

Simultaneous improvement of the thermostability and catalytic activity of epoxidase Lsd18 for the synthesis of Lasalocid A

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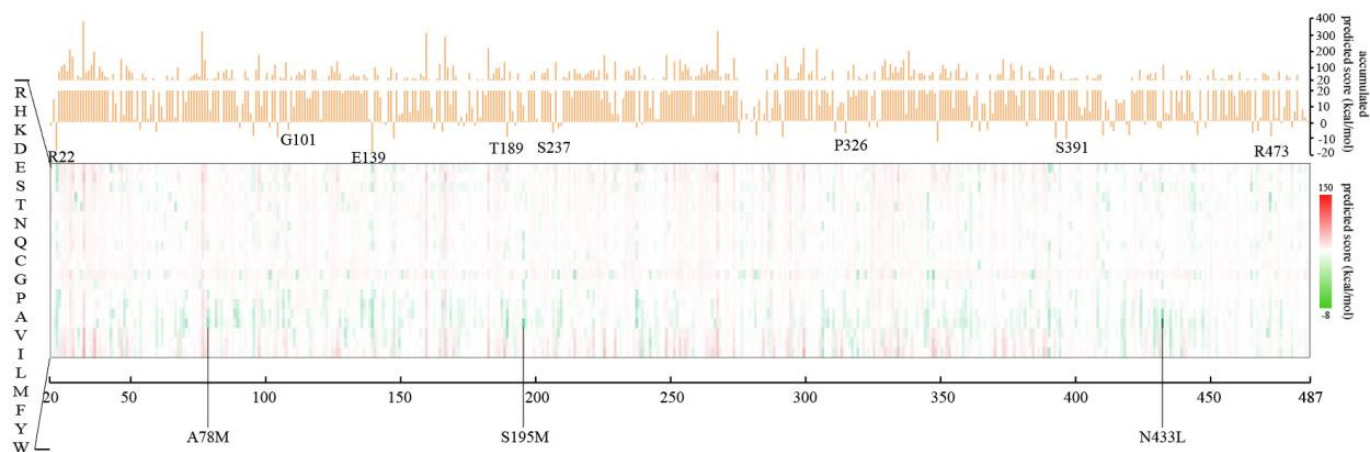


Figure S1. FoldX evaluates all possible mutation sites of Lsd18.

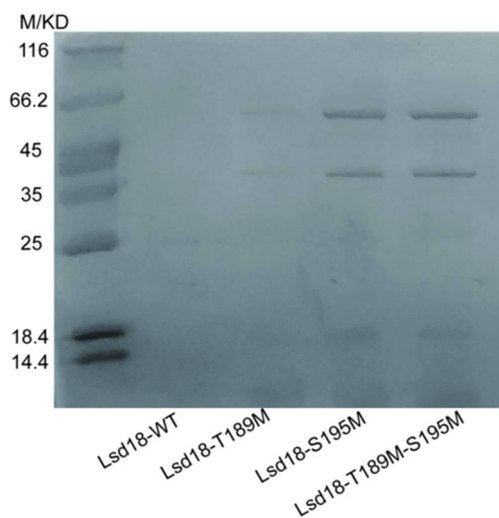


Figure S2. SDS-PAGE of the limited proteolysis of Lsd18 with trypsin.

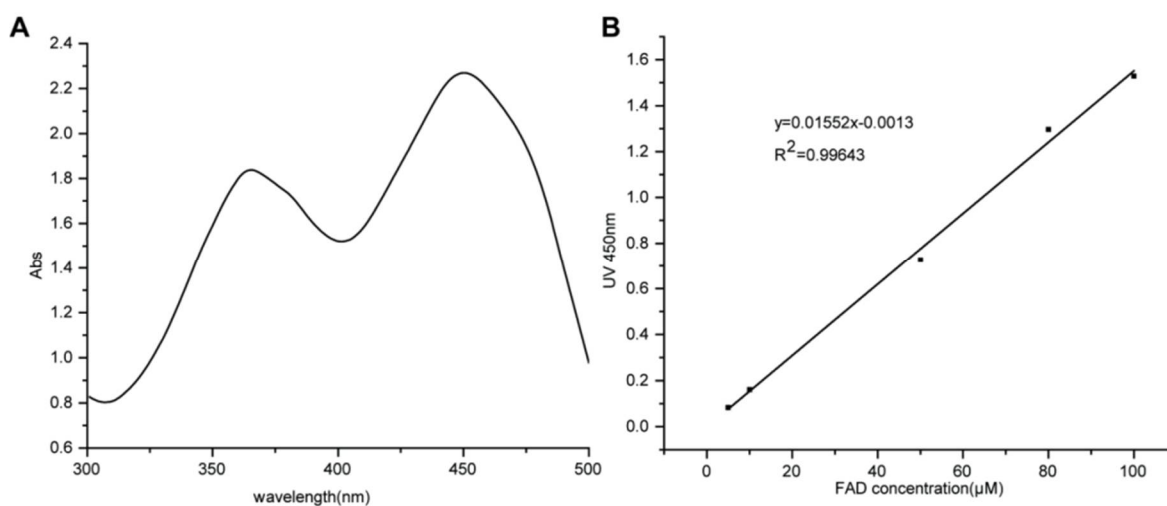


Figure S3. Standard FAD fluorescence spectrum (A) and standard curve of the UV absorbance and the concentration of FAD (B).

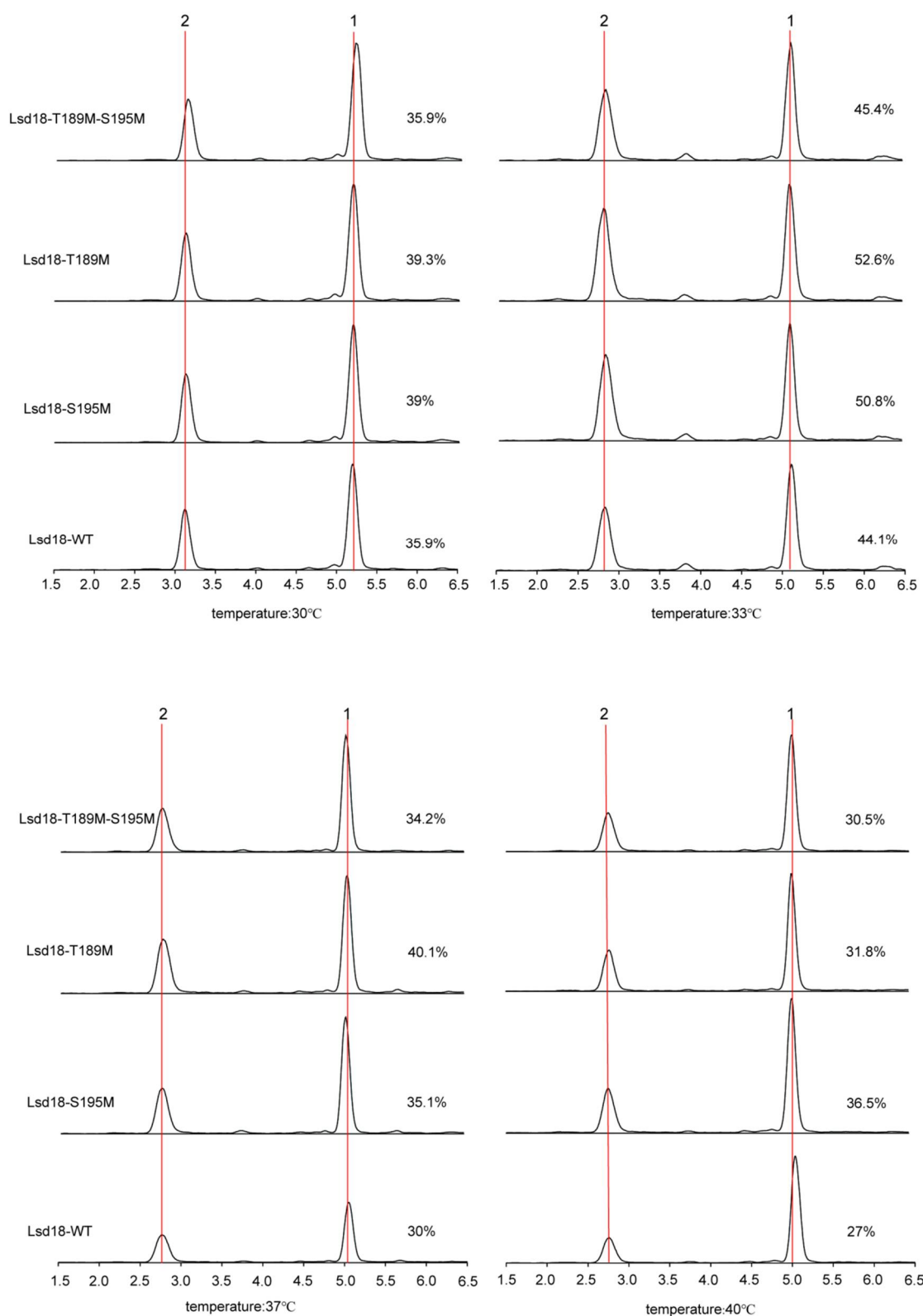


Figure S4. LC-MS detection of the enzymatic activity of wild-type Lsd18 and the mutants at different temperatures.

Table S1. Semi-rational design mutants of Lsd18

Mutant	$\Delta\Delta G$ (kcal/mol)
R51W	-0.69
D52S	-0.40
V64D	-1.12
S108V	-1.79
S237V	-2.31
H239L	-1.14

Table S2. Data collection and refinement statistics

	Lsd18-S195M	Lsd18-T189M-S195M
PDB	8WVB	8WVF
Data collection		
Space group	P 1 21 1	P 1 21 1
Cell dimensions		
<i>a</i> , <i>b</i> , <i>c</i> (Å)	62.041, 48.671, 136.049	63.005, 48.116, 135.569
(°)	90, 91.337, 90	90, 91.559, 90
Resolution (Å)	29.46 - 2.5 (2.589 - 2.5)	19.9- 3.764 (3.897 - 3.764)
<i>R</i> _{merge}	0.370 (0.994)	0.268 (0.389)
<i>I</i> / <i>I</i>	3.9 (2.6)	3.7 (2.2)
Completeness (%)	99.03 (98.52)	87.95 (83.62)
Redundancy	6.7 (6.8)	1.0 (1.0)
Refinement		
Resolution (Å)	2.5	3.764
No. reflections	190400	7506
<i>R</i> _{work} / <i>R</i> _{free}	0.1955/0.2538	0.2323 /0.3194
No. atoms	7084	6623
Protein	930	936
Ligand/ion	108	106
Solvent	186	0
<i>B</i> -factors	22.42	33.26
Protein	22.54	33.26
Ligand/ion	16.94	33.27
Solvent	21.17	1
R.m.s. deviations		
Bond lengths (Å)	0.003	0.002
Bond angles (°)	0.57	0.58