nature portfolio

Corresponding author(s): PCA van der Wel; MS Miettinen
Last updated by author(s): Nov 3, 2024

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	The ssNMR data were collected from Bruker Biospin - TopSpin 4.1.3 and processed using NMRPipe version 2019.218.13.13 software. The MD data were generated with the freely available open-source engine Gromacs (www.gromacs.org) versions 2018.3 and 2021.4.
Data analysis	The EM data were analyzed using FIJI (based on ImageJ2) software (v. 2.14.0). The ssNMR data were analyzed using the CCPNMR 2.4 software and visualized with GraphPad Prism 10. The MD data were analyzed using the GROMACS tools gmx_angle, gmx_distance, gmx_traj, gmx_do_dssp, and in-house Python scripts freely openly available on the Zenodo repository with the DOI:10.5281/zenodo.13926360.

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

The data (experimental and MD data, and the in-house analysis scripts) that support the findings of this study are openly available on Zenodo (DOI:

10.5281/zenodo.13926360).

Research involving human participants, their data, or biological material

Policy information about studies with human participants or human data. See also policy information about sex, gender (identity/presentation), and sexual orientation and race, ethnicity and racism.

Reporting on sex and gender	N/A
Reporting on race, ethnicity, or other socially relevant groupings	N/A
Population characteristics	N/A
Recruitment	N/A
Ethics oversight	N/A

Note that full information on the approval of the study protocol must also be provided in the manuscript.

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	The paper includes experimental data obtained by EM and ssNMR spectroscopy. As is common in these fields, the reported results are obtained on individual samples. The resulting spectra are shown in the manuscript. Notably, the reported data build on prior work in which many such samples were studied, and where reproducibility of these analyses was determined. We do not have such experiments that failed to not replicate the reported findings or contradicted them. Reproducibility of MD findings was assessed by the use of different force field families: Amber, OPLS, and Charmm.
Data exclusions	No experimental or simulation data were excluded.
Replication	See sample size explanation.
Randomization	No randomization was applied in the performed experiments. No significant issues are expected from covariation of parameters in the applied experimental studies.
Blinding	No blinding was applied in the described experiments or simulations. Blinding is not customary in the field of NMR studies also given the small number of samples studied (see sample size above).

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
☒	☐ Clinical data
☒	☐ Dual use research of concern
☒	☐ Plants

Methods

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

Plants

Seed stocks	N/A
Novel plant genotypes	N/A
Authentication	N/A