

Additional file 1:

Towards an understanding of oleate hydratase and their application in industrial processes

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Table S1 Overview of available structures of Ohys with cofactor or ligand decoration. Assignment to the respective family of oleate hydratases is given according to Schmidt *et al.* [1]. The PEG molecule originates from the crystallization condition. In the structure of OhySa [2], there are three copies in the asymmetric unit, that are described with differently bound substrates or products.

Protein	Organism	HFam Family	Resolution	Cofactor/ Ligand	PDB-ID	Reference
OhyLa	<i>L. acidophilus</i>	HFam2	2.22 Å	none	4IA5	[3]
OhyLa	<i>L. acidophilus</i>	HFam2	1.80 Å	linoleic acid	4IA6	[3]
OhySa	<i>S. aureus</i>	HFam2	1.84 Å	PEG	7KAV	[2]
OhySa	<i>S. aureus</i>	HFam2	2.10 Å	FAD / PEG	7KAW	[2]
OhySa (E82A)	<i>S. aureus</i>	HFam2	3.51 Å	none	7KAX	[2]
OhySa (E82A)	<i>S. aureus</i>	HFam2	1.95 Å	oleate	7KAY	[2]
OhySa (E82A)	<i>S. aureus</i>	HFam2	1.85 Å	FAD / oleate / 10-HSA	7KAZ	[2]
OhyRe	<i>R. erythropolis</i>	HFam3	2.64 Å	none	5ODO	[4]
OhySt	<i>Stenotrophomonas</i> sp. KCTC 12332	HFam11	2.91 Å	none	5Z70	[5]
OhyEm	<i>E. meningoseptica</i>	HFam11	2.75 Å	FAD / PEG	4UIR	[3]

Table S2 Pairwise amino acid sequence comparison. Given are identities and in parenthesis the homology. Pairwise alignments were performed with EMBOSS [6].

	OhyLa	OhySa	OhyRe	OhySt
OhyLa	-	-	-	-
OhySa	61% (76%)	-	-	-
OhyRe	33% (48%)	33% (48%)	-	-
OhySt	37% (55%)	35% (50%)	27% (42%)	-
OhyEm	39% (56%)	41% (56%)	28% (44%)	56% (72%)

Table S3 Results of a DALI search [7] for Ohys with the OhySa [2] as reference structure.

PDB-ID	rmsd [Å]	sequence identity [%]	Z-score	Organism	HFam Family	Cofactor/ Ligand	Reference
7KAZ	0.0	100	66.7	<i>S. aureus</i>	HFam2	FAD / oleate	[2]
7KAY	0.6	100	58.2	<i>S. aureus</i>	HFam2	oleate	[2]
4IA6	1.1	61	58.0	<i>L. acidophilus</i>	HFam2	linoleic acid	[3]
4UIR	2.1	44	48.8	<i>E. meningoseptica</i>	HFam11	FAD / PEG	[8]
5ODO	1.7	36	34.4	<i>R. erythropolis</i>	HFam3	none	[4]
5Z70	1.9	42	34.1	<i>Stenotrophomonas</i> sp. KCTC 12332	HFam11	none	[3]

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