Submission guidelines

- Registered Reports

Format of articles

Scientific Reports publishes original research in two formats: Article and Registered Report. For Registered Reports, see section below. In most cases, we do not impose strict limits on word count or page number. However, we strongly recommend that you write concisely and stick to the following guidelines:

- Articles should ideally be no more than 11 typeset pages
- The main text should be no more than 4,500 words (not including Abstract, Methods, References and figure legends)
- The title should be no more than 20 words, should describe the main message of the article using a single scientifically accurate sentence, and should not contain puns or idioms
- The abstract should be no more than 200 words

For a definitive list of which limits are mandatory please visit the submission checklist page.

Abstract

Please do not include any references in your Abstract. Make sure it serves both as a general introduction to the topic and as a brief, non-technical summary of the main results and their implications. Abstract should be unstructured, i.e. should not contain sections or subheadings.

Manuscript

Your manuscript text file should start with a title page that shows author affiliations and contact information, identifying the corresponding author with an asterisk. We recommend that each section includes an introduction of referenced text that expands on the background of the work. Some overlap with the Abstract is acceptable.

Large Language Models (LLMs), such as ChatGPT, do not currently satisfy our authorship criteria. Notably an attribution of authorship carries with it accountability for the work, which cannot be effectively applied to LLMs.

Use of an LLM should be properly documented in the Methods section (and if a Methods section is not available, in a suitable alternative part) of the manuscript. In response to emerging information, advice, guidance and policy around artificial intelligence (AI), we have created a dedicated AI section in our Editorial Policy page. Please familiarize yourself with this content and comply with relevant policies.

For the main body of the text, there are no specific requirements. You can organise it in a way that best suits your research. However, the following structure will be suitable in many cases:

- Introduction
- Results (with subheadings)
- Discussion (without subheadings)
- Methods

You should then follow the main body of text with:

- References (limited to 60 references, though not strictly enforced)
- Acknowledgements (optional)
- Author contributions (names must be given as initials)
- Data availability statement (mandatory)
- Additional Information (including a Competing Interests Statement)
- Figure legends (these are limited to 350 words per figure)
- Tables (maximum size of one page)

Please note, footnotes should not be used. Please also do not include keywords, as these are not published in *Scientific Reports* articles.

We do not automatically include page or line numbers in the materials sent to Editorial Board Members and reviewers. Please consider including those in your manuscript; this can help facilitate the evaluation of the paper and makes giving feedback on specific sections easier.

You may include a limited number of uncaptioned molecular structure graphics and numbered mathematical equations if necessary. Display

items are limited to 8 (figures and/or tables). However, to enable typesetting of papers, we advise making the number of display items commensurate with your overall word length. So, for Articles of 2,000 words or less, we suggest including no more than 4 figures/tables. Please note that schemes should not be used and should be presented as figures instead.

Your submission must also include:

- A cover letter
- Individual figure files and optional supplementary information files

For first submissions (i.e. not revised manuscripts), you may incorporate the manuscript text and figures into a single file up to 3 MB in size. Whilst Microsoft Word is preferred we also accept LaTeX, or PDF format. Figures can be inserted in the text at the appropriate positions, or grouped at the end.

Supplementary information should be combined and supplied as a single separate file, preferably in PDF format.

A submission template is available in the Overleaf template gallery to help you prepare a LaTeX manuscript within the *Scientific Reports* formatting criteria.

Cover letter

In your cover letter, you should include:

- The affiliation and contact information of your corresponding author
- A brief explanation of why the work is appropriate for *Scientific Reports*
- The names and contact information of any reviewers you consider suitable
- The names of any referees you would like *excluded* from reviewing

Finally, you should state whether you have had any prior discussions with a *Scientific Reports* Editorial Board Member about the work described in your manuscript.

Revised manuscripts

For revised manuscripts, you should provide all textual content in a single file, prepared using either Microsoft Word or LaTeX. Please note, we do not accept PDF files for the article text of revised manuscripts. Make sure you:

- Format the manuscript file as single-column text without justification.
- Number the pages using an Arabic numeral in the footer of each page.
- Use the default Computer Modern fonts for your text, and the 'symbols' font for any Greek characters.
- Supply any figures as individual files.
- Combine and supply any Supplementary Information as a separate file, preferably in PDF format.
- Include the title of the manuscript and author list in the first page of the Supplementary Information file.

If you do not wish to incorporate the manuscript text and figures into a single file, please provide all textual content in a separate single file, prepared using either Microsoft Word or LaTeX.

TeX/LaTeX files

If you're submitting LaTeX files, you can either use the standard 'Article' document class (or similar) or the wlscirep.cls file and template provided by Overleaf. For graphics, we recommend your use graphicx.sty. Use numerical references only for citations.

Our system cannot accept .bib files. If you prepare references using BibTeX (which is optional), please include the .bbl file with your submission (as a 'LaTeX supplementary file') in order for it to be processed correctly; this file is included automatically in the zip file generated by

Overleaf for submissions. Please see this help article on Overleaf for more details.

Alternatively, you can make sure that the references (source code) are included within the manuscript file itself. As a final precaution, you should ensure that the complete .tex file compiles successfully on its own system with no errors or warnings, before submission.

Writing your manuscript

Scientific Reports is read by a truly diverse range of scientists. Please therefore give careful thought to communicating your findings as clearly as possible.

Although you can assume a shared basic knowledge of science, please don't expect that everyone will be familiar with the specialist language or concepts of your particular field. Therefore:

- Avoid technical jargon wherever possible, explaining it clearly when it is unavoidable.
- Keep abbreviations to a minimum, particularly when they are not standard.
- If you must use an abbreviation, make sure you spell it out fully in the text or legend the first time it appears.
- Clearly explain the background, rationale and main conclusions of your study.
- Write titles and abstracts in language that will be readily understood by any scientist.

We strongly recommend that you ask a colleague with different expertise to review your manuscript before you submit it. This will help you to identify concepts and terminology that non-specialist readers may find hard to grasp.

Copy editing services

We don't provide in-depth copy editing as part of the production process. So, if you feel your manuscript would benefit from someone looking at

the copy, please consider using a copy editing or language editing service. You can either do this before submission or at the revision stage. You can also get a fast, free grammar check of your manuscript that takes into account all aspects of readability in English.

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Please note that the use of an editing service is at your own expense, and doesn't ensure that your article will be selected for peer-review or accepted for publication.

Methods

We don't impose word limits on the description of methods. Make sure it includes adequate experimental and characterisation data for others to be able to reproduce your work. You should:

- Include descriptions of standard protocols and experimental procedures.
- Only identify commercial suppliers of reagents or instrumentation when the source is critical to the outcome of the experiments.
- Identify sources for any kits you use in your procedures.
- Include any experimental protocols that describe the synthesis of new compounds.
- Use the systematic name of any new compound and put its bold Arabic numeral in the heading for the experimental protocol, indicating it thereafter by its assigned, bold numeral.
- Describe the experimental protocol in detail, referring to amounts of reagents in parentheses, when possible (eg 1.03 g, 0.100 mmol).
- Use standard abbreviations for reagents and solvents.

- Clearly identify safety hazards posed by reagents or protocols.
- Report isolated mass and percent yields at the end of each protocol.

If you're reporting experiments on live vertebrates (or higher invertebrates), humans or human samples, you must include a statement of ethical approval in the Methods section (see our detailed requirements for further information on preparing these statements).

References

We don't copy edit your references. Therefore, it's essential you format them correctly, as they will be linked electronically to external databases where possible. At *Scientific Reports*, we use the standard *Nature* referencing style. So, when formatting your references, make sure they:

- Run sequentially (and are always numerical).
- Sit within square brackets.
- Only have one publication linked to each number.
- Only include papers or datasets that have been published or accepted by a named publication, recognised preprint server or data repository (if you include any preprints of accepted papers in your reference list, make sure you submit them with the manuscript).
- Include published conference abstracts and numbered patents, if you wish.
- Don't include grant details and acknowledgements.

Sorry, we cannot accept BibTeX (.bib) bibliography files for references. If you are making your submission by LaTeX, it must either contain all references within the manuscript .tex file itself, or (if you're using the Overleaf template) include the .bbl file generated during the compilation process as a 'LaTeX supplementary file' (see the "Manuscripts" section for more details).

In your reference list, you should:

- Include all authors unless there are six or more, in which case only the first author should be given, followed by 'et al.'.

- List authors by last name first, followed by a comma and initials (followed by full stops) of given names.
- Use Roman text for Article and dataset titles, with only the first word of the title having an initial capital and written exactly as it appears in the work cited, ending with a full stop.
- Use italics for book titles, giving all words in the title an initial capital.
- Use italics for journal and data repository names, abbreviating them according to common usage (with full stops).
- Use bold for volume numbers and the subsequent comma.
- Give the full page range (or article number), where appropriate.

Examples

Published papers:

Printed journals

Schott, D. H., Collins, R. N. & Bretscher, A. Secretory vesicle transport velocity in living cells depends on the myosin V lever arm length. *J. Cell Biol*. **156**, 35-39 (2002).

Online only

Bellin, D. L. *et al*. Electrochemical camera chip for simultaneous imaging of multiple metabolites in biofilms. *Nat. Commun*. **7**, 10535; 10.1038/ncomms10535 (2016).

For papers with more than five authors include only the first author's name followed by '*et al.*'.

Books:

Smith, J. Syntax of referencing in *How to reference books* (ed. Smith, S.) 180-181 (Macmillan, 2013).

Online material:

Babichev, S. A., Ries, J. & Lvovsky, A. I. Quantum scissors: teleportation of single-mode optical states by means of a nonlocal single photon. Preprint at https://arxiv.org/abs/quant-ph/0208066 (2002).

Manaster, J. Sloth squeak. *Scientific American Blog Network* http://blogs.scientificamerican.com/psi-vid/2014/04/09/sloth-squeak (2014).

Hao, Z., AghaKouchak, A., Nakhjiri, N. & Farahmand, A. Global integrated drought monitoring and prediction system (GIDMaPS) data sets. *figshare* https://doi.org/10.6084/m9.figshare.853801 (2014).

Acknowledgements

Please keep any acknowledgements brief, and don't include thanks to anonymous referees and editors, or any effusive comments. You may acknowledge grant or contribution numbers. You should also acknowledge assistance from medical writers, proof-readers and editors.

Author contributions

You must supply an Author Contribution Statement as described in the Author responsibilities section of our Editorial and Publishing Policies.

Please be aware:

- The author name you give as the corresponding author will be the main contact during the review process and should not change.
- The information you provide in the submission system will be used as the source of truth when your paper is published.

Competing interests

You must supply a competing interests statement. If there is no conflict of interest, you should include a statement declaring this.

Your statement must be explicit and unambiguous, describing any potential competing interest (or lack thereof) for EACH contributing author. The information you provide in the submission system will be used as the source of truth when your paper is published.

Examples of declarations are:

Competing interests

The author(s) declare no competing interests.

Competing interests

Dr X's work has been funded by A. He has received compensation as a member of the scientific advisory board of B and owns stock in the company. He also has consulted for C and received compensation. Dr Y and Dr Z declare no potential conflict of interest.

Data availability

You must include a Data Availability Statement in all submitted manuscripts (at the end of the main text, before the References section); see 'Availability of materials and data' section for more information.

Ethics declarations

If your research includes human or animal subjects, you will need to include the appropriate ethics declarations in the Methods section of your manuscript.

Approval for animal experiments

For experiments involving live vertebrates and/or higher invertebrates, your Methods section must include a statement that:

1. Identifies the institutional and/or licensing committee that approved the experiments, including any relevant details.
2. Confirms that all experiments were performed in accordance with relevant named guidelines and regulations.
3. Confirms that the authors complied with the ARRIVE guidelines.

Approval for human experiments

For experiments involving human subjects (or tissue samples), your Methods section must include a statement that:

1. Identifies the institutional and/or licensing committee that approved the experiments, including any relevant details.
2. Confirms that all experiments were performed in accordance with relevant named guidelines and regulations.

3. Confirms that informed consent was obtained from all participants and/or their legal guardians.

Consent to participate/Consent to publish

Please note that:

1. Study participant names (and other personally identifiable information) must be removed from all text/figures/tables/images.
2. The use of coloured bars/shapes or blurring to obscure the eyes/facial region of study participants is not an acceptable means of anonymisation. For manuscripts that include information or images that could lead to identification of a study participant, your Methods section must include a statement that confirms informed consent was obtained to publish the information/image(s) in an online open access publication.

Supplementary Information

You should submit any Supplementary Information together with the manuscript so that we can send it to referees during peer-review. This will be published online with accepted manuscripts.

It's vital that you carefully check your Supplementary Information before submission as any modification after your paper is published will require a formal correction.

Please avoid including any "data not shown" statements and instead make your data available via deposition in a public repository (see 'Availability of materials and data' for more information).

If any data that is necessary to evaluate the claims of your paper is not available via a public depository, make sure you provide it as Supplementary Information.

We do not edit, typeset or proof Supplementary Information, so please present it clearly and succinctly at initial submission, making sure it conforms to the style and terminology of the rest of the paper.

To avoid any delays to publication, please follow the guidelines below for creation, citation and submission of your Supplementary Information:

1. You can combine multiple pieces of Supplementary Information and supply them as a single composite file. If you wish to keep larger information (e.g. supplementary videos, spreadsheets [.csv or .xlsx] or data files) as another separate file you may do so.

2. Designate each item as Supplementary Table, Figure, Video, Audio, Note, Data, Discussion, Equations or Methods, as appropriate. Number Supplementary Tables and Figures as, for example, "Supplementary Table S1". This numbering should be separate from that used in tables and figures appearing in the main article. Supplementary Note or Methods should not be numbered; titles for these are optional.

3. Refer to each piece of supplementary material at the appropriate point(s) in the main article. Be sure to include the word "Supplementary" each time one is mentioned. Please do not refer to individual panels of supplementary figures.

4. Use the following examples as a guide (note: abbreviate "Figure" as "Fig." when in the middle of a sentence): "Table 1 provides a selected subset of the most active compounds. The entire list of 96 compounds can be found as Supplementary Table S1 online." "The biosynthetic pathway of L-ascorbic acid in animals involves intermediates of the D-glucuronic acid pathway (see Supplementary Fig. S2 online). Figure 2 shows...".

5. Remember to include a brief title and legend (incorporated into the file to appear near the image) as part of every figure submitted, and a title as part of every table.

6. Keep file sizes as small as possible, with a maximum size of 50 MB, so that they can be downloaded quickly.

7. Supplementary video files should be provided in the standard video aspects: 4:3, 16:9, 21:9.

If you have any further questions about the submission and preparation of Supplementary Information, please email: scirep.admin@nature.com.

Figure legends

Please begin your figure legends with a brief title sentence for the whole figure and continue with a short description of what is shown in each panel. Use any symbols in sequence and minimise the methodological details as much as possible. Keep each legend total to no more than 350 words. Provide text for figure legends in numerical order after the references.

Tables

Please submit any tables in your main article document in an editable format (Word or TeX/LaTeX, as appropriate), and not as images. Tables that include statistical analysis of data should describe their standards of error analysis and ranges in a table legend.

Equations

Include any equations and mathematical expressions in the main text of the paper. Identify equations that are referred to in the text by parenthetical numbers, such as (1), and refer to them in the manuscript as "equation (1)" etc.

For submissions in a .doc or .docx format, please make sure that all equations are provided in an editable Word format. You can produce these with the equation editor included in Microsoft Word.

General figure guidelines

You are responsible for obtaining permission to publish any figures or illustrations that are protected by copyright, including figures published elsewhere and pictures taken by professional photographers. We cannot publish images downloaded from the internet without appropriate permission.

You should state the source of any images used. If you or one of your co-authors has drawn the images, please mention this in your acknowledgements. For software, you should state the name, version number and URL.

Number any figures separately with Arabic numerals in the order they occur in the text of the manuscript. Include error bars when appropriate. Include a description of the statistical treatment of error analysis in the figure legend.

Please do not use schemes. You should submit sequences of chemical reactions or experimental procedures as figures, with appropriate captions. You may include in the manuscript a limited number of uncaptioned graphics depicting chemical structures - each labelled with their name, by a defined abbreviation, or by the bold Arabic numeral.

Use a clear, sans-serif typeface (for example, Helvetica) for figure lettering. Use the same typeface in the same font size for all figures in your paper. For Greek letters, use a 'symbols' font. Put all display items on a white background, and avoid excessive boxing, unnecessary colour, spurious decorative effects (such as three-dimensional 'skyscraper' histograms) and highly pixelated computer drawings. Never truncate the vertical axis of histograms to exaggerate small differences. Ensure any labelling is of sufficient size and contrast to be legible, even after appropriate reduction. The thinnest lines in the final figure should be no smaller than one point wide. You will be sent a proof that will include figures.

- Figures divided into parts should be labelled with a lower-case, bold letter (**a, b, c** and so on) in the same type size as used elsewhere in the figure.
- Lettering in figures should be in lower-case type, with only the first letter of each label capitalised.
- Units should have a single space between the number and the unit, and follow SI nomenclature (for example, ms rather than msec) or the nomenclature common to a particular field.

- Thousands should be separated by commas (1,000).
- Unusual units or abbreviations should be spelled out in full or defined in the legend.
- Scale bars should be used rather than magnification factors, with the length of the bar defined on the bar itself rather than in the legend.

In legends, please use visual cues rather than verbal explanations such as "open red triangles". Avoid unnecessary figures: data presented in small tables or histograms, for instance, can generally be stated briefly in the text instead. Figures should not contain more than one panel unless the parts are logically connected; each panel of a multipart figure should be sized so that the whole figure can be reduced by the same amount and reproduced at the smallest size at which essential details are visible.

Figures for peer review

At the initial submission stage, you may choose to upload separate figure files or to incorporate figures into the main article file, ensuring that any figures are of sufficient quality to be clearly legible.

When submitting a revised manuscript, you must upload all figures as separate figure files, ensuring that the image quality and formatting conforms to the specifications below.

Figures for publication

You must supply each complete figure as a separate file upload. Multi-part/panel figures must be prepared and arranged as a single image file (including all sub-parts; a, b, c, etc.). Please do not upload each panel individually.

Please read the digital images integrity and standards section of our Editorial and Publishing Policies. When possible, we prefer to use original digital figures to ensure the highest-quality reproduction in the journal. When creating and submitting digital files, please follow the guidelines below. Failure to do so, or to adhere to the following guidelines, can significantly delay publication of your work.

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1. Line art, graphs, charts and schematics

For optimal results, you should supply all line art, graphs, charts and schematics in vector format, such as EPS or AI. Please save or export it directly from the application in which it was made, making sure that data points and axis labels are clearly legible.

2. Photographic and bitmap images

Please supply all photographic and bitmap images in a bitmap image format such as tiff, jpg, or psd. If saving tiff files, please ensure that the compression option is selected to avoid very large file sizes. Please do not supply Word or Powerpoint files with placed images. Images can be supplied as RGB or CMYK (note: we will not convert image colour modes).

Figures that do not meet these standards will not reproduce well and may delay publication until we receive high-resolution images.

3. Chemical structures

Please produce Chemical structures using ChemDraw or a similar program. All chemical compounds must be assigned a bold, Arabic numeral in the order in which the compounds are presented in the manuscript text. Structures should then be exported into a 300 dpi RGB tiff file before being submitted.

4. Stereo images

You should present stereo diagrams for divergent 'wall-eyed' viewing, with the two panels separated by 5.5 cm. In the final accepted version of the manuscript, you should submit the stereo images at their final page size.

Statistical guidelines

If your paper contains statistical testing, it should state the name of the statistical test, the n value for each statistical analysis, the comparisons of interest, a justification for the use of that test (including, for example, a discussion of the normality of the data when the test is appropriate only

for normal data), the alpha level for all tests, whether the tests were one-tailed or two-tailed, and the actual P value for each test (not merely "significant" or "P < 0.05"). Please make it clear what statistical test was used to generate every P value. Use of the word "significant" should always be accompanied by a P value; otherwise, use "substantial," "considerable," etc.

Data sets should be summarised with descriptive statistics, which should include the n value for each data set, a clearly labelled measure of centre (such as the mean or the median), and a clearly labelled measure of variability (such as standard deviation or range).

Ranges are more appropriate than standard deviations or standard errors for small data sets. Graphs should include clearly labelled error bars. You must state whether a number that follows the ± sign is a standard error (s.e.m.) or a standard deviation (s.d.).

You must justify the use of a particular test and explain whether the data conforms to the assumptions of the tests. Three errors are particularly common:

- Multiple comparisons: when making multiple statistical comparisons on a single data set, you should explain how you adjusted the alpha level to avoid an inflated Type I error rate, or you should select statistical tests appropriate for multiple groups (such as ANOVA rather than a series of t-tests).
- Normal distribution: many statistical tests require that the data be approximately normally distributed; when using these tests, you should explain how you tested your data for normality. If the data does not meet the assumptions of the test, you should use a non-parametric alternative instead.
- Small sample size: when the sample size is small (less than about 10), you should use tests appropriate to small samples or justify the use of large-sample tests.

Chemical and biological nomenclature and abbreviations

You should identify molecular structures by bold, Arabic numerals assigned in order of presentation in the text. Once identified in the main text or a figure, you may refer to compounds by their name, by a defined abbreviation, or by the bold Arabic numeral (as long as the compound is referred to consistently as one of these three).

When possible, you should refer to chemical compounds and biomolecules using systematic nomenclature, preferably using IUPAC. You should use standard chemical and biological abbreviations. Make sure you define unconventional or specialist abbreviations at their first occurrence in the text.

Gene nomenclature

You should use approved nomenclature for gene symbols, and employ symbols rather than italicised full names (for example Ttn, not titin). Please consult the appropriate nomenclature databases for correct gene names and symbols. A useful resource is Entrez Gene.

You can get approved human gene symbols from HUGO Gene Nomenclature Committee (HGNC), e-mail: hgnc@genenames.org; see also www.genenames.org.

You can get approved mouse symbols from The Jackson Laboratory, e-mail: nomen@informatics.jax.org; see also www.informatics.jax.org/mgihome/nomen.

For proposed gene names that are not already approved, please submit the gene symbols to the appropriate nomenclature committees as soon as possible, as these must be deposited and approved before publication of an article.

Avoid listing multiple names of genes (or proteins) separated by a slash, as in 'Oct4/Pou5f1', as this is ambiguous (it could mean a ratio, a complex,

alternative names or different subunits). Use one name throughout and include the other at first mention: 'Oct4 (also known as Pou5f1)'.

Characterisation of chemical and biomolecular materials

Scientific Reports is committed to publishing technically sound research. Manuscripts submitted to the journal will be held to rigorous standards with respect to experimental methods and characterisation of new compounds.

You must provide adequate data to support your assignment of identity and purity for each new compound described in your manuscript. You should provide a statement confirming the source, identity and purity of known compounds that are central to the scientific study, even if they are purchased or resynthesised using published methods.

1. Chemical identity

Chemical identity for organic and organometallic compounds should be established through spectroscopic analysis. Standard peak listings (see formatting guidelines below) for 1H NMR and proton-decoupled 13C NMR should be provided for all new compounds. Other NMR data should be reported (31P NMR, 19F NMR, etc.) when appropriate. For new materials, you should also provide mass spectral data to support molecular weight identity. High-resolution mass spectral (HRMS) data is preferred. You may report UV or IR spectral data for the identification of characteristic functional groups, when appropriate. You should provide melting-point ranges for crystalline materials. You may report specific rotations for chiral compounds. You should provide references, rather than detailed procedures, for known compounds, unless their protocols represent a departure from or improvement on published methods.

2. Combinational compound libraries

When describing the preparation of combinatorial libraries, you should include standard characterisation data for a diverse panel of library components.

3. Biomolecular identity

For new biopolymeric materials (oligosaccharides, peptides, nucleic acids, etc.), direct structural analysis by NMR spectroscopic methods may not be possible. In these cases, you must provide evidence of identity based on sequence (when appropriate) and mass spectral characterisation.

4. Biological constructs

You should provide sequencing or functional data that validates the identity of their biological constructs (plasmids, fusion proteins, site-directed mutants, etc.) either in the manuscript text or the Methods section, as appropriate.

5. Sample purity

We request evidence of sample purity for each new compound. Methods for purity analysis depend on the compound class. For most organic and organometallic compounds, purity may be demonstrated by high-field 1H NMR or 13C NMR data, although elemental analysis (±0.4%) is encouraged for small molecules. You may use quantitative analytical methods including chromatographic (GC, HPLC, etc.) or electrophoretic analyses to demonstrate purity for small molecules and polymeric materials.

6. Spectral data

Please provide detailed spectral data for new compounds in list form (see below) in the Methods section. Figures containing spectra generally will not be published as a manuscript figure unless the data are directly relevant to the central conclusions of the paper. You are encouraged to include high-quality images of spectral data for key compounds in the Supplementary Information. You should list specific NMR assignments after integration values only if they were unambiguously determined by multidimensional NMR or decoupling experiments. You should provide information about how assignments were made in a general Methods section.

Example format for compound characterisation data. mp: 100-102 °C (lit.[ref] 99-101 °C); TLC ($CHCl_3$:MeOH, 98:2 v/v): R_f = 0.23; $[\alpha]_D$ = -21.5 (0.1 M in n-hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.30 (s, 1H), 7.55-7.41 (m,

6H), 5.61 (d, J = 5.5 Hz, 1H), 5.40 (d, J = 5.5 Hz, 1H), 4.93 (m, 1H), 4.20 (q, J = 8.5 Hz, 2H), 2.11 (s, 3H), 1.25 (t, J = 8.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.4, 165.0, 140.5, 138.7, 131.5, 129.2, 118.6, 84.2, 75.8, 66.7, 37.9, 20.1; IR (Nujol): 1765 cm-^{1}; UV/Vis: λ_{max} 267 nm; HRMS (m/z): $[M]^+$ calcd. for $C_{20}H_{15}C_{l2}NO_5$, 420.0406; found, 420.0412; analysis (calcd., found for $C_{20}H_{15}C_{l2}NO_5$): C (57.16, 57.22), H (3.60, 3.61), Cl (16.87, 16.88), N (3.33, 3.33), O (19.04, 19.09).

7. Crystallographic data for small molecules

If your manuscript is reporting new three-dimensional structures of small molecules from crystallographic analysis, you should include a .cif file and a structural figure with probability ellipsoids for publication as Supplementary Information. These must have been checked using the IUCR's CheckCIF routine, and you must include a PDF copy of the output with the submission, together with a justification for any alerts reported. You should submit crystallographic data for small molecules to the Cambridge Structural Database and the deposition number referenced appropriately in the manuscript. Full access must be provided on publication.

8. Macromolecular structural data

If your manuscript is reporting new structures, it should contain a table summarising structural and refinement statistics. Templates are available for such tables describing NMR and X-ray crystallography data. To facilitate assessment of the quality of the structural data, you should submit with the manuscript a stereo image of a portion of the electron density map (for crystallography papers) or of the superimposed lowest energy structures (≳10; for NMR papers). If the reported structure represents a novel overall fold, you should also provide a stereo image of the entire structure (as a backbone trace).

Registered Reports

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