Multivariate optimization in the biosynthesis of a triethanolamine (TEA)-based esterquat cationic surfactant using an artificial neural network.

ABSTRACT

An Artificial Neural Network (ANN) based on the Quick Propagation (QP) algorithm was used in conjunction with an experimental design to optimize the lipase-catalyzed reaction conditions for the preparation of a triethanolamine (TEA)-based esterquat cationic surfactant. Using the best performing ANN, the optimum conditions predicted were an enzyme amount of 4.77 w/w%, reaction time of 24 h, reaction temperature of 61.9 °C, substrate (oleic acid: triethanolamine) molar ratio of 1:1 mole and agitation speed of 480 r.p.m. The relative deviation percentage under these conditions was less than 4%. The optimized method was successfully applied to the synthesis of the TEA-based esterquat cationic surfactant at a 2,000 mL scale. This method represents a more flexible and convenient means for optimizing enzymatic reaction using ANN than has been previously reported by conventional methods.

Keyword: Multivariate optimization; Biosynthesis; Triethanolamine (TEA)-based esterquat cationic surfactant; Artificial neural network.