given range of the main parameters.

Keyword: Artificial neural network; Lipase; Dioctyl adipate; Neural network; Modeling; Prediction.