

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	All high-resolution images were collected using a HS-AFM (SS-NEX, Research Institute of Biomolecule Metrology Co.). The AFM-SMFS measurements were collected using a JPK Nanowizard 4. All MDS were performed using the GROMACS2020 simulation package using the Amber99sb-ildn force field. MST experiments were performed using a Monolith NT.115 Pico (NanoTemper Technologies, Germany) and Monolith NT.115 Premium capillaries (NanoTemper Technologies, Germany).
Data analysis	All AFM-SMFS data were analyzed by using JPK force curve processing software (7.0.72). All force histograms were fitted in Origin 2019b. The MST traces were analyzed using the software M.O. Affinity Analysis v2.3 (NanoTemper Technologies, Germany).

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 source data files contain all data (force distribution histograms, H-bond distributions) necessary to interpret, verify and extend the presented work. In the absence of dedicated data repositories for raw data AFM force curves and MDS trajectories, and in light of the instructions needed to open these files in proprietary software (in the case of the AFM force curves) and the additional information (parameters and conditions) needed to understand and use the data, raw data AFM force curves and MDS trajectories can be received from Simon Scheuring (sis2019@med.cornell.edu) and Helmut Grubmüller (hgrubmu@gwdg.de), respectively, upon reasonable request.

Human research participants

Policy information about [studies involving human research participants and Sex and Gender in Research](#).

Reporting on sex and gender	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	No statistical methods were used to determine the sample size. Sample size was determined based on the amount that is sufficient for the histograms creating and Gaussian fitting applied in this study. For each pulling speed or different contact time, at least 38 events were used for the histogram creating and Gaussian fitting (in most cases above hundred events).
Data exclusions	No data exclusions were made.
Replication	All the experiments were replicated 2-3 times.
Randomization	For AFM-SMFS experiments, force distance curves at different pulling speed were collected from multiple random areas. For high resolution AFM imaging experiments, multiple areas were randomly acquired. As the CNBD molecules formed uniform 2D crystal in our experiments, we didn't allocate experimental groups.
Blinding	No blinding was required for single molecule biophysics research. We did quantitative analysis of our collected data. For the data analysis, we used the commercial JPK data processing software (7.0.72). All the data were analyzed in the same software and using the same criteria.

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 and archaeology
<input checked="" type="checkbox"/>	<input type="checkbox"/> Animals and other organisms
<input checked="" type="checkbox"/>	<input type="checkbox"/> Clinical data
<input checked="" type="checkbox"/>	<input type="checkbox"/> Dual use research of concern

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