

Supplementary Material

Molecular Characterization of a Thermostable L-Aparaginase from *Geobacillus* Strain SBS-4S

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Protein sequence

MTKRKVVLTTGGTIASKRNERSGRLRA-
GALSGEELAAMCHLPKEIEIIVESVFQLPS-
MH LTFSHWLELKKRIEAHFTDPSVDGIVVTH-
GTDAL EETAYFLDLTIDDPRTIVVTGSQRAP
SDLGSDVYINIRHAIYAACAESLRGAGAVVVF-
NERIFA AKYVKKEHASNIQGFNAFGFGY LGIDN-
DEVYVYQKPIRREYYKLVRPLPPVDIVKCYLEADG-
KFIKAARESGVAGIVLEGV
GRGQVAPKVMVDEIVKAI EAGIKVVVTTSAEEG-
AVYTTYDYPGSAYDLHKKGVILGSDYDA KKA-
RIKLAVALAADA AAVDGLFAY

Supplementary Fig. 1. Amino acid sequence of L-asparaginase

Supplementary Table I. Docking energies of L-asparagine with geoAsnase enzyme.

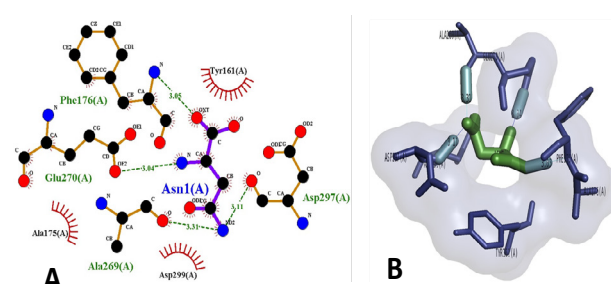
Vina score	Cavity size	Center			Size		
		X	Y	Z	X	Y	Z
-5	642	4	-5	8	16	16	25
-4.7	709	1	7	10	23	16	16
-4.1	131	8	-3	-6	16	16	16
-3.7	250	17	3	15	24	16	16
-3.6	218	6	17	-5	16	16	16

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0030-9923/2026/0001-0415 \$ 9.00/0

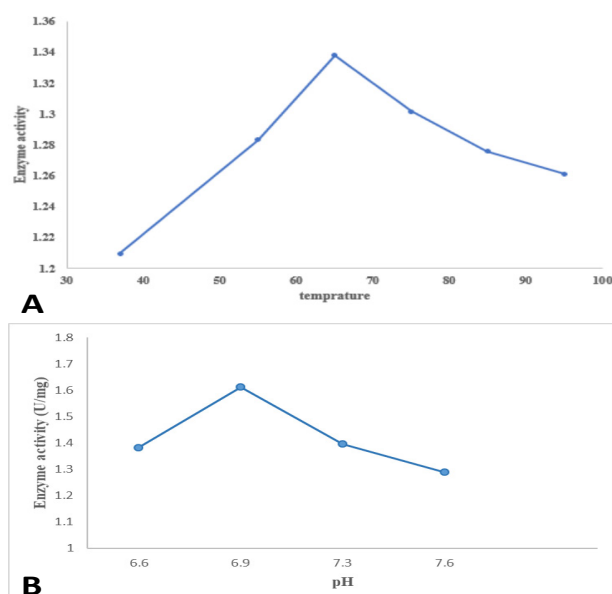


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Supplementary Fig. 2. Structure-based docking of geoAsnase with substrate D-asparagine. (A) 2D image and (B) 3D image of the docking complex showing Asn1 in the center forming hydrogen bonds with Phe176, Ala269, Glu270 and Asp297 residues of the enzyme. Hydrophobic interactions indicated by (Tyr161, Ala175 and Asp299) in the periphery (A) are involved in stabilizing the complex.



Supplementary Fig. 3. Effect of temperature (A) and pH (B) on geoAsnase on enzyme activity.