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.

For all statistical analyses, confirm that the following items are present in the figure legend, table legend, main text, or Methods section.

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St	at	ıstı	CS

n/a	Cor	nfirmed
	X	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
	x	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 Give <i>P</i> values as exact values whenever suitable.
x		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 Publicly available software

Publicly available software package GROMACS v2020.3 was used for the simulations (https://www.gromacs.org).

Data analysis

Publicly available software package VMD v1.9.4 was used for the analysis and visualization (https://www.ks.uiuc.edu/Research/vmd/). Inhouse scripts employed to analyse the MD trajectories are available in an open public repository: https://doi.org/10.5281/zenodo.7028021

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

MD trajectories, parameter files, and input files have been deposited in an open public repository [https://doi.org/10.5281/zenodo.7028021].

Human rese	earch parti	cipants
Policy information	n about <u>studies i</u>	nvolving human research participants and Sex and Gender in Research.
Reporting on sex a	and gender	Not applicable to our study.
Population charac	teristics	Not applicable to our study.
Recruitment		Not applicable to our study.
Ethics oversight		Not applicable to our study.
Note that full inform	nation on the appr	oval of the study protocol must also be provided in the manuscript.
Field-spe	ecific re	porting
Please select the o	one below that i	s the best fit for your research. If you are not sure, read the appropriate sections before making your selection.
x Life sciences	□ E	Behavioural & social sciences 🔲 Ecological, evolutionary & environmental sciences
For a reference copy of	f the document with	all sections, see <u>nature.com/documents/nr-reporting-summary-flat.pdf</u>
Life scie	nces sti	udy design
All studies must di	isclose on these	points even when the disclosure is negative.
Sample size		le, data sample size was determined based on previous reports in the literature. //pubs.acs.org/doi/full/10.1021/acscentsci.8b00143 and https://pubs.rsc.org/en/content/articlehtml/2016/sm/c6sm01186a
Data exclusions	No data were ϵ	excluded from the analyses.
Replication		ults are based on multiple independent copies. Membrane deformation patterns were confirmed by four independent icas, all yielding the same deformation patterns.
Randomization	All the membra	ane systems were independently generated initially based on a random model generator.
Blinding	Not applicable	to our study. The study does not include samples from individuals that could be subject to blinding.
•		pecific materials, systems and methods
system or method li	sted is relevant to	about some types of materials, experimental systems and methods used in many studies. Here, indicate whether each material, your study. If you are not sure if a list item applies to your research, read the appropriate section before selecting a response.
Materials & ex	ystems Methods n/a Involved in the study	
		ChIP-seq
x Eukaryoti	c cell lines	Flow cytometry
✗ ☐ Palaeonto	ology and archaeo	logy MRI-based neuroimaging

Animals and other organisms

Dual use research of concern