nature portfolio

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Reporting Summary

Nature Portfolio 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 Portfolio policies, see our Editorial Policies and the Editorial Policy Checklist.

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	Confirmed
☐	☒ The exact sample size (*n*) for each experimental group/condition, given as a discrete number and unit of measurement
☐	☒ A statement on whether measurements were taken from distinct samples or whether the same sample was measured repeatedly
☐	☒ 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.*
☒	☐ A description of all covariates tested
☒	☐ 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)
☒	☐ 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.*
☒	☐ For Bayesian analysis, information on the choice of priors and Markov chain Monte Carlo settings
☒	☐ For hierarchical and complex designs, identification of the appropriate level for tests and full reporting of outcomes
☒	☐ 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 availability of computer code

Data collection

X-ray diffraction data were collected at Advanced Photon Source using beamline 23-ID-B (wavelength 1.03317 Å).
Melting temperature (Tm) of PET films and enzymes were determined by Differential scanning calorimetry (DSC). Data were collected using a DSC250 (TA Instruments) with a Trios software (TA Instruments).
NMR data were collected at a 400 MHz Bruker AVANCE NEO spectrometer using a Mestrenova software (Mestrelab).
Atomic force microscopy (AFM) data were collected using an Asylum MFP-3D atomic force microscope (Asylum Research) using Igor Pro.
Scanning electron microscope (SEM) imaging was performed under vacuum using a Zeiss Supra40 SEM. The electron beam intensity was 5 kV. Samples were sputter-coated with 8 nm platinum/palladium using a Cressington 208HR Sputter Coater.
Gel permeation chromatography (GPC) was performed at an on an Agilent system with a 1260 Infinity isocratic pump, degasser, and thermostated column chamber held at 30 °C.
Chromoleon software was used for acquisition of spectra on High Performance Liquid Chromatography (HPLC)-Dionex UltiMate 3000 (Thermo Fisher Scientific, Waltham, MA) equipped with an Agilent Eclipse Plus C18 column.
The CNN predictions were obtained from mutcompute.com

Data analysis	The X-ray diffraction pattern were processed by using HKL2000. The protein crystal structure was solved by molecular replacement with molecular replacement package in Phenix. The molecular replacement solution was iteratively built and refined using Coot and Phenix refinement package. Structure analysis and visualization were carried out by Chimera X. DSC data were analyzed using a Trios software (TA Instruments). NMR data were analyzed using a Mestrenova software (Mestrelab). AFM data were analyzed using Igor Pro. GPC data were analyzed using Agilent Bio SEC software. HPLC data were analyzed using Chromoleon software for integration of chromatograms. CNN model predictions were analyzed and processed by the Pandas python package.

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 Portfolio 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 description of any restrictions on data availability
- For clinical datasets or third party data, please ensure that the statement adheres to our policy

Structural coordinates have been deposited into the PDB database.

The mutcompute - view has been added and is publicly accessible at mutcompute.com

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 ☐ Behavioural & social sciences ☐ Ecological, evolutionary & environmental sciences

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

Life sciences study design

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

Sample size	For enzymatic activity assays, Tm determination, and the experiments incorporating various enzymes and cell, triplicates were performed to determine mean and standard deviation and was stated when relevant. Results are reproducible. Attempts at replication were successful.
Data exclusions	No data was excluded.
Replication	All in vitro and in vivo experiments with explicit standard deviation were performed in triplicates. Attempts at replication were successful.
Randomization	No data was randomized since it was not applicable to our set of experiments.
Blinding	For DSC, SEM, GPC, AFM, HPLC analysis, The analytical team who performed the experiments and analyze the data were blind to the samples that they were handling with and analyzing.

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
☒	☐ Antibodies
☒	☐ Eukaryotic cell lines
☒	☐ Palaeontology and archaeology
☒	☐ Animals and other organisms
☒	☐ Human research participants
☒	☐ Clinical data
☒	☐ Dual use research of concern

Methods

n/a	Involved in the study
☒	☐ ChIP-seq
☒	☐ Flow cytometry
☒	☐ MRI-based neuroimaging