Structure-based redesign of the bacterial prolidase active-site pocket for efficient enhancement of methyl-parathion hydrolysis

(Supplementary information)

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Table S1 X-ray data collection and refinement statistics

Parameters	*Pl*OPAA[3R]
PDB ID	7E5C
Data collection	
Beamline	SSRF-BL17U1
Space group	H32
Cell dimensions	
a, b, c, Å	182.9, 182.9, 372.0
Wavelength, Å	0.97918
Resolution, Å[a]	67.36-2.22 (2.29-2.22)
Total reflections	2,239,248
Unique reflections	111,133 (3,942)
Redundancy	20.1 (18.4)
R_{sym} [a,b]	0.134 (0.079)
R_{pim}	0.030 (0.018)
Mean (I/σ)	15.9 (34.3)
CC (1/2)	0.998 (0.998)
Completeness, %	93.9 (99.6)
Refinement	
R_{work}/R_{free}[c]	0.217/0.240
No. of protein atoms	14,271
No. of ligand atoms	8
No. of water atoms	360
Average B factor, Å^2	36.8
RMS bond lengths, Å	0.014
RMS bond angles, °	1.49
Ramachandran distribution	
Favored, %	99.08
Allowed, %	0.92
Outliers, %	0

[a] Numbers in parentheses are values for the highest-resolution shell.

[b] $R_{sym} = \sum_{hkl}\sum_{i}|I_i - \langle I \rangle| / \sum_{hkl}\sum_{i}|\langle I \rangle|$, where I_i is the intensity for the ith measurement of an equivalent reflection with indices h, k, and l.

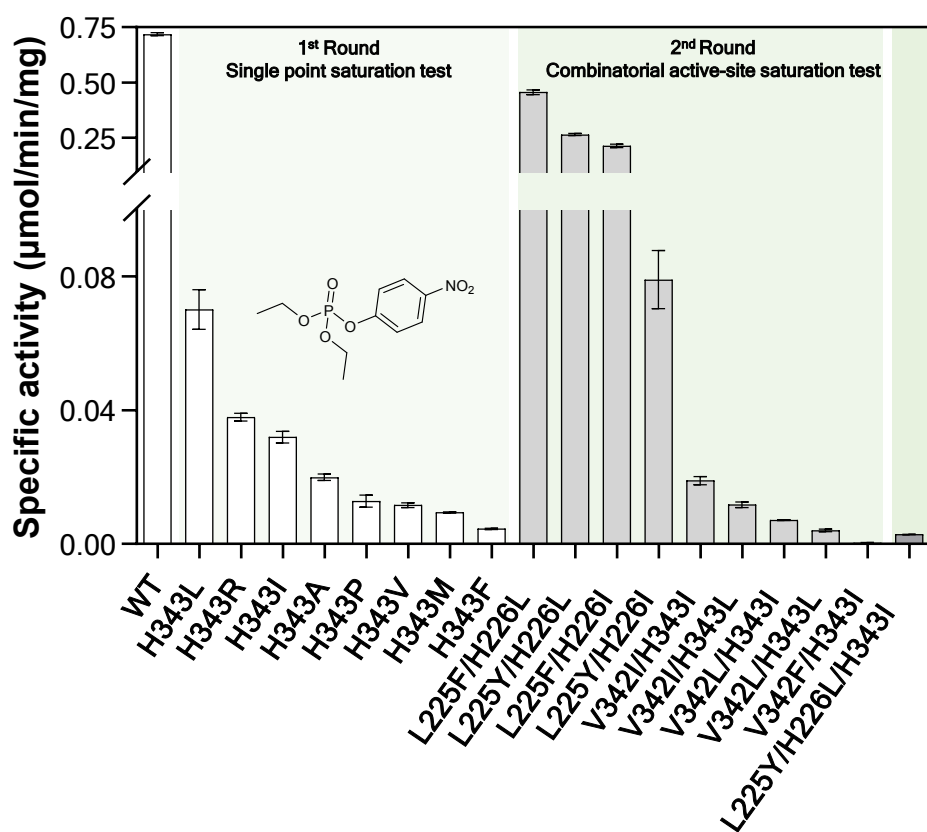[c] R_{free} was calculated with 5% of the reflections set aside randomly throughout the refinement.

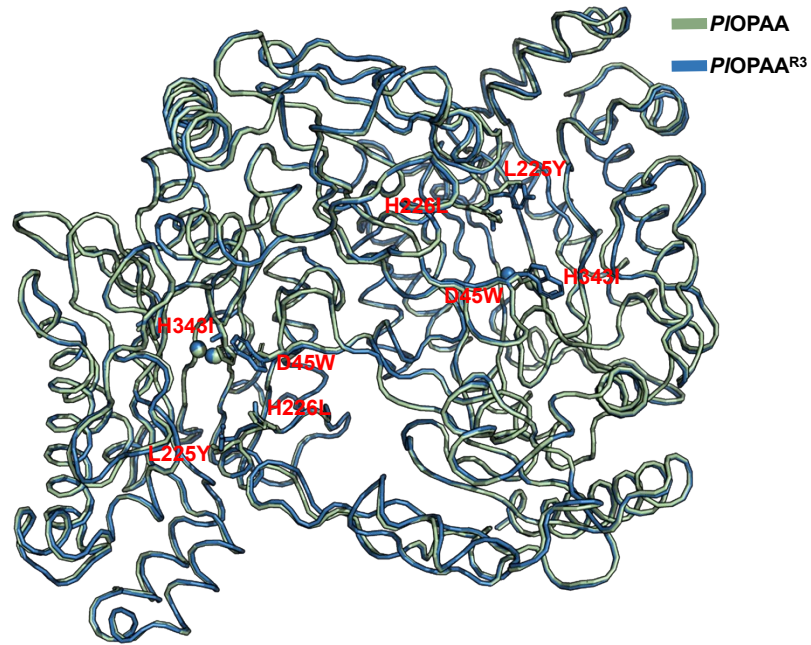**Figure S1** Catalytic activities of the wild-type enzyme and its variants on paraoxon.

Figure S2 Structural superposition of *Pl*OPAA (PDB entry 6AH8) and *Pl*OPAA[3R] (PDB entry 7E5C). Cα atoms

of *Pl*OPAA[3R] and wild-type superpose with an rmsd of 0.22 Å. The four mutations are indicated (green sticks,

wild-type *Pl*OPAA residues; blue sticks, *Pl*OPAA[3R] residues).