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: not applicable.

- 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 all hypothesis testing, the test statistic (e.g. F, t, r) with degrees of freedom and P value noted Give P values as exact values whenever possible
- 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

For manuscripts utilizing custom algorithms or software that are not yet described in published literature, software must be made available to editors and reviewers. We strongly encourage code deposition in open community repositories such as GitHub. See the Nature Portfolio guidelines for submitting code & software for further information.

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.

All data generated or analyzed in this study are included in the main text or the supplementary materials. Atomic coordinates and NMR data for the reduced NineAcrlC1 have been deposited in the Protein Data Bank (PDB) under entry ID 7X31 [https://doi.org/10.2210/pdb7X31/pdb] and Biological Magnetic Resonance Bank (BMRB) under entry ID 36471 [https://doi.org/10.1016/B978-0-12-819471-1]. Atomic coordinates and structure factors for the crystal structures of the oxidized state of NineAcrlC1 have been deposited in the PDB under entry ID 7X48 [https://doi.org/10.2210/pdb7X48/pdb]. One other published PDB (cited in this paper)
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.

- [x] Life sciences
- [ ] Behavioural & social sciences
- [ ] Ecological, evolutionary & environmental sciences

For a reference copy of this document with all sections, see nature.com/documents/reporing-summary-flat.pdf

Life sciences study design

All studies must disclose on these points even when the disclosure is negative.

| Sample size | For structural calculation of the reduced NmeAcR1C1, 100 starting structures were initially calculated and 2C structures with the lowest AMBER energy were reported. The sample size was chosen based on previous similar studies. The RMSD of the 2C structures for the backbone of the secondary structural region is only 0.19 Å, indicating the sample size is sufficient. For all functional assays, three independent experiments (n=3) were performed. |
| Data exclusions | No data were excluded. |
| Replication | All the assays were replicated more than three times with similar results. |
| Randomization | Randomization is not relevant to our study, because there is no specific grouping in data collection or analysis. |
| Blinding | Blinding is not relevant to our study, because there is no specific grouping in data collection or analysis. |

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

- [x] Antibodies
- [x] Eukaryotic cell lines
- [x] Palaeontology and archaeology
- [x] Animals and other organisms
- [x] Human research participants
- [x] Clinical data
- [x] Dual-use research of concern

Methods

- [x] ChIP-seq
- [x] Flow cytometry
- [x] MRI-based neuroimaging