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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 <u>Authors & Referees</u> and the <u>Editorial Policy Checklist</u>.

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FOI	all statistical analyses, confirm that the following items are present in the figure regend, table regend, 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.
	X 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)
x	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 <i>Give P values as exact values whenever suitable.</i>
	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 <i>d</i> , Pearson's <i>r</i>), indicating how they were calculated
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Our web collection on <u>statistics for biologists</u> contains articles on many of the points above.

Software and code

Policy information about availability of computer code

Data collection

Python 3.6 with the package edd_utils 0.0.5

Data analysis

Data analysis is performed by the custom algorithm/software ART described in the manuscript.

ART is developed under Python 3.6 and relies on packages:

- seaborn 0.7.1
- scikit-learn 0.20.2
- pymc3 3.5
- pandas 0.23.4
- numpy 1.14.3
- matplotlib 3.0.2
- scipy 1.1.0
- PTMCMCSampler 2015.2

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.

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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

The experimental data analyzed in this paper can be found in the public repository "Experiment Data Depot" in the following studies:					
Biofuel	Biofuel https://public-edd.jbei.org/s/pcap/				
Hopless beer https://public-edd.agilebiofoundry.org/s/hopless-beer/					
	https://public-edd.agilebiofoundry.org/s/hopless-beer-cycle-2/				

Dodecanol https://public-edd.jbei.org/s/ajinomoto/

Freely available accounts on public-edd.jbei.org are required to view and download these studies.

All data sets are also provided as Source Data files.

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x Life sciences	Behavioural & social sciences Ecological, evolutionary & environmental sciences				
For a reference copy of the document with all sections, see <u>nature.com/documents/nr-reporting-summary-flat.pdf</u>					

Life sciences study design

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All studies must disclose on these points even when the disclosure is negative.				
Sample size	N/A. This study used previously published data sets and we chose to use all samples, i.e. no exclusions were made.			
Data exclusions	No data were excluded from the analysis.			
Replication	N/A. This study used previously published data sets and no additional experimental work was involved.			
Randomization	N/A. This study used previously published data sets.			
Blinding	Blinding was not relevant to this study as all predictive models were trained on the entire data set using cross-validation.			

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.

Ma	terials & experimental systems	Methods		
n/a	Involved in the study	n/a	Involved in the study	
×	Antibodies	x	ChIP-seq	
×	Eukaryotic cell lines	x	Flow cytometry	
×	Palaeontology	x	MRI-based neuroimaging	
×	Animals and other organisms			
×	Human research participants			
×	Clinical data			