

## 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 [Authors & Referees](#) 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  |
| <input type="checkbox"/>            | <input checked="" type="checkbox"/> The exact sample size ( $n$ ) for each experimental group/condition, given as a discrete number and unit of measurement  |
| <input type="checkbox"/>            | <input checked="" type="checkbox"/> A statement on whether measurements were taken from distinct samples or whether the same sample was measured repeatedly  |
| <input checked="" type="checkbox"/> | <input type="checkbox"/> The statistical test(s) used AND whether they are one- or two-sided<br><i>Only common tests should be described solely by name; describe more complex techniques in the Methods section.</i>  |
| <input checked="" type="checkbox"/> | <input type="checkbox"/> A description of all covariates tested  |
| <input checked="" type="checkbox"/> | <input type="checkbox"/> A description of any assumptions or corrections, such as tests of normality and adjustment for multiple comparisons   |
| <input type="checkbox"/>            | <input checked="" type="checkbox"/> 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) |
| <input checked="" type="checkbox"/> | <input type="checkbox"/> For null hypothesis testing, the test statistic (e.g. $F$ , $t$ , $r$ ) with confidence intervals, effect sizes, degrees of freedom and $P$ value noted<br><i>Give <math>P</math> values as exact values whenever suitable.</i>                                       |
| <input checked="" type="checkbox"/> | <input type="checkbox"/> For Bayesian analysis, information on the choice of priors and Markov chain Monte Carlo settings  |
| <input checked="" type="checkbox"/> | <input type="checkbox"/> For hierarchical and complex designs, identification of the appropriate level for tests and full reporting of outcomes  |
| <input checked="" type="checkbox"/> | <input type="checkbox"/> 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 custom codes used to generate the contour plots in Fig. 4b and c and the simulations in Fig. S4 (both Wolfram Mathematica 12) can be downloaded from: [http://hore.chem.ox.ac.uk/Nature\\_2021/Codes.zip](http://hore.chem.ox.ac.uk/Nature_2021/Codes.zip).

The custom codes written to control and acquire data from our home-built magnetic field effect spectrometers (LabView v.15 and C++) are available from PJH on request. Given that these instruments are unique, the control software is unlikely to be of use to anyone else which is why they are not made publicly available.

NAMD 2.10 (<http://www.ks.uiuc.edu/Research/namd/>) and VIKING (<https://viking-suite.com/>) were used for the molecular dynamics simulations.

All relevant input and output files for the molecular dynamics simulations are available for download from the University of Oldenburg repository: <https://cloud.uol.de/s/NrTYpoEzL6RbPq7>.

#### Data analysis

VMD 1.9.3 (<http://www.ks.uiuc.edu/Research/vmd/>) was used for analysis of molecular dynamics data.

UNICORN, GE Healthcare, versions 7.1 and 7.3, control software for chromatography.

The ShakeH algorithm is a standard component of NAMD.

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 [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 list of figures that have associated raw data
- A description of any restrictions on data availability

All relevant spectroscopic data are presented in Figures in the manuscript or in the Supplementary Information. The data used to prepare the figures are available as Supplementary Data files.

The complete set of molecular dynamics simulation data is available for download from the University of Oldenburg repository: <https://cloud.uol.de/s/NrTYpoEzL6RbPq7>. Specific molecular dynamics data can also be obtained directly from IAS on request.

## 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](https://www.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	All experimental data were spectroscopic measurements on samples of proteins. Measurements were repeated and the signals averaged until the signal-to-noise ratio was judged satisfactory. The number of measurements on each sample depended on the particular instrument used and the strength of the signals. Detailed information is provided in the Statistics & Reproducibility subsection in the Methods section.
Data exclusions	Occasional spectroscopic measurements failed to yield usable data as a result of instrument breakdowns, protein precipitation, etc.
Replication	The number of repeats of each measurement using independently produced batches of protein is given in the Statistics & Reproducibility subsection in the Methods section.
Randomization	Not relevant for spectroscopic measurements.
Blinding	Blinding is not appropriate for the spectroscopic measurements reported here. No statistical tests were required to interpret the results.

## 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
<input checked="" type="checkbox"/>	<input type="checkbox"/> Antibodies
<input checked="" type="checkbox"/>	<input type="checkbox"/> Eukaryotic cell lines
<input checked="" type="checkbox"/>	<input type="checkbox"/> Palaeontology
<input checked="" type="checkbox"/>	<input type="checkbox"/> Animals and other organisms
<input checked="" type="checkbox"/>	<input type="checkbox"/> Human research participants
<input checked="" type="checkbox"/>	<input type="checkbox"/> Clinical data

### Methods

n/a	Involved in the study
<input checked="" type="checkbox"/>	<input type="checkbox"/> ChIP-seq
<input checked="" type="checkbox"/>	<input type="checkbox"/> Flow cytometry
<input checked="" type="checkbox"/>	<input type="checkbox"/> MRI-based neuroimaging