

Supplementary materials

A Novel Organophosphorus Acid Anhydrolase from Deep Sea Sediment with High Degradation Efficiency for Organophosphorus Pesticides and Nerve Agent

Nucleotide sequence

ATGGAAGCTAACATAACTATTCTGCACATATTGCAGAACTTCAAC-GCAGAACTAAAAAAGCCTTAGCACGAGAAAATTAGATGCTT-GGTGATCCACTCAGGCAAAGAAATTAAAGTTTTTAGACGAC-TATAGTTACCTTCAAAGTTAACCTCATTTAAAGCTGGTGCCTAAC-CGATGTTGCTAACTGTTGGCTATTGTAATGGCGAAGATAAACCTACAC-TTATTATTACCAACCTATTGATTTGGCATAAAGTAATTGAATTAAACAGA-CAGTTACTGGCAAGAGTTTTGATATTAAAATATTAAGTT-GCCAGCGAAGTGGATAAGCTTTACCTTATGATAAAAAAGGTTATGCC-TACATAGGTGAGCATATTGAAGTTGCTAACGCTTAGGATTGAAGCAA-TAAATCCAGAGCCTTAATGAATTA-TATGCATTATCATCGAGCTTATAAAACAGCTTATGAATT-TGATTGTATGCGAAAATCTAACGCGTTAGCGGTAAAGGCTCATCAAGCGG-CACAACAAGCTTTAGCGGGTGAAGCTGAATTGCTATTCAACAA-GCTTATTAAAGGCTATCGCTTATTCAAGAAAATGATACACCTATGGCAA-TATTGTTGCGCTTAATGAAAATGCAGCAATATTACATTACACCCTAGTTGCG-GAACAAACCTCAAGAACCGACGGTCATTAAATT-GATGCGGGCGCTAATTAAATGGTTATGCTGCTGACATTACACGCAC-TTATGCTTTAAACAAAATAATTGCAAGATTAAATTGCTCGTATGGATCAG-TTAATGCTTAAAGCTGTTGATGGCTTAAAGCCAATAAAAGCTATGTAGAT-TTACATATTGAAACTTATGCGGAAATAGGAAGGTTAAAAGAATTGAT-TTATTAAATGTTGAAGCAGACACGGCAGTGGAAACAGGGAT-TATTCAACATTTCGGCATGGTTAGGG-CATCATTTAGGTTACAAACCCATGATGTTGGCTTATGGCGATGAAC-GAGGCACACATATTAATGCACCTAAAATCATCCTTTAA-GAACTTCTCGAGTTATTGAAGCTAATCAAGTATTACTATTGAACCGGGCTT-GTATTATCGATTCACTACTTAAAGAGCTGAAACAGTCAAA-TATGCACAAATGGTAAATTGG-CAAAAAGTAGATGAAATGCGTCCTTATGGGGCATTGCTATAGAAGATAA-TATTATTGTTCATAAAATCATAATGAAAATATGACACGCGAAGCAGGAT-TAAATTAA

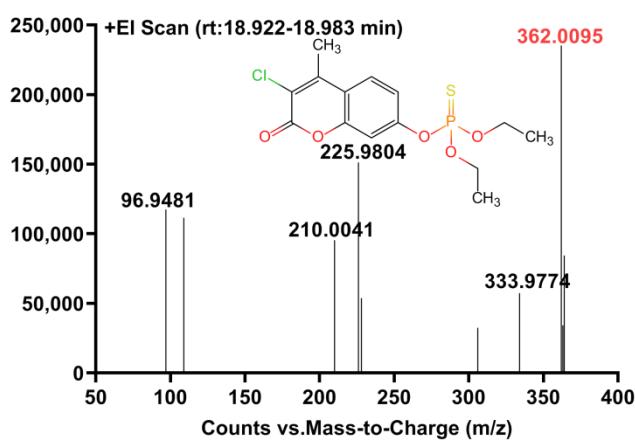
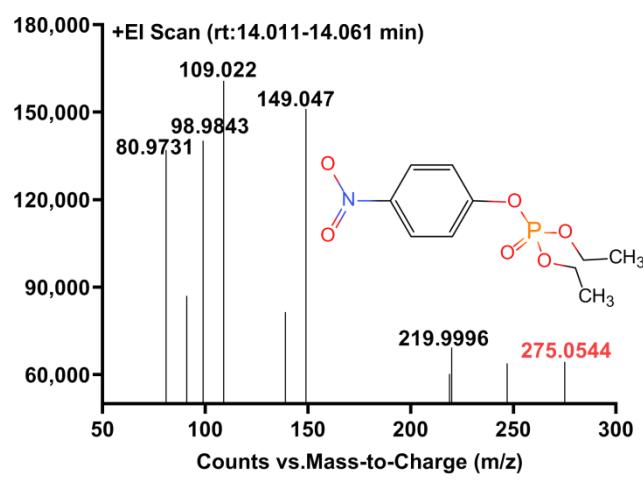
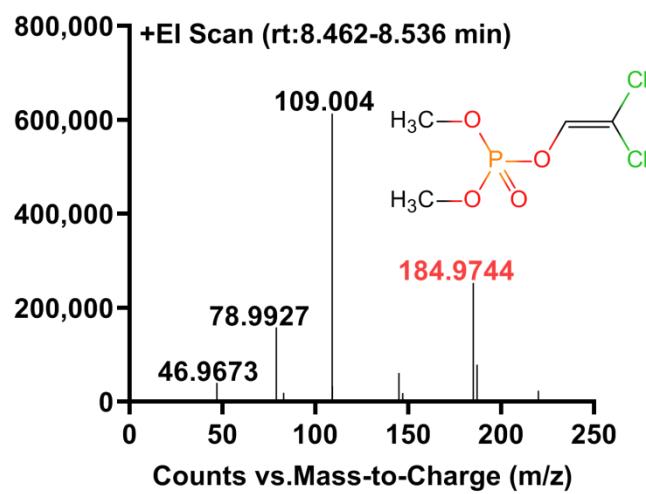
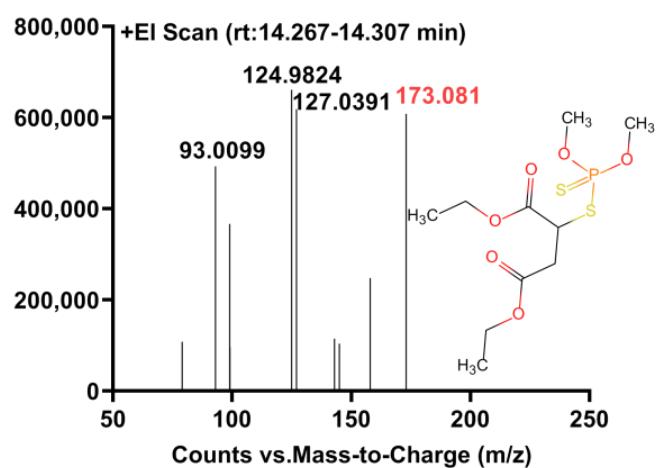
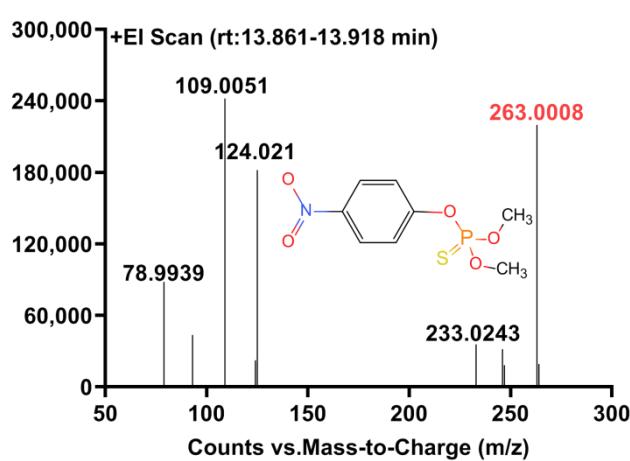
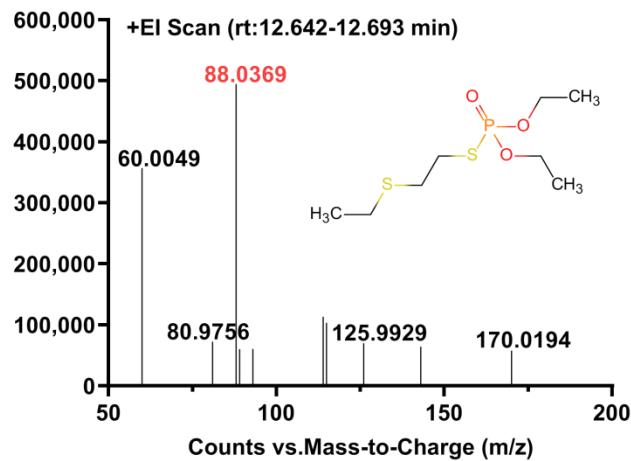
Amino acid sequence

MEANNNYSAHIAELQRRTKKALARENLDALVIHSGKEIKVFLDDY-SYPFKVNPHFKAWLPITDVANCWLIVNGEDKPTLIYYQPIDFWHKVIELT-DSYWQEFFDIKILKVASEVDKLLPYDKKGYAYIGEHIEVAKALGFEAINPEPLM-NYMHYHRAYKTAYEFDCMRKSNALAVKAHQAAQQAFLAGESFAIQQAYLKA-IAYSENDTPYGNIVALNENAAILHYTALVRNKPQEPRSLIDAGANFNGYAADIT-RTYAFKQNKFELIARMQMLKAVDGLKPNKSYVDLHIETYAEIGKVLKEFDFIN-VEADTAVETGIISTFFPHGLGHHLGLQTHDVGGMADERGTHINAP-KNHPFLRTSRVIEANQVFTIEPGLYFIDSLLKELKQSKYAQMVNWQKVDEMRPYGGI-RIEDNIIVHKHNHNENMTREA

Table S1. Characteristics of the organophosphorus-degrading enzymes^a.

Enzyme	OPH	OpdA	MPH	OPAA	OPN 1	DFPase
Organism source	<i>Brevundimonas diminuta</i> ; <i>Flavobacterium</i> sp.	<i>Agrobacterium radiobacter</i>	<i>Pseudomonas</i> sp. WBC3; <i>Plesiomonas</i> sp. strain M6	<i>Alteromonas</i> sp. strain JD6.5	Mammalian serum	<i>Loligo vulgaris</i> squid
Structure	(α/β) ₈ -barrel fold	(α/β) ₈ -barrel fold	β-Lactamase fold	Pita bread fold	β-Propeller fold	β-Propeller fold
Molecular Weight	36 kDa	35 kDa	34 kDa	58 kDa	43 kDa	35 kDa
Metals	Zn ²⁺ , Co ²⁺ , Ni ²⁺ , Cd ²⁺ , Mn ²⁺	Fe ²⁺ , Zn ²⁺ , Co ²⁺	Co ²⁺ , Ni ²⁺ , Mn ²⁺ , Zn ²⁺ , Fe ²⁺ , Cd ²⁺	Mn ²⁺ , Co ²⁺ , Fe ²⁺ , Cd ²⁺	Ca ²⁺	Mg ²⁺ , Ba ²⁺ , Ca ²⁺
Substrate	Paraoxon, Parathion, Malathion, Chlorpyrifos, Demeton-S, Diazinon, Coumaphos, DFP, VX, VR, GA, GB, GD, GF	Paraoxon, Parathion, Diazinon, Coumaphos, GA; GB; GD	Me-thyl-parathion, Parathion, Paraoxon	Paraoxon, DFP, GD, GB, GA	Lactones, Paraoxon, GD	DFP, GD, GB, GA
Optimum pH	9.0	9.0	9.0	8.5	8.0	8.0
Optimum temperature	35 °C	40 °C	37 °C	45 °C	45 °C	30°C
PDB ID	1DPM; 1EZ2; 1HZY	2R1N	1P9E	3L7G	1V04	2GVV

^a represents the cited literature [6].



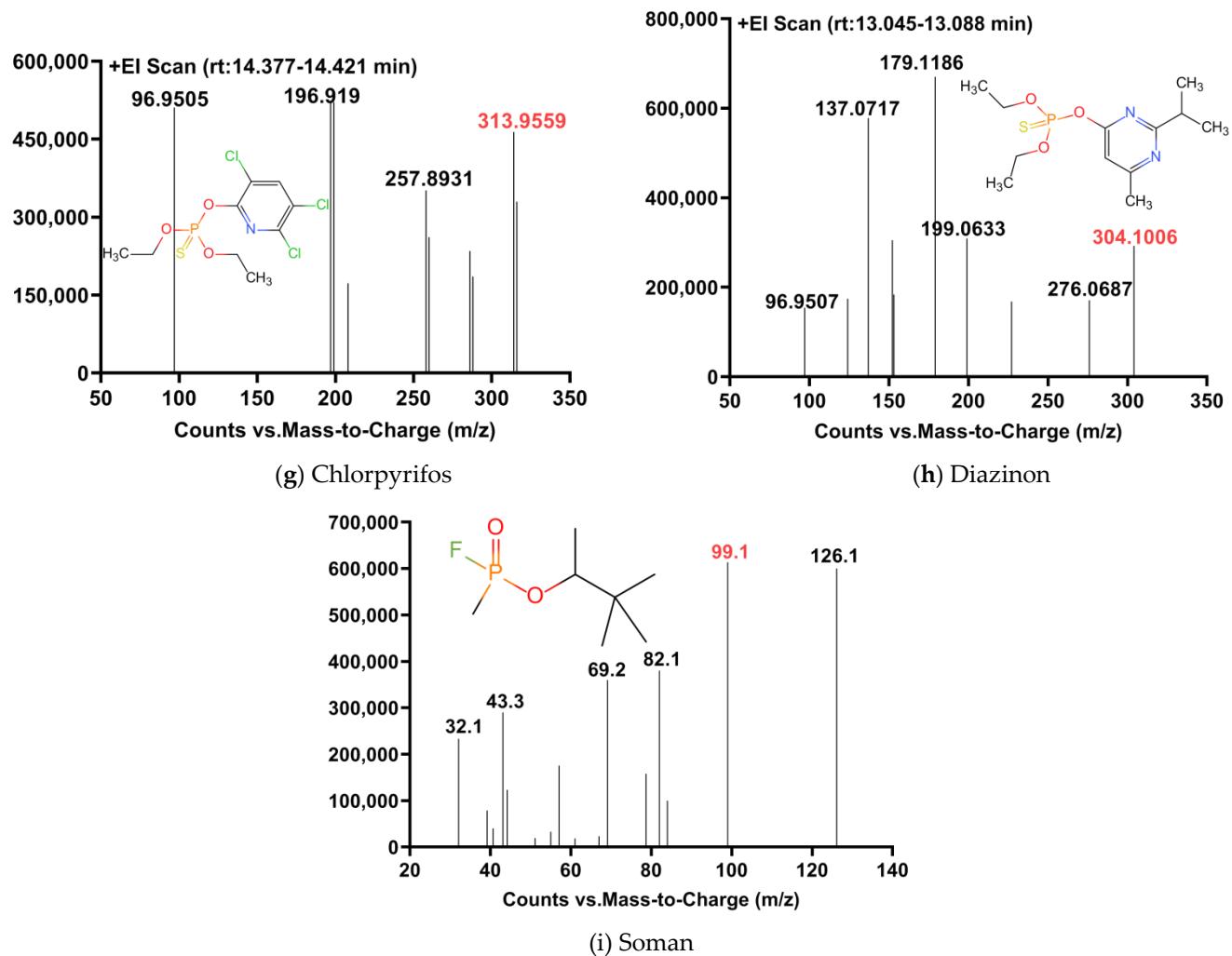


Figure S1. Chemical structures and mass spectrums of OP pesticides and nerve agent.

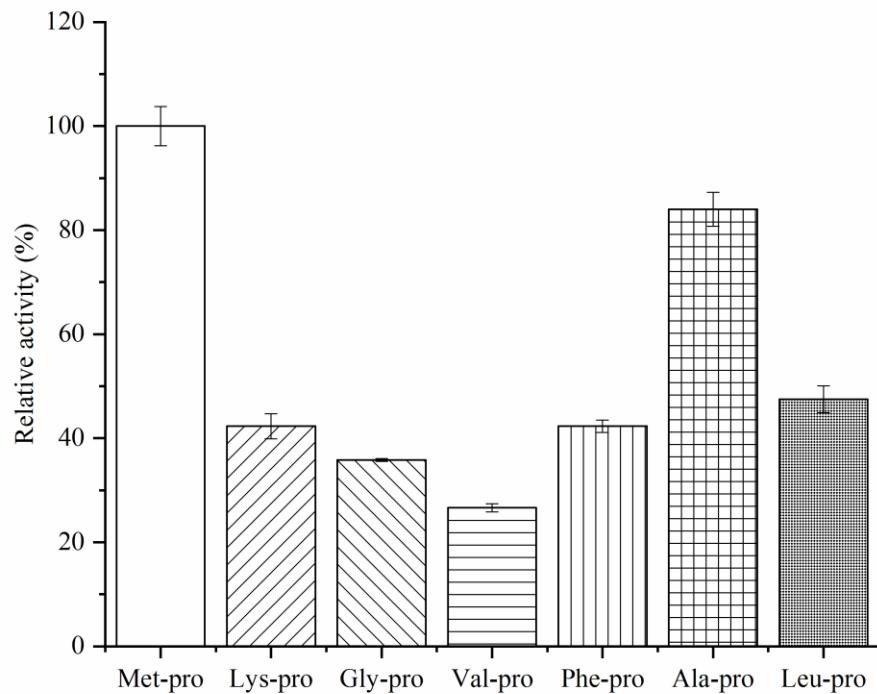


Figure S2. Activity of OPAA114644 against Xaa-Pro dipeptides. The final concentration of Xaa-Pro dipeptides was 4 mM, and the relative activity for Met-Pro was set as 100%, corresponding to specific activity of 3095 U/mg. The values were an average of three independent experiments and error bars represented standard deviation.

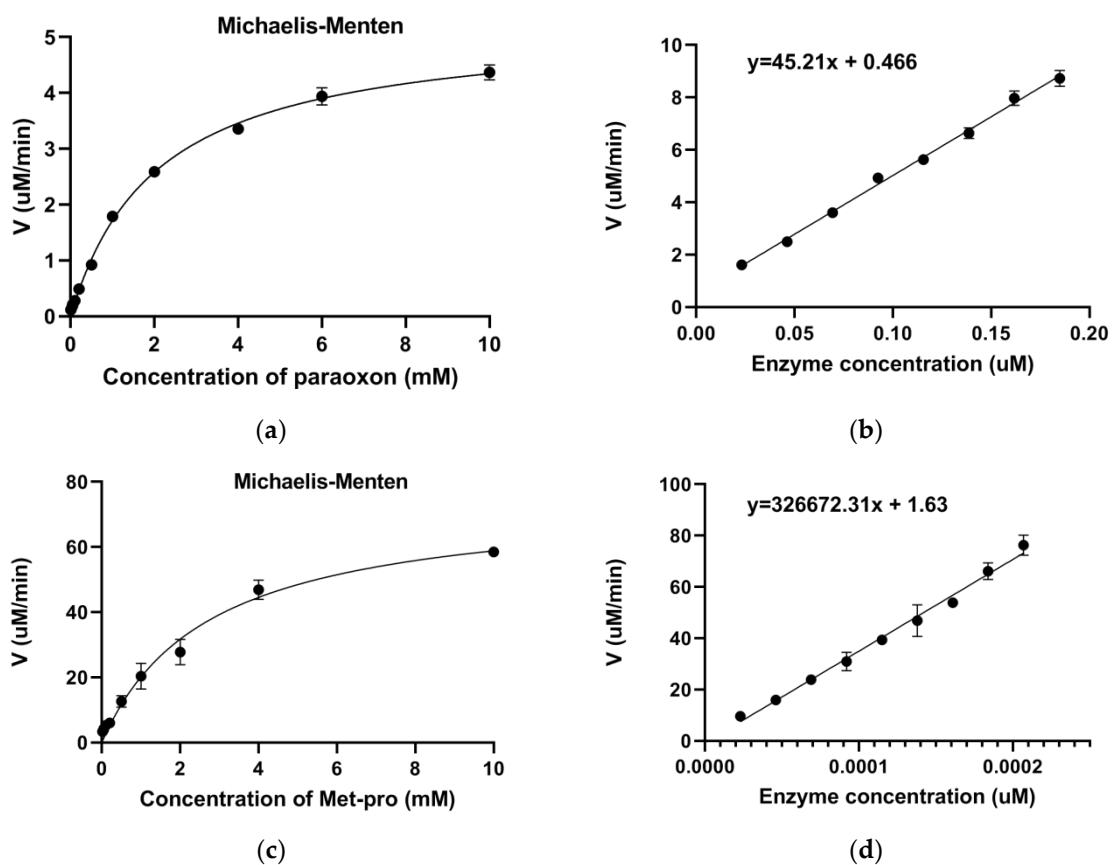


Figure S3. Kinetic analysis of OPAA114644 for paraoxon and Met-Pro. (fitted to the Michaelis-Menten kinetics). (A) Michaelis-Menten kinetics for paraoxon. (B) k_{cat} for paraoxon. (C) Michaelis-Menten kinetics for Met-Pro. (D) k_{cat} for Met-Pro.

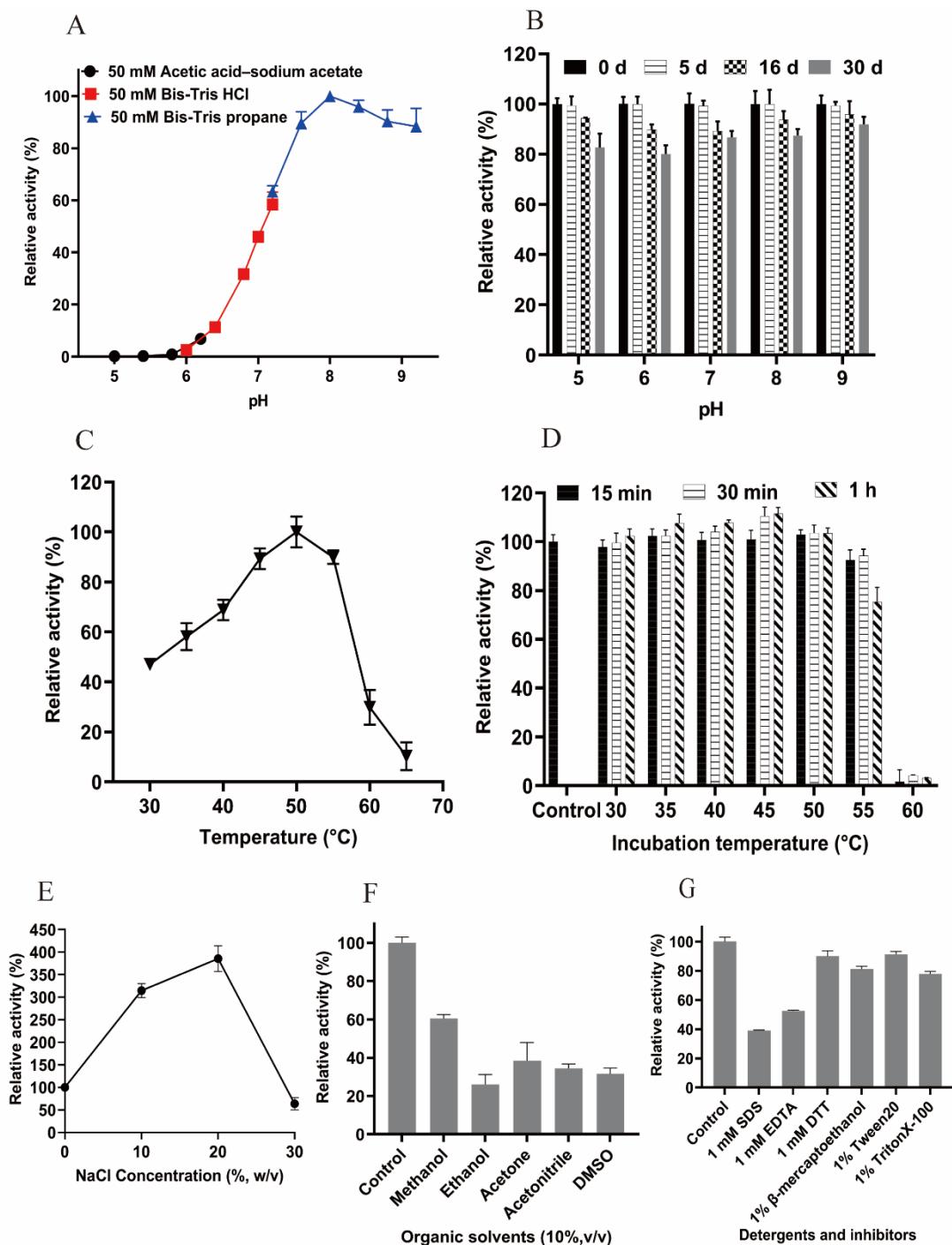


Figure S4. Biochemical characterization of OPAA114644. (A) Effects of pH on enzyme activity. (B) Effects of pH on enzyme stability. (C) Effects of temperature on enzyme activity. (D) Thermostability. (E) Effects of NaCl on enzyme activity. (F) Effects of organic solvents on enzyme activity. (G) Effects of other chemical agents on enzyme activity. Control was set as 100% of activity without NaCl, organic solvents and other chemical agents in the mixture reaction. The values were an average of three independent experiments.