Evaluating Ylehd, a recombinant epoxide hydrolase from *Yarrowia lipolytica* as a potential biocatalyst for resolution of benzyl glycidyl ether

Chandrika Bendigiri[a], K. Harini[c], Sajal Yenkar[a], Smita Zinjarde[a], R.Sowdhamini[c] and Ameeta RaviKumar[a,b] *
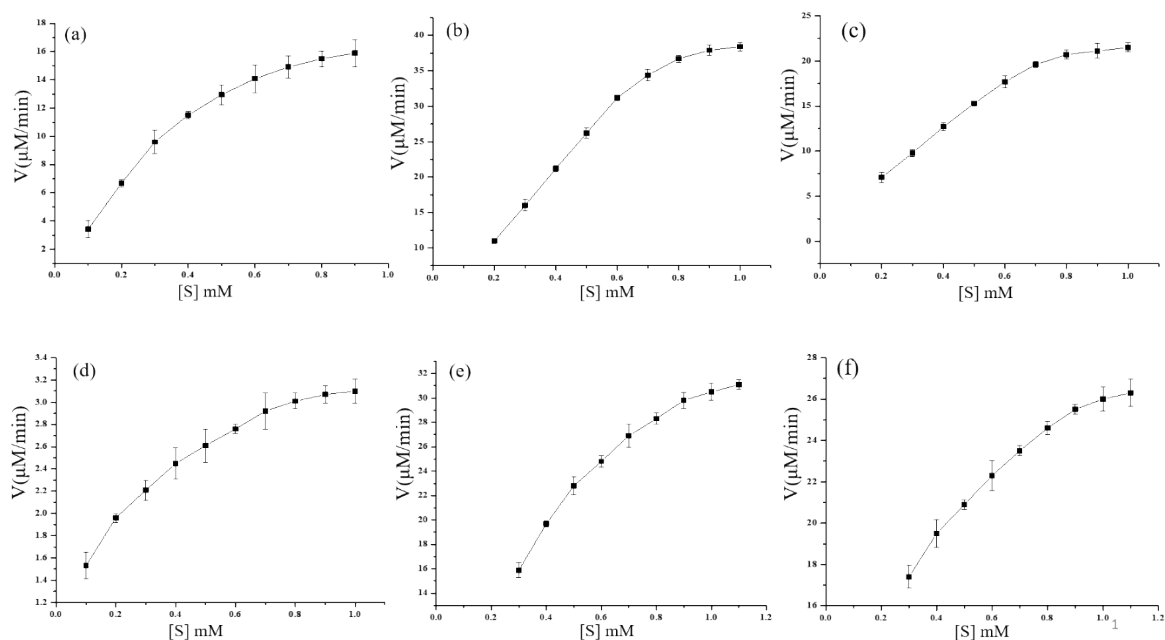
Fig. S1: Substrate saturation plots

Curves indicate the substrate saturation of Ylehd with rac-PGE(a), *(R)*-PGE(b), *(S)*-PGE(c), rac-BGE(d), *(R)*-BGE(e) and *(S)*-BGE(f)
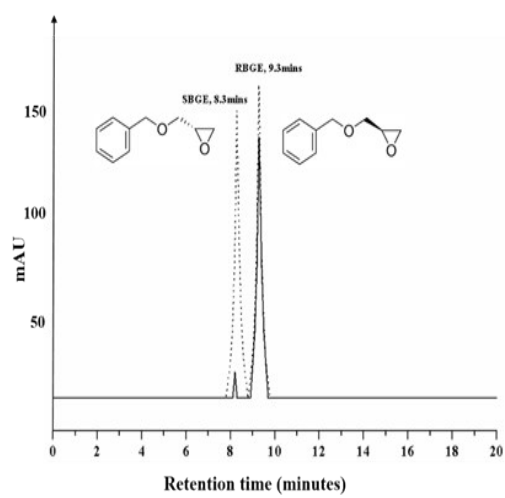
Figure S2: Resolution of BGE

Racemic BGE(dotted),Racemic BGE +Ylehd after 20 minutes of reaction(solid)

1,2-Epoxypropane	1,2-Epoxybutane	1,2-Epoxypentane	1,2-Epoxyhexane	1,2-Epoxyoctane
-3.56 kJ/mol	-3.81 kJ/mol	-4.06 kJ/mol	-4.39 kJ/mol	-5.81 kJ/mol

1,2-Epoxydodecane	2,3-Epoxybutane	Epichlorohydrin	Glycidol
-4.33 kJ/mol	-5.23 kJ/mol	-3.65 kJ/mol	-3.2 kJ/mol

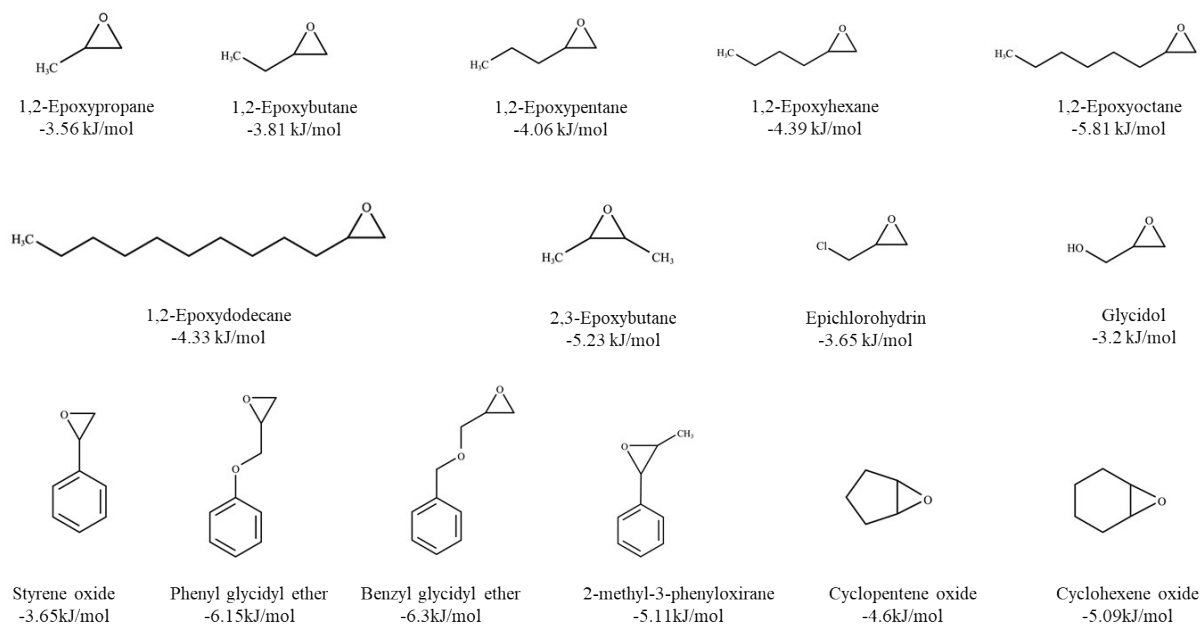| Styrene oxide	Phenyl glycidyl ether	Benzyl glycidyl ether	2-methyl-3-phenyloxirane	Cyclopentene oxide	Cyclohexene oxide
-3.65kJ/mol	-6.15kJ/mol	-6.3kJ/mol	-5.11kJ/mol	-4.6kJ/mol	-5.09kJ/mol

Fig. S3: Binding energy of compounds docked with Ylehd

3D coordinates of ligands were downloaded from Pubchem and docked flexibly with Ylehd protein model. Pubchem CID numbers are serially given as follows: 6378, 7834, 13853, 15036, 18126, 17858, 30664, 7835, 11164, 7276, 31217, 94247 and 12339.
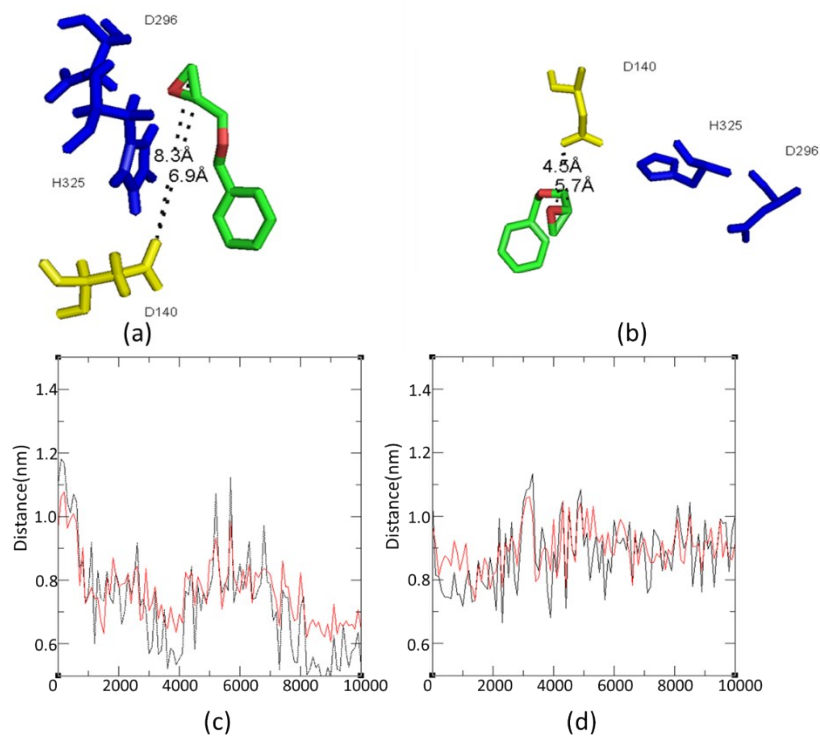
Fig. S4: Distance between nucleophile and ligand

(a,b) Distance between nucleophile D140 and carbon atoms of the oxirane ring of *(R)*-BGE(a) and (S)-BGE(b) bound to Ylehd model after docking and energy minimisation.

(c,d) Distance trajectories for C1(red) and C2(black) from D140 in hydrated active site pocket of Ylehd bound to *(R)*-BGE(c) and (S)-BGE(d) during the course of simulations.