Synthesis of (S)-omeprazole catalyzed by soybean pod peroxidase in water-in-oil microemulsions: optimization and modeling

yuanyuan Zhang[1], Hui Tang [1], Yashan Deng[1], Depeng Li[1], Zhiyong Wang[1], Huiling Li[1], Xin Xin Gao[1], and Fanye Wang[1]

[1]Qingdao University of Science and Technology

October 6, 2020

Abstract

Response surface methodology (RSM) was used to optimize the oxidation of the omeprazole sulfide to (S)-omeprazole catalyzed by environmentally friendly catalyst soybean pod peroxidase (SPP) in cetyltrimethylammonium bromide (CTAB)/isooctane/n-butyl alcohol/water water-in-oil microemulsions. With the initial concentration of SPP of 3200 U ml-1, the conversion of the omeprazole sulfide, the (S)-omeprazole yield and ee were 93.75%, 91.56% and 96.08%, respectively, under the optimal conditions: Wo of 15.85, the concentration of H2O2 of 22.44 mM and reaction temperature of 49.68 , respectively. The proposed mechanism of asymmetric sulfoxidations catalyzed by SPP involves three concomitant mechanisms as follows: (1) a two-electron reduction of SPP-I, (2) a single-electron transfer to SPP-I and (3) nonenzymatic reactions, including five enzymatic and two nonenzymatic reactions, which is reasonable and can express the oxidations. With 5.44% of the average relative error, a kinetic model based on the mechanisms fitting observed data very well was established, and the SPP-catalyzed reactions including both the two-electron reduction and the single-electron transfer mechanisms obey ping-pong mechanism with substrate and product inhibition, while nonenzymatic reactions follow a power law. This study has also demonstrated the feasibility of SPP as a substitute with low cost, excellent enantioselectivity and better thermal stability.

Hosted file

`Biotechnology and Bioengineering.pdf` available at https://authorea.com/users/364771/articles/485069-synthesis-of-s-omeprazole-catalyzed-by-soybean-pod-peroxidase-in-water-in-oil-microemulsions-optimization-and-modeling