

Molecular Dynamic Simulation of space-grown and earth-grown crystal structures of thermostable T1 lipase *Geobacillus zalihae* revealed a better structure.

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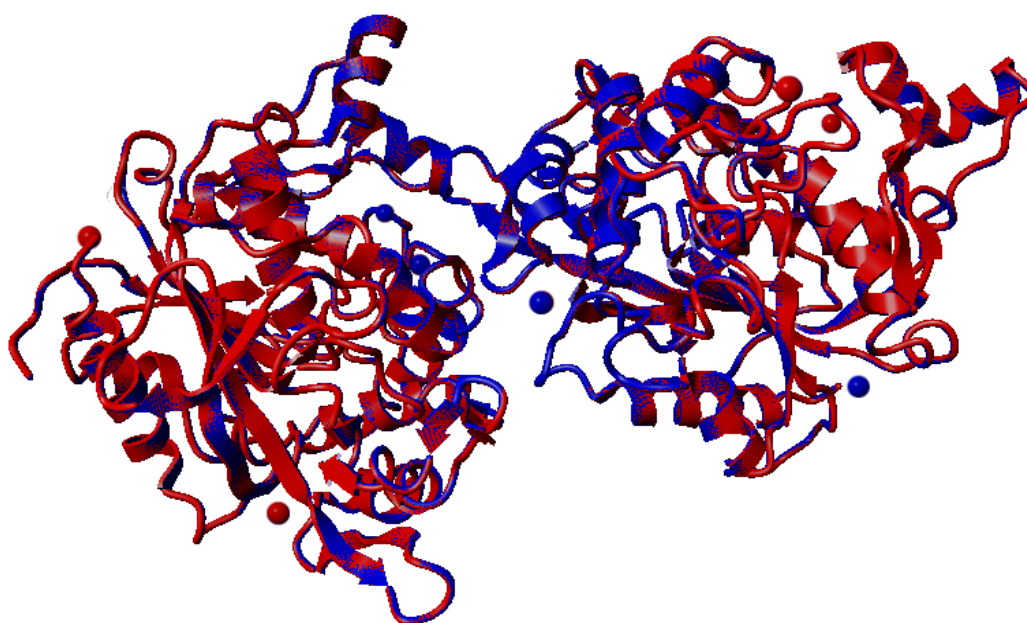


Figure S1. Superimposed of space-grown (blue) and ground-grown (red) T1 lipase crystal structures.

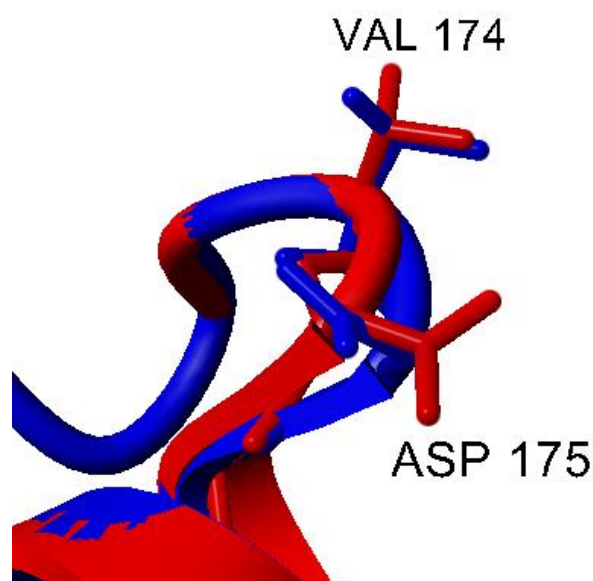


Figure S2. Superimposed of space-grown (blue) and ground-grown (red) of T1 lipase structure showed a region with different conformation at residue Asp175.

Table S1. Total number of hydrogen bond of T1 lipase space-grown and earth-grown crystal structures.

Number of hydrogen bonds better than 6025 kJ/mol	
Space-grown	1834
Earth-grown	1800

Table S2. Different location of hydrogen bond in T1 lipase space-grown crystal compared to earth-grown crystal structures.

Earth-grown structure	Space-grown structure
O Leu 208 < N Trp 211	ND2 Asn 42 > O Thr 48
N Asn 321 > OD1 Asn 321	O Glu 250 < N Gln 254
OD1 Asn 367 < N Ser 369	O Thr 342 < NZ Lys 344
	OD1 Asn 304 < OG1 Thr 306
	NH1 Arg 34 > O Phe 370
	NE2 39 Gln > OD1 Asp 43
	OD1 Asn 59 < OG1 Thr 118
	O Glu 226 < NH1 Arg 230

Hydrogen bond which are same in both structures are not shown. The symbols of > represent 'donated to' while < represent 'accepted from'.

Table S3. Average number of hydrogen bond between given residues in ground-grown and space-grown structures throughout 20ns of simulation.

Residues	Ground-grown structure	Space-grown structure
Glu250 and Gln254	0.16	0.60
Asn304 and Thr306	0.03	0.18
Gln39 and Asp43	0.59	0.88
Asn59 and Thr118	0.43	0.66