Title: Prediction of enantioselectivity of lipase catalyzed kinetic resolution using umbrella sampling

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Prediction of enantioselectivity of lipase catalyzed kinetic resolution using umbrella sampling

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Highlights

- Molecular dynamics (MD) simulation of *Candida rugosa* lipase (CRL) and *Burkholderia cepacia* lipase (BCL) in n-hexane have been carried out.
- Initial conformation for protein-ligand interaction were obtained from docking simulations.
- Simulation of acylated complex of R and S form of four racemic alcohols with BCL and CRL in n-hexane have been carried out.
- Umbrella sampling was carried out to get the free energy change along the reaction coordinate.
- The enantiomeric ratio (E) estimated from umbrella sampling were experimental values with less than 20% error.