# nature research

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# **Reporting Summary**

Nature Research wishes to improve the reproducibility of the work that we publish. This form provides structure for consistency and transparency in reporting. For further information on Nature Research policies, see our <u>Editorial Policies</u> and the <u>Editorial Policy Checklist</u>.

#### **Statistics**

For all statistical analyses, confirm that the following items are present in the figure legend, table legend, main text, or Methods section.						
n/a	Cor	nfirmed				
		The exact sample size (n) for each experimental group/condition, given as a discrete number and unit of measurement				
	$\square$	A statement on whether measurements were taken from distinct samples or whether the same sample was measured repeatedly				
$\boxtimes$		The statistical test(s) used AND whether they are one- or two-sided Only common tests should be described solely by name; describe more complex techniques in the Methods section.				
$\boxtimes$		A description of all covariates tested				
$\boxtimes$		A description of any assumptions or corrections, such as tests of normality and adjustment for multiple comparisons				
		A full description of the statistical parameters including central tendency (e.g. means) or other basic estimates (e.g. regression coefficient) AND variation (e.g. standard deviation) or associated estimates of uncertainty (e.g. confidence intervals)				
$\boxtimes$		For null hypothesis testing, the test statistic (e.g. F, t, r) with confidence intervals, effect sizes, degrees of freedom and P value noted Give P values as exact values whenever suitable.				
$\ge$		For Bayesian analysis, information on the choice of priors and Markov chain Monte Carlo settings				
$\boxtimes$		For hierarchical and complex designs, identification of the appropriate level for tests and full reporting of outcomes				
$\boxtimes$		Estimates of effect sizes (e.g. Cohen's d, Pearson's r), indicating how they were calculated				
		Our web collection on statistics for biologists contains articles on many of the points above.				

### Software and code

Policy information	about <u>availability of computer code</u>
Data collection	Data was collected using commercially available software. Plate reader: Magellan V6.5 (Tecan) HPLC: ChemStation Rev. B.01.03 SR1 and OpenLAB CDS Rev. C.01.07 SR3 (Agilent) GC: ChemStation Rev. B.04.03-SP2 (Agilent) Tube-in-Tube Reactor: LabVIEW 2016 16.0.0 (National Instruments) and MATLAB 9.0 R2016A (MathWorks), PLS Toolbox Version 8.2 (Eigenvector Research)
Data analysis	0.2 L Scale Reactions: my-Control Version V1_11 (Applikon) Data analysis was performed using commercially available software. Enzyme Kinetics: GraphPad Prism, versions 6 and 7 HPLC: ChemStation Rev. B.01.03 SR1 and OpenLAB CDS Rev. C.01.07 SR3 (Agilent) GC: ChemStation Rev. B.04.03-SP2 (Agilent) Tube-in-Tube Reactor: MATLAB 9.0 R2016A (MathWorks)

For manuscripts utilizing custom algorithms or software that are central to the research but not yet described in published literature, software must be made available to editors and reviewers. We strongly encourage code deposition in a community repository (e.g. GitHub). See the Nature Research guidelines for submitting code & software for further information.

#### Data

Policy information about availability of data

All manuscripts must include a data availability statement. This statement should provide the following information, where applicable:

- Accession codes, unique identifiers, or web links for publicly available datasets
- A list of figures that have associated raw data
- A description of any restrictions on data availability

Source Data are provided with the paper. Data supporting the findings presented in this article can be obtained from the authors upon reasonable request.

# Field-specific reporting

Please select the one below that is the best fit for your research. If you are not sure, read the appropriate sections before making your selection.

Life sciences

For a reference copy of the document with all sections, see <u>nature.com/documents/nr-reporting-summary-flat.pdf</u>

Ecological, evolutionary & environmental sciences

# Life sciences study design

All studies must disclose on these points even when the disclosure is negative.

Behavioural & social sciences

Sample size	No sample size calculations were performed. This work analyzed specific enzyme transformation of one substrate to one or two product(s), all of which are defined and commercially available. Data processing did not involve statistical analysis of large numbers of samples for sample size calculation to be impactful. Enzyme kinetic characterizations and specific activity measurements were performed in triplicate (n=3) as this is sufficient for statistical analysis.
Data exclusions	No data were excluded.
Replication	Kinetic studies (plate reader and TiTR) as well as specific activity measurements were performed in triplicate. Screening of biotransformation reaction conditions were performed as single reactions, however some reactions were independently repeated a second time and showed similar results.
Randomization	Not applicable to this study since there were no experimental groups.
Blinding	Not applicable to this study since experiments were performed with purified enzymes.

# Reporting for specific materials, systems and methods

We require information from authors about some types of materials, experimental systems and methods used in many studies. Here, indicate whether each material, system or method listed is relevant to your study. If you are not sure if a list item applies to your research, read the appropriate section before selecting a response.

#### Materials & experimental systems

n/a	Involved in the study
$\boxtimes$	Antibodies
$\boxtimes$	Eukaryotic cell lines
$\boxtimes$	Palaeontology and archaeology
$\boxtimes$	Animals and other organisms
$\boxtimes$	Human research participants
$\boxtimes$	Clinical data
$\boxtimes$	Dual use research of concern

#### Methods

n/a	Involved in the study
$\boxtimes$	ChIP-seq

MRI-based neuroimaging