

Supporting Information

Exploring multifunctional residues of ribose-5-phosphate isomerase B from *Ochrobactrum* sp. CSL1 enhancing isomerization of D-allose

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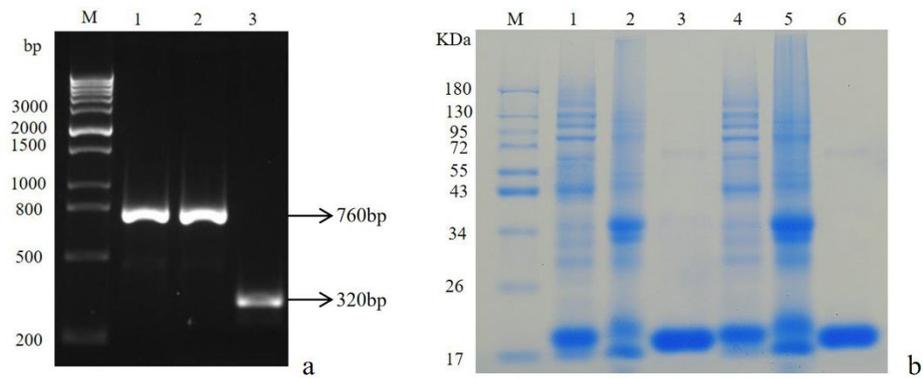


Fig. S1 Electrophoresis analysis of DNAs and proteins.

a: Colony PCR analysis of generated OsRpiB mutants (M: DNA Marker; 1: S9T mutant; 2: S98H/S134H mutant; 3: *E. coli* without insertion of the gene of interest). b: SDS-PAGE analysis of generated OsRpiB mutants (M: Protein Marker; 1: Crude wild type in supernatant; 2: Crude wild type in precipitation; 3: Purified wild type in supernatant; 4: Crude S98H/S134H mutant in supernatant; 5: Crude S98H/S134H in precipitation; 6: Purified S98H/S134H mutant in supernatant).

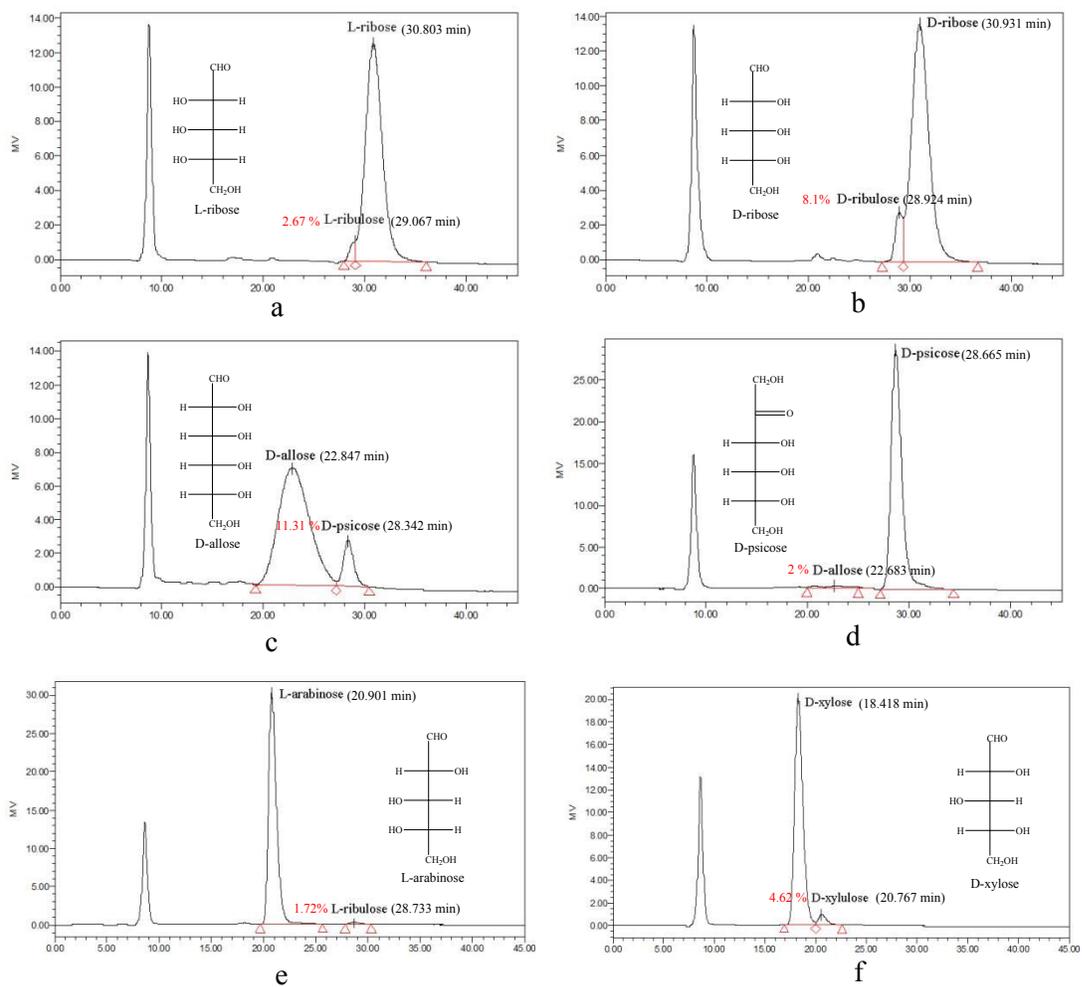


Fig. S2 HPLC chromatogram of isomerizing different substrates.

a: Substrate:L-ribose; b: Substrate:D-ribose; c: Substrate:D-allose; d:Substrate:D-psicose ; e: Substrate:L-arabinose; f: Substrate:D-xylose.

Table S1 Binding free energy analysis using the Molecular Mechanics Poisson Boltzmann (generalized Born) surface area (MM-PB(GB)/SA) method.

Energy (kcal/mol)	RpiB-wt	S9T	S98H/S134H	S9T/S98H/S134H
VDW	-16.74± 0.51	-13.35±0.51	-10.80±0.60	-7.03±0.33
EEL	-44.32± 1.86	-21.84±1.75	-53.96±3.58	-46.21±2.06
EGB	50.79±1.89	37.57±1.25	58.51±2.56	55.34±1.93
ESURF	-3.46±0.041	-2.72±0.07	-3.10±0.06	-1.91±0.03
Ggas	-61.06±1.74	-35.19±1.44	-64.77±3.37	-53.24±1.99
Gsolv	47.33± 1.88	34.85±1.21	55.40±2.51	53.43±1.92
EtotGB	-13.73±1.08	-0.34±0.31	-9.36±1.27	0.18±0.43
EPB	63.47±1.45	46.02±2.35	63.86±2.61	55.04±2.21
ENPOLAR	-15.68±0.20	-12.59±0.30	-14.05±0.34	-9.28±0.20
EDISPER	25.74± 0.09	23.30±0.28	22.91±0.27	15.12±0.27
GsolvPB	73.53±1.57	56.7323±2.30	72.71±2.43	60.88±2.26
EtotPB	12.46± 1.49	21.53±1.81	7.94±1.64	7.63±0.90