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Reporting Summary

X Life sciences

Behavioural & social sciences

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 <u>Authors & Referees</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 Confirmed					
\square 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. <i>F</i> , <i>t</i> , <i>r</i>) with confidence intervals, effect sizes, degrees of freedom and <i>P</i> value noted Give <i>P</i> 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					
\square Estimates of effect sizes (e.g. Cohen's d , Pearson's r), indicating how they were calculated					
Our web collection on <u>statistics for biologists</u> contains articles on many of the points above.					
Software and code					
Policy information about <u>availability of computer code</u>					
Data collection Data collection was performed with custom python and bash scripts. These are available upon request.					
Data analysis was performed with Python (Jupyter notebooks). In the manuscript we link a repository with all analysis code to reproduce all figures.					
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/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 <u>availability of data</u> All manuscripts must include a <u>data availability statement</u> . 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					
All data are available in the main text or the supplementary materials.					
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.					

Ecological, evolutionary & environmental sciences

Life sciences study design

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

Sample size

Sample size was determined in a prospective manner such that it would likely be more than enough before the analysis was performed. Sample sizes were not determined using a formal statistical analysis. Instead, sample sizes were chosen such that we could estimate at minimum single-digit percentage differences in performance between the methods examined.

Data exclusions

There were two proteins excluded from the analysis of the Grey et al. (2017) paper (Figure 3e). These were excluded on the basis that they were excluded in the original reference due to poor statistical signal. This exclusion criteria was pre-established.

Replication

For all computational analyses, random seeds were set. Jupyter notebooks were run repeatedly to ensure reproducibility of analysis. All replication attempts were successful.

Randomization

Train-Validation-Test splits were randomly allocated when described as such, except when a split was designed to examine specific behavior of a model (e.g. transfer learning).

Blinding

Authors were blinded to validation set sequences when developing models. After a panel of models were assembled, the validation set was then used to select the modeling paradigm. The test set was kept hidden until the manuscript was being written. We note that this blinding was not enforced by a 3rd party.

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.

ivia	teriais & experimental systems	IVIETNOAS	
n/a	Involved in the study	n/a	Involved in the study
\boxtimes	Antibodies	\boxtimes	ChIP-seq
\boxtimes	Eukaryotic cell lines	\boxtimes	Flow cytometry
\boxtimes	Palaeontology	\boxtimes	MRI-based neuroimaging
\boxtimes	Animals and other organisms		
\boxtimes	Human research participants		
\boxtimes	Clinical data		