Abstract:

In this study, the reaction of caffeic acid and ٢-phenyl ethanol in the presence of immobilized lipase from *Candida antractica* (Novozym ٤٣٥) was modeled and optimized in isooctane system using artificial neural network and genetic algorithm methods in order to obtain caffeic acid phenethyl ester. For this purpose, a ٥- level-٤ variable central composite rotatable design was used for modeling the enzymatic reaction using artificial neural network. Independent variables were temperature, time, molar ratio of substrates and enzyme amount; while the molar conversion of caffeic acid to ester was considered as a dependent variable. The Levenberg-Marquardt algorithm was used as learning algorithm of artificial neural network. Therefore, first, the modeling was carried out by artificial neural network and using the Levenberg-Marquardt algorithm. The best model is including a network with four inputs, ١٠ neurons in hidden layer and one output (٤-١٠-١). After modeling by artificial neural network, genetic algorithm was used for optimization of the model. The optimized conditions were: time ٦٠ hrs, temperature ٦٩°C, molar ratio of substrates ٧٣:١ (٢-phenyl ethanol: caffeic acid) and enzyme amount ٣٢٢ PLU. Under these conditions, the actual and predicted of molar conversion of caffeic acid to ester were ٩٨.١٢ and ١٠٠.٥٤, respectively.

Key words: Modeling; optimization; enzymatic synthesis; caffeic acid phenethyl ester; artificial neural network; genetic algorithm

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