

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

Hui Tang¹, yuanyuan zhang¹, Yashan Deng¹, depeng Li¹, zhiyong Wang¹, huiling Li¹, xin Gao¹, and Fanye Wang¹

¹Qingdao University of Science and Technology

March 30, 2022

Abstract

Response surface methodology(RSM)was used to optimize the oxidizing the omeprazole sulfide to(S)-omeprazole catalyzed by 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. The 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. With 5.44% of the average relative error, a kinetic model based on the mechanisms 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

Synthesis of (S)-omeprazole catalyzed by soybean pod peroxidaseAJ.doc available at <https://authorea.com/users/364772/articles/562043-synthesis-of-s-omeprazole-catalyzed-by-soybean-pod-peroxidase-in-water-in-oil-microemulsions-optimization-and-modeling>