Supporting Information

Efficient enzymatic synthesis of chiral 2,3-dihydro-1,4-benzodioxane ring motif using engineered *Candida antarctica* lipase B

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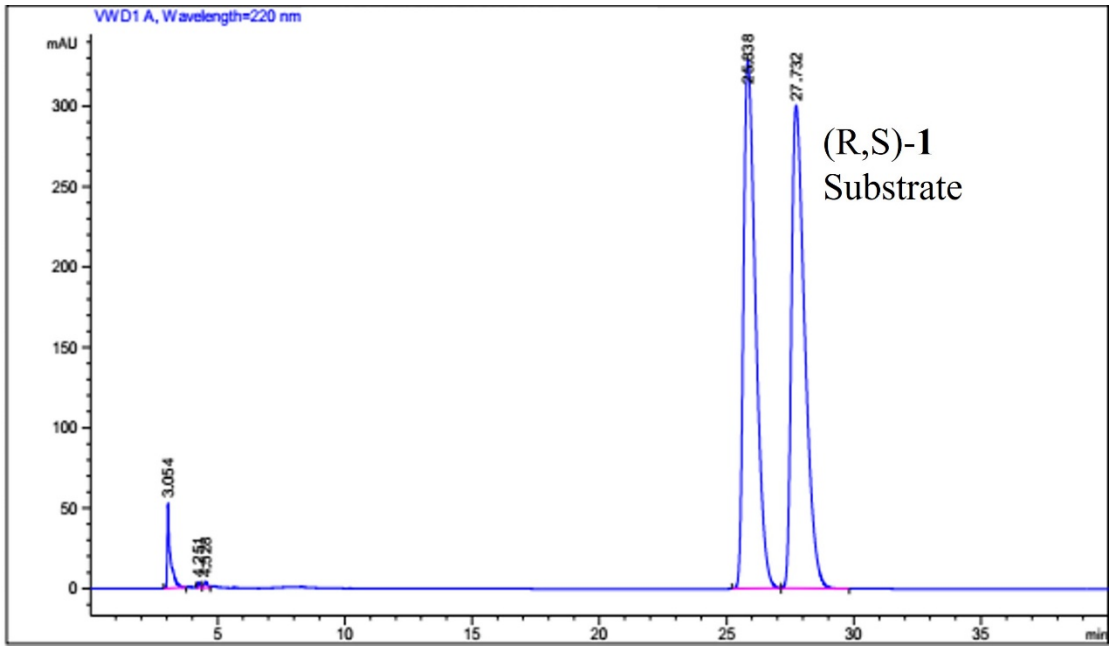

Fig. S1. HPLC Chromatogram of substrate 1,4-Benzodioxane-2-carboxylic acid methyl ester (R, S)-**1**

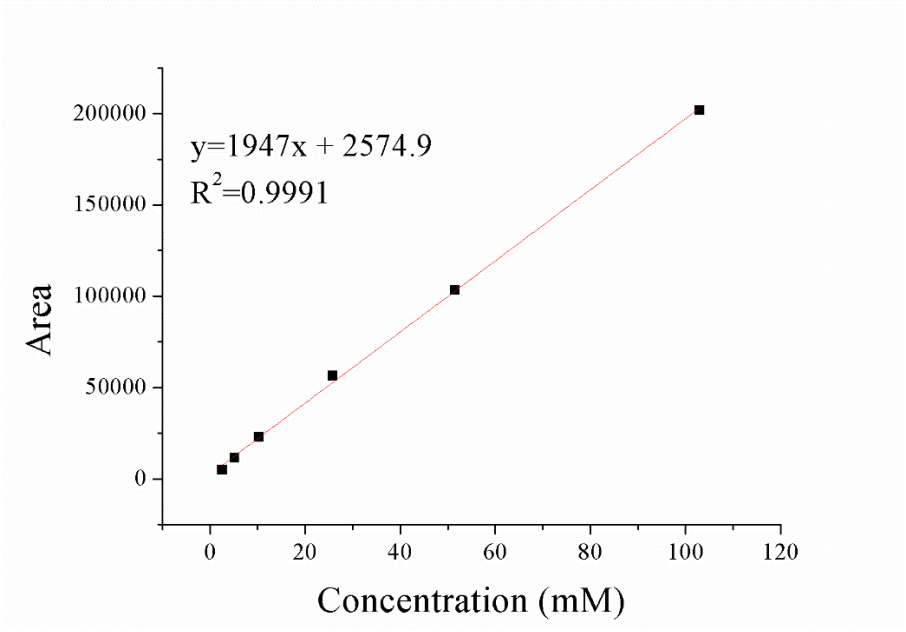

Fig. S2. Standard curve of 1,4-Benzodioxane-2-carboxylic acid methyl ester by HPLC analysis

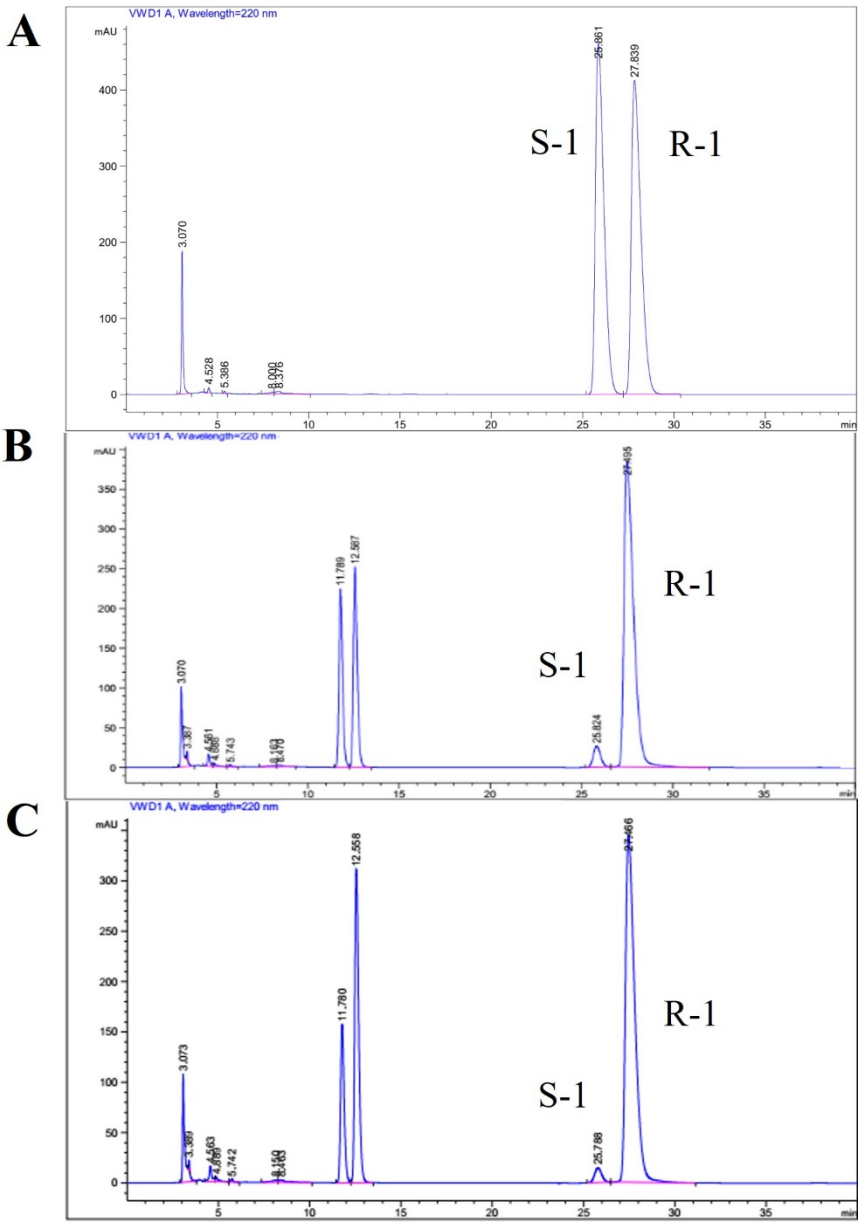

Fig. S3. HPLC Chromatogram of CALB and mutants catalyze 1,4- Benzodioxane-2-carboxylic acid methyl ester. (A) CALB; (B) A225F; (C) A225F/T103A

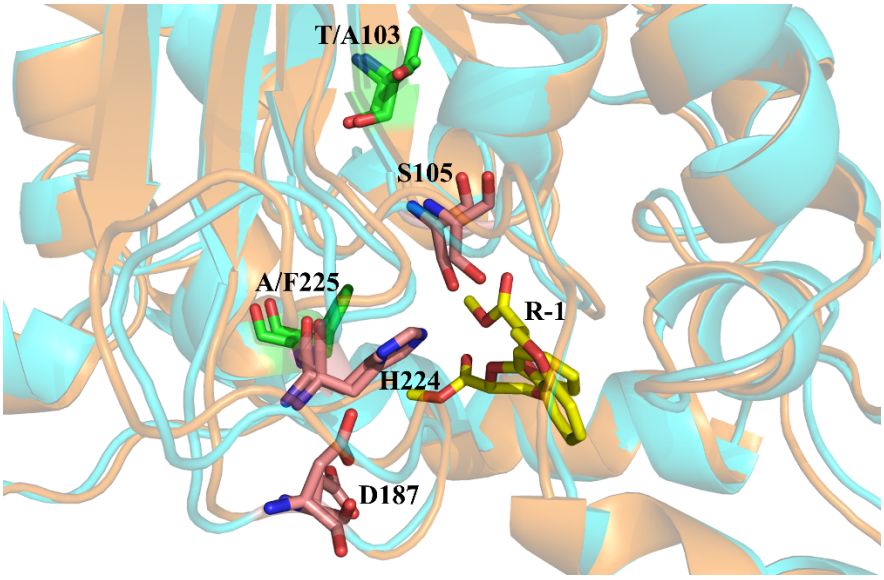

Fig. S4. Superposition of active sites of wild type CALB and A225F/T103A mutant. Wild type CALB and A225F/T103A mutant are in cyan and wheat. Substrate R-**1** is shown as yellow; catalytic triad (S105-D187-H224) is shown as orange; the mutation sites 103 and 225 are shown as green.

Table S1. Specific activities and enantioselectivity of the purified CALB and mutants in resolution of (*R, S*)-**1** [a]

Enzyme	Specific activity [b] (U mg^{-1})	E
CALB	3.33±0.15	N.D.
A225F	6.68±0.21	>200
A225F/T103A	5.83±0.19	>200

[a] The activity of the CALB and mutants were measured in 10 mL PBS buffer containing 20% *n*-butanol and 50 mM (*R, S*)-**1** at 30 °C. [b] One unit of enzyme activity (U) was defined as the amount of enzyme consuming 1.0 μmol of (*R, S*)-**1** per minute under the assay conditions used.