Tables

An effective computational-screening strategy for simultaneously improving both catalytic activity and thermostability of α-L-rhamnosidase

Table 1

Sequence analysis of r-Rha1 with six different sources α-L-rhamnosidases

Sources	Region 1	Region 2	Region 3	Sequences
Aspergillus niger	299YDTVSFTY	355ASADWLR	525DGSLVYA	AGN92963.1
Bacillus sp. GL1	621AWSSVIPN	677AIWNLLD	845NFAENRS	2OKX_A[a]
Aspergillus tubingensis	509GQSAVYVD	576NIGAFFS	749GTTWEYL	ANZ93894.1
Thermomicrobia bacterium	308PPQASFTY	365AYNDWLR	534NTGELHY	AAR96047.1
Alternaria sp. L1	624GWSSVIPN	680NSIKTAA	847GALGARY	AFA41506.1
Streptomyces avermitilis	687NLGNGVAG	743GYGDWLN	898DSIQPDG	3W5M_A[a]
Bacteroides thetaiotaomicron	687NLGNGVAG	435GYWVFVD	600NPEESGT	3CIH_A[a]

Note: Residues on grey background are conservative residues

Table 2

The kinetic analysis of r-Rha1 and its mutants.

Sample	K_m (mM)	V_{max} (μmol·mL^{-1}·min^{-1})	k_{cat} (min^{-1})	k_{cat}/K_m (min^{-1}·mM)
WT	12.90	188.68	12.62×10^4	9.78×10^3
A355N	9.29	142.86	9.53×10^4	10.26×10^3
S356Y	7.34	117.65	7.84×10^4	10.68×10^3
D525N	5.03	113.64	7.57×10^4	15.05×10^3

Table 3.

Binding free energies of wild type r-Rha1 (WT) and mutants A355N, S356Y, D525N with *p*NPR based on MM-PBSA analysis.

Components	The free energy (kJ/mol)			
	WT	A355N	S356Y	D525N
Electrostatic energy	-13.24	-19.00	-4.74	-20.05
Van der Waal energy	-139.94	-142.52	-172.54	-177.78
Polar solvation energy	76.26	80.25	84.01	100.78
Non polar solvation energy	-15.08	-15.20	-16.74	-16.40
Binding energy (Sum)	-92.00	-96.47	-110.01	-113.45