

Catalytic Mechanism of Acetolactate Decarboxylase from *Brevibacillus brevis* Towards both Enantiomers of α -acetolactate

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Table S1. Key distances in the five optimized geometries. Distances are given in angstroms.

	R _A	TS1 _A	IM1 _A	TS2 _A	P _A
d _{Zn-N194}	2.11	2.14	2.14	2.13	2.09
d _{Zn-N196}	2.11	2.11	2.15	2.13	2.12
d _{Zn-N207}	2.25	2.17	2.12	2.12	2.10
d _{Zn-OA1}	2.06	2.75	3.56	5.44	5.33
d _{Zn-OA2}	2.21	2.22	2.28	2.22	2.18
d _{Zn-OA3}	2.39	1.98	1.92	2.03	2.14
d _{CA2-CA3}	1.52	1.40	1.37	1.43	1.52

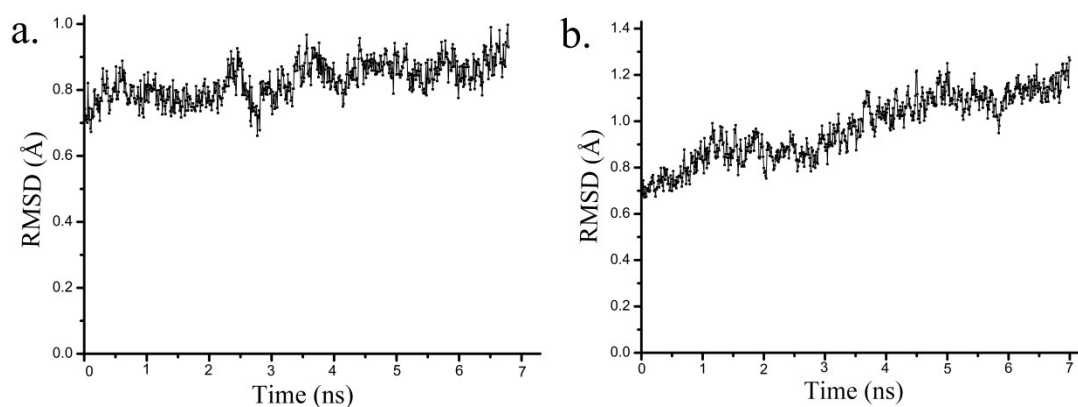
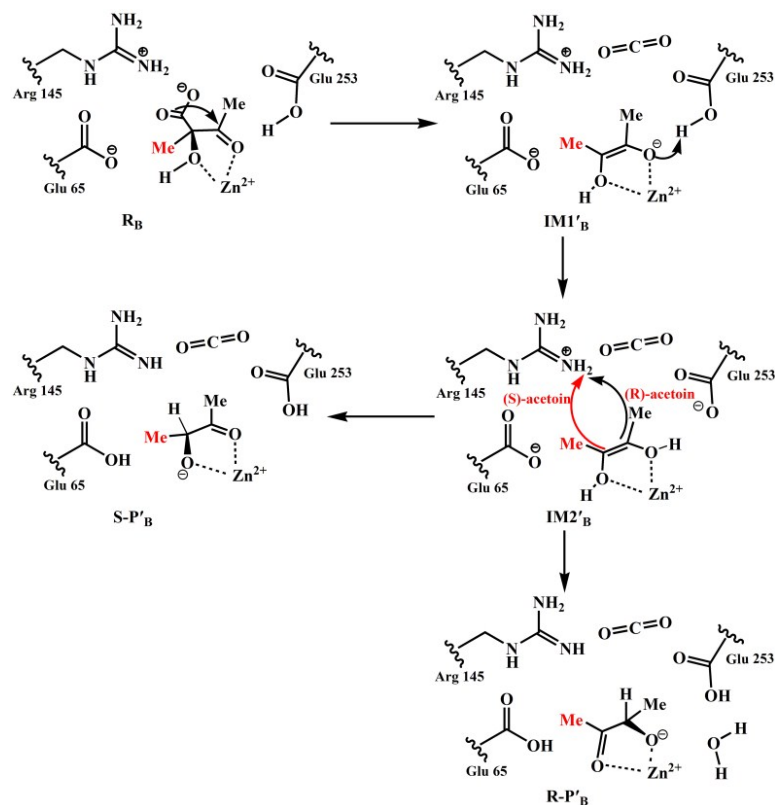


Figure S1. Time dependences of RMSDs from 7ns MD simulations for Michaelis complexes of ALDC-(S)-AL (a) and ALDC-(R)-AL (b).



Scheme S1. Possible pathways of the conversion of (R)- α -acetolactate to (R)-acetoin catalyzed by ALDC, in which the (R)-AL firstly undergoes direct decarboxylation rather than carboxylate migration.

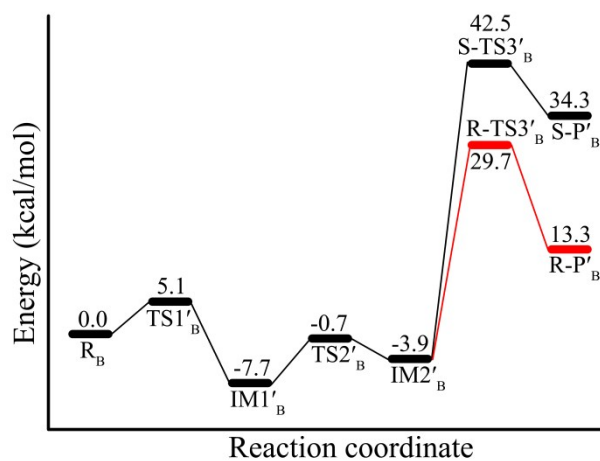


Figure S2. Energy profile for the pathways of the conversion of (R)- α -acetolactate to (R)-acetoin, in which the (R)-AL firstly undergoes direct decarboxylation rather than carboxylate migration. The energy data have included the dispersion corrections.

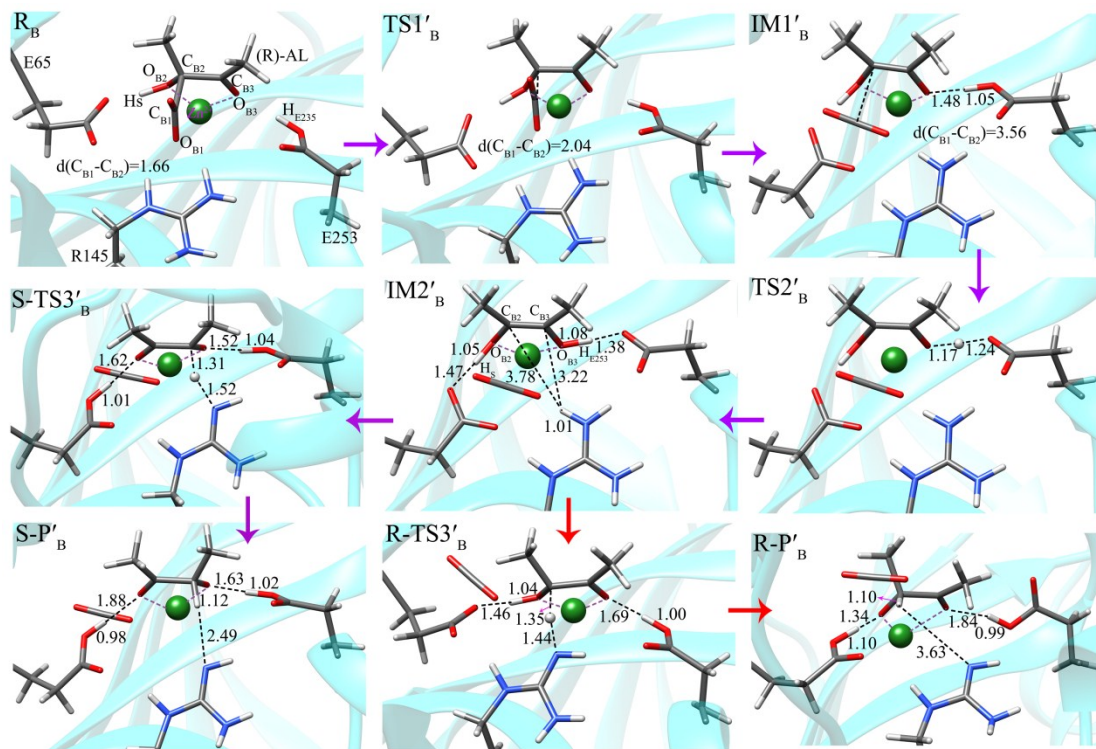


Figure S3. Optimized structures involved in the pathways of the conversion of (R)- α -acetolactate to (R)-acetoin, in which the (R)-AL firstly undergoes direct decarboxylation rather than carboxylate migration. All distance are given in angstroms.