

\*\*\* Data underlying the chapter: Peroxygenase-promoted enzymatic cascades for the valorisation of fatty acids \*\*\*

Authors: Yinqi Wu, Caroline E. Paul, Thomas Hilberath, Ewald P.J. Jongkind, Wuyuan Zhang, Miguel Alcalde and Frank Hollmann

Biocatalysis Group, Applied Sciences, Delft University of Technology

Tianjin Institute of Industrial Biotechnology, Chinese Academy of Sciences

Department of Biocatalysis, Institute of Catalysis and Petrochemistry (CSIC)

Corresponding author: Frank Hollmann

Contact Information: F.Hollmann@tudelft.nl

Delft University of Technology - Faculty of Applied Sciences

van der Maasweg 9, 2629 HZ, Delft, The Netherlands

### \*\*\*General Introduction\*\*\*

This dataset contains data collected during experiments at Delft University of Technology, as chapter 2 of Yinqi Wu's PhD Thesis project (September 2023):

It is being made public for both to act as supplementary data for publications and the PhD thesis of Yinqi Wu and in order for other researchers to use this data in their own work.

The data in this dataset was collected in the Biocatalysis Laboratory of the Delft University of Technology - Faculty of Applied Sciences, between October 2019 and September 2023.

This research project was made possible by a grant from the China Scholarship Council (CSC) and European Union (ERC, PeroxyZyme, No101054658).

### \*\*\*Purpose of the test campaign\*\*\*

The purpose of these experiments was to investigate the peroxygenase-promoted enzymatic cascades for the valorisation of fatty acids.

### \*\*\*Test equipment\*\*\*

Test equipment information could be found in the supplementary information of the chapter.

### \*\*\*Description of the data in this data set\*\*\*

Corresponding methods and conditions could be found in the supporting information of the chapter.

Experiment	Category	Description Category	Analysis	Experiment Description
P8.E3	EC	Enzyme Characterization	CO Dif spectra, SDS-PAGE	measure the UPO concentration and check the expression level of UPO A77L stock from JenaBios
P8.E14	BC	Bioconversion	GC	Bioconversion of fatty acids and methyl esters (see summary file) by UPO WT, A77L_2 mM/h H2O2_4h
P8.E18	BC	Bioconversion	GC	Optimization A77L crude enzyme conc. (1-10 uM) in 2LPS (1mL) and 10%ACN (10 mL)_methyl hexanoate_5 mM/h H2O2 pumping
P8.E19	LC	Lactonization	GC, GC/MS, NMR	isolate the w-1 hydroxy methyl hexanoate and perform lactonization, and identify the product structure
P8.E20	BC	Bioconversion	GC	optimization of hydroxylation of methyl decanoate in 10% ACN
P8.E21	BC	Bioconversion	GC	cascade reaction from methyl decanoate to w-1 ketone and w-1 amide_enzymes screening_ADH and RedAm
P8.E22	BC	Bioconversion	GC, NMR	scale up the methyl decanoate hydroxylation and isolate_10 mL
P8.E24	BC	Bioconversion	GC	cascade reaction from methyl decanoate_UPO_ADH_BVMO
P8.E28	BC	Bioconversion	GC	cascade reaction_UPO_ADH_RedAm
P8.E32	BC	Bioconversion	GC	methyl decanoate_UPO_ADH_purified RedAm