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online data

SUPPLEMENTARY ONLINE DATA

Structure and activity of the cold-active and anion-activated carboxyl esterase OLEI01171 from the oil-degrading marine bacterium *Oleispira antarctica*

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Table S1 The number of the surface-located charged residues (calculated using a cut-off value 2 Å^2) in the structures of homologous PF00746 esterases from psychrophilic and mesophilic organisms

			Number of the surface-located residues				
Protein ID	Total number of amino acids	Percentage of sequence identity with OLEI01171	Aspartic acid	Glutamic acid	Arginine	Lysine	Total amino acids
OLEI01171	280	100	11	17	11	10	49
Ps. haloplanktis FGH	280	65	12	10	2	15	39
Atu1476	277	48	15	21	14	11	61
Saccharomyces cerevisiae FGH	299	43	17	15	8	20	60

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Co-ordinates and structure factors of the OLEI01171 complexes with Cl^- or Br^- have been deposited in the PDB under the accession codes 3I6Y and 3S8Y respectively.

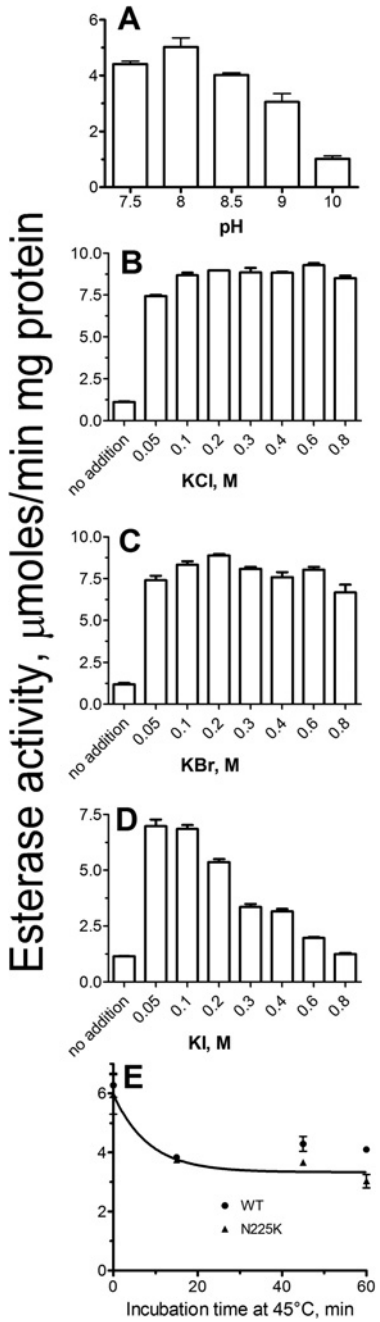

Figure S1 Hydrolysis of α-naphthyl acetate by OLEI01171 as a function of pH (A), KCl concentration (B), KBr concentration (C), KI concentration (D) and pre-incubation time at 45°C (E)

The reaction mixtures contained 2 mM α-naphthyl acetate and 1 μg of OLEI01171, and the assay temperature was 15°C.

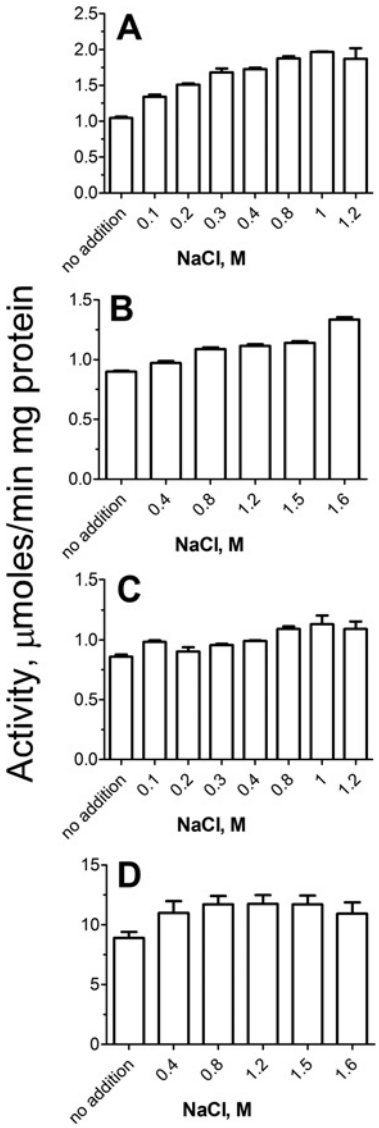

Figure S2 Effect of NaCl on esterase activity of Atu1476 (A), SMc01273 (B), *E. coli* YeiG (C) and *E. coli* BioH (D)

The reaction mixtures contained 2 mM naphthyl acetate and 1 μg of purified enzyme.

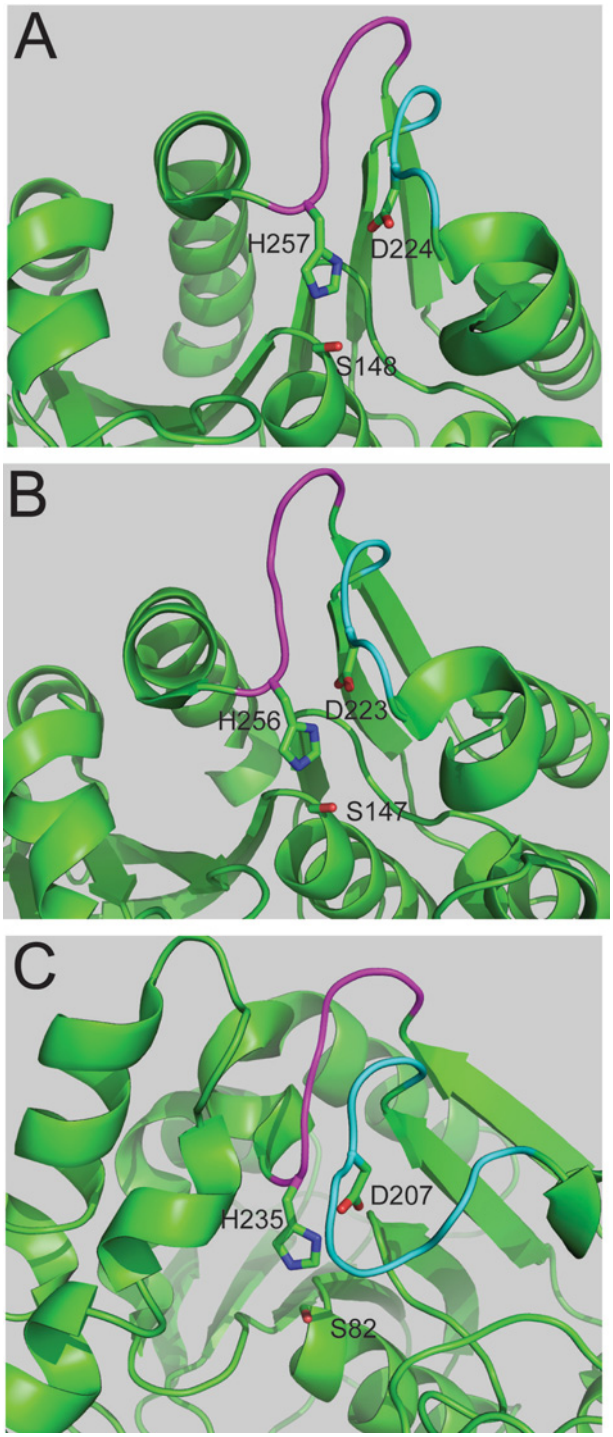

Figure S3 The active site histidine residue loop of OLEI01171 and other structurally characterized esterases

(**A**) OLEI01171. (**B**) *Ph*FGH. (**C**) *E. coli* BioH. Side chains of the catalytic triad residues are shown as sticks and labelled, whereas the histidine loop is coloured in magenta.

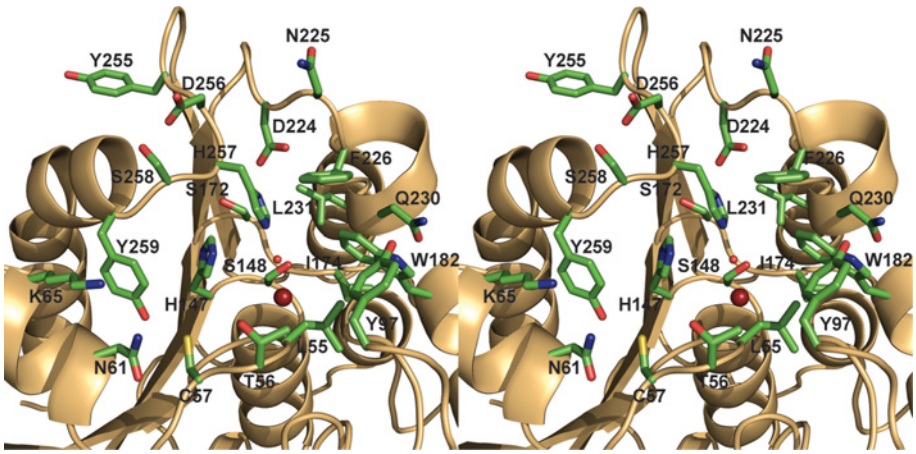

Figure S4 Close-up stereo view of the OLEI01171 active site with a bromide ion bound

The bromide ion is shown as the fire-brick-coloured ball. The amino acid side chains are shown as sticks along the OLEI01171 ribbon. The orange ball represents the potential catalytic water molecule.

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