

Supplementary material

Semi-rational design of diaminopimelate dehydrogenase from *Symbiobacterium thermophilum* improved its activity toward hydroxypyruvate for D-serine synthesis

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Table S1 Primers used in this study

152G-F	TTACACAAACTTTGGCCCCGGCATGGGCATGGGC
152A-F	TTACACAAACTTTGGCCCCGGCATGGCCATGGGC
152V-F	TTACACAAACTTTGGCCCCGGCATGGTCATGGGC
152L-F	TTACACAAACTTTGGCCCCGGCATGTTAATGGGC
152I-F	TTACACAAACTTTGGCCCCGGCATGATCATGGGC
152W-F	TTACACAAACTTTGGCCCCGGCATGTGGATGGGC
152F-F	TTACACAAACTTTGGCCCCGGCATGTTTCATGGGC
152P-F	TTACACAAACTTTGGCCCCGGCATGCCCATGGGC
152S-F	TTACACAAACTTTGGCCCCGGCATGAGCATGGGC
152T-F	TTACACAAACTTTGGCCCCGGCATGACCATGGGC
152C-F	TTACACAAACTTTGGCCCCGGCATGTGCATGGGC
152Y-F	TTACACAAACTTTGGCCCCGGCATGTACATGGGC
152N-F	TTACACAAACTTTGGCCCCGGCATGAACATGGGC
152Q-F	TTACACAAACTTTGGCCCCGGCATGCAAATGGGC
152D-F	TTACACAAACTTTGGCCCCGGCATGGACATGGGC
152E-F	TTACACAAACTTTGGCCCCGGCATGGAAATGGGC
152K-F	TTACACAAACTTTGGCCCCGGCATGAAGATGGGC
152R-F	TTACACAAACTTTGGCCCCGGCATGAGAATGGGC
152H-F	TTACACAAACTTTGGCCCCGGCATGCACATGGGC
152-R	CGGGGCCAAAGTTTGTGTAAGTAATTCCTTGGG
92G-F	CTTTGGCCCCGGCATGTCCATGGGCGGATCAGTAG
92A-F	CTTTGGCCCCGGCATGTCCATGGGCGCATCAGTAG
92V-F	CTTTGGCCCCGGCATGTCCATGGGCGTATCAGTAG
92L-F	CTTTGGCCCCGGCATGTCCATGGGCTTATCAGTAG
92I-F	CTTTGGCCCCGGCATGTCCATGGGCATATCAGTAG
92M-F	CTTTGGCCCCGGCATGTCCATGGGCATGTCAGTAG
92W-F	CTTTGGCCCCGGCATGTCCATGGGCTGGTCAGTAG
92F-F	CTTTGGCCCCGGCATGTCCATGGGCTTCTCAGTAG
92P-F	CTTTGGCCCCGGCATGTCCATGGGCCCCCTCAGTAG
92S-F	CTTTGGCCCCGGCATGTCCATGGGCTCCTCAGTAG
92T-F	CTTTGGCCCCGGCATGTCCATGGGCACCTCAGTAG
92C-F	CTTTGGCCCCGGCATGTCCATGGGCTGCTCAGTAG
92Y-F	CTTTGGCCCCGGCATGTCCATGGGCTACTCAGTAG
92N-F	CTTTGGCCCCGGCATGTCCATGGGCAACTCAGTAG
92Q-F	CTTTGGCCCCGGCATGTCCATGGGCCAATCAGTAG
92E-F	CTTTGGCCCCGGCATGTCCATGGGCGAATCAGTAG
92K-F	CTTTGGCCCCGGCATGTCCATGGGCAAGTCAGTAG
92R-F	CTTTGGCCCCGGCATGTCCATGGGCCGCTCAGTAG
92H-F	CTTTGGCCCCGGCATGTCCATGGGCCACTCAGTAG
92-R	TGGACATGCCGGGGCCAAAGTTTGTGTAAG
253G-F	TGCCCAATGCATACCTTTGGGATCGGGACTAGGCC
253A-F	TGCCCAATGCATACCTTTGGGATCGGCCCTAGGCC

253V-F	TGCCCAATGCATACCTTTGGGATCGGTCCCTAGGCC
253L-F	TGCCCAATGCATACCTTTGGGATCGTTACTAGGCC
253I-F	TGCCCAATGCATACCTTTGGGATCGATCCTAGGCC
253M-F	TGCCCAATGCATACCTTTGGGATCGATGCTAGGCC
253W-F	TGCCCAATGCATACCTTTGGGATCGTGGCTAGGCC
253F-F	TGCCCAATGCATACCTTTGGGATCGTTCCTAGGCC
253P-F	TGCCCAATGCATACCTTTGGGATCGCCCCTAGGCC
253S-F	TGCCCAATGCATACCTTTGGGATCGAGCCTAGGCC
253T-F	TGCCCAATGCATACCTTTGGGATCGACCCTAGGCC
253C-F	TGCCCAATGCATACCTTTGGGATCGTGCCTAGGCC
253Y-F	TGCCCAATGCATACCTTTGGGATCGTCCCTAGGCC
253Q-F	TGCCCAATGCATACCTTTGGGATCGCAACTAGGCC
253D-F	TGCCCAATGCATACCTTTGGGATCGGCACTAGGCC
253E-F	TGCCCAATGCATACCTTTGGGATCGGAACTAGGCC
253K-F	TGCCCAATGCATACCTTTGGGATCGAAGCTAGGCC
253R-F	TGCCCAATGCATACCTTTGGGATCGGAGCTAGGCC
253H-F	TGCCCAATGCATACCTTTGGGATCGCACCTAGGCC
253-R	G TTCAGCCCCGATTATCATTCGCGTACCCG
122G-F	GCTTAGACAAACGTTGCCAGCTAAGGATAACGGC
122A-F	GCTTAGACAAACGTTGCCAGCTAAGCCTAACGGC
122V-F	GCTTAGACAAACGTTGCCAGCTAAGTCTAACGGC
122L-F	GCTTAGACAAACGTTGCCAGCTAATTATAACGGC
122I-F	GCTTAGACAAACGTTGCCAGCTAAATCTAACGGC
122M-F	GCTTAGACAAACGTTGCCAGCTAAATGTAACGGC
122W-F	GCTTAGACAAACGTTGCCAGCTAATGGTAACGGC
122F-F	GCTTAGACAAACGTTGCCAGCTAATTCTAACGGC
122P-F	GCTTAGACAAACGTTGCCAGCTAACCCTAACGGC
122S-F	GCTTAGACAAACGTTGCCAGCTAAAGCTAACGGC
122T-F	GCTTAGACAAACGTTGCCAGCTAAACCTAACGGC
122C-F	GCTTAGACAAACGTTGCCAGCTAATGCTAACGGC
122Y-F	GCTTAGACAAACGTTGCCAGCTAATCCTAACGGC
122N-F	GCTTAGACAAACGTTGCCAGCTAAAACTAACGGC
122Q-F	GCTTAGACAAACGTTGCCAGCTAACAATAACGGC
122E-F	GCTTAGACAAACGTTGCCAGCTAAGAATAACGGC
122K-F	GCTTAGACAAACGTTGCCAGCTAAAAGTAACGGC
122R-F	GCTTAGACAAACGTTGCCAGCTAAGAGTAACGGC
122H-F	GCTTAGACAAACGTTGCCAGCTAACACTAACGGC
122-R	CCCGCGTATTAACTACGGCGCGCGTCGGCC

Table S2 The rank of docking results of HPPA

Ligand	Rank	Dock energy
HPPA	HPPA1_1	-4.21
	HPPA1_2	-4.13
	HPPA1_3	-3.99
	HPPA1_4	-3.92
	HPPA1_5	-3.84
	HPPA1_6	-3.76
	HPPA1_7	-3.71
	HPPA1_8	-3.68

Table S3 The retention times of the substances analyzed by high-performance liquid chromatography (HPLC)

Substance	Retention time (min)
D-Ser	14.322
L-Ser	13.780
HPPA	15.873

Table S4 Hydrogen bond occupancy

Donor	Acceptor	Hydrogen bond occupancy
M152S	HPPA	87.3%
HPPA	M152S	92.1%
D92E	HPPA	89.4%
152M	HPPA	79.8%