

Optimization of synthesis of (S)-omeprazole catalyzed by soybean pod peroxidase in water-in-oil microemulsions using RSM

Hui Tang¹, Yuanyuan Zhang¹, Yashan Deng¹, Shanshan Du¹, Depeng Li¹, Zhiyong Wang¹, Huiling Li¹, Xin Xin Gao¹, and Fanye Wang¹

¹Qingdao University of Science and Technology

April 05, 2024

Abstract

Response surface methodology (RSM) was used to optimize the oxidizing 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 °C, 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

Optimization of synthesis of (S)-omeprazole BIOT.doc available at <https://authorea.com/users/364772/articles/709353-optimization-of-synthesis-of-s-omeprazole-catalyzed-by-soybean-pod-peroxidase-in-water-in-oil-microemulsions-using-rsm>