

## Combination of oxyanion Gln114 Mutation and medium engineering to influence the enantioselectivity of thermophilic lipase from *Geobacillus zalihae*

### Abstract

The substitution of the oxyanion Q114 with Met and Leu was carried out to investigate the role of Q114 in imparting enantioselectivity on T1 lipase. The mutation improved enantioselectivity in Q114M over the wild-type, while enantioselectivity in Q114L was reduced. The enantioselectivity of the thermophilic lipases, T1, Q114L and Q114M correlated better with  $\log p$  as compared to the dielectric constant and dipole moment of the solvents. Enzyme activity was good in solvents with  $\log p < 3.5$ , with the exception of hexane which deviated substantially. Isooctane was found to be the best solvent for the esterification of (R,S)-ibuprofen with oleyl alcohol for lipases Q114M and Q114L, to afford E values of 53.7 and 12.2, respectively. Selectivity of T1 was highest in tetradecane with E value 49.2. Solvents with low  $\log p$  reduced overall lipase activity and dimethyl sulfoxide (DMSO) completely inhibited the lipases. Ester conversions, however, were still low. Molecular sieves employed as desiccant were found to adversely affect catalysis in the lipase variants, particularly in Q114M. The higher desiccant loading also increased viscosity in the reaction and further reduced the efficiency of the lipase-catalyzed esterifications.