DESCRIPTION

The *Journal of Molecular Graphics and Modelling* is devoted to the publication of papers on the uses of computers in theoretical investigations of molecular structure, function, interaction, and design. The scope of the journal includes all aspects of molecular modeling and computational chemistry, including, for instance, the study of molecular shape and properties, molecular simulations, protein and polymer engineering, drug design, materials design, structure-activity and structure-property relationships, database mining, and compound library design.

As a primary research journal, *JMGM* seeks to bring new knowledge to the attention of our readers. As such, submissions to the journal need to not only report results, but must draw conclusions and explore implications of the work presented. Authors are strongly encouraged to bear this in mind when preparing manuscripts. Routine applications of standard modelling approaches, providing only very limited new scientific insight, will not meet our criteria for publication. Reproducibility of reported calculations is an important issue. Wherever possible, we urge authors to enhance their papers with Supplementary Data, for example, in QSAR studies machine-readable versions of molecular datasets or in the development of new force-field parameters versions of the topology and force field parameter files. Routine applications of existing methods that do not lead to genuinely new insight will not be considered.

*JMGM* is published in association with two of the largest and most active professional societies in the field: the Molecular Graphics and Modelling Society (MGMS) and the Computers in Chemistry (COMP) Division of the American Chemical Society. Several thousand computational chemists worldwide belong to these two societies and any research topic that may of interest to the membership is within the wide scope of the journal. It is not necessary to be a member of these professional societies to publish in the journal.

Published in association with the Molecular Graphics and Modelling Society [www.mgms.org](http://www.mgms.org) and the ACS Division of Computers in Chemistry.

AUDIENCE

Researchers in computer graphics, molecular modelling, and automation for chemical engineering, engineered materials, and pharmaceutical research.
IMPACT FACTOR

2016: 1.754 © Thomson Reuters Journal Citation Reports 2017

ABSTRACTING AND INDEXING

Biotechnology Citation Index
Elsevier BIOBASE
Chemical Abstracts
Chemistry Citation Index
Computer and Information Systems Abstracts Journal
Current Contents
MEDLINE®
Research Alert
Science Citation Index
Scisearch
Scopus

EDITORIAL BOARD

Editors:
E.X. Esposito, exeResearch, East Lansing, Michigan, USA
J. Platts, Cardiff University, Cardiff, UK

Honorary Editor
J.D. Madura †

International Editorial Board:
J. Briggs, University of Houston, Houston, Texas, USA
R. Bryce, University of Manchester, Manchester, UK
T. Cagin, Texas A&M University, College Station, Texas, USA
T.E. Cheatham, The University of Utah, Salt Lake City, Utah, USA
E. Deliyanii, Aristotle University of Thessaloniki, Thessaloniki, Greece
M. Feig, Michigan State University, East Lansing, Michigan, USA
D.R. Flower, Aston University, Birmingham, UK
V. Gillet, University of Sheffield, Sheffield, England, UK
J.M. Goodman, University of Cambridge, Cambridge, UK
M. Gür, Istanbul Technical University, Beyoğlu, Istanbul, Turkey
D. Hamelberg, Georgia State University, Atlanta, Georgia, USA
J.D. Hirst, Nottingham, Nottingham, UK
A.J. Holder, University of Missouri at Kansas City, Kansas City, Missouri, USA
H. Jiang, Chinese Academy of Sciences (CAS), Shanghai, China
C.K. Kim, Inha University, Incheon, The Republic of Korea
D.R. Koes, University of Pittsburgh, Pittsburgh, Pennsylvania, USA
P. Kolb, Philipps-Universität Marburg, Marburg, Germany
A. Leach, GlaxoSmithKline, Stevenage, UK
R. Lewis, Novartis Pharma AG, Basel, Switzerland
J. Mitchell, University of St. Andrews, Haugh, St. Andrews, UK
M. Orozco, Institute for Research in Biomedicine (IRB Barcelona), Barcelona, Spain
E. Papaleo, University of Copenhagen, Copenhagen, Denmark
A.L. Parrill, University of Memphis, Memphis, Tennessee, USA
R. Paton, University of Oxford, Oxford, UK
Z. Qasmi, University of Karachi, Karachi, Pakistan
K. Roy, Jadavpur University, Kolkata, India
G.N. Sastry, Indian Institute of Chemical Technology, Hyderabad, India
J. Stone, University of Illinois at Urbana-Champaign, Urbana, Illinois, USA
M. Swart, Universitat de Girona, Girona, Spain
Y.J. Tseng, National Taiwan University, Taipei, Taiwan, ROC
D. Wei, Shanghai Jiao Tong University, Shanghai, China
W.J. Welsh, University of Medicine and Dentistry New Jersey (UMDNJ), Newark, New Jersey, USA
X. Yao, Lanzhou University, Lanzhou, China
E. Yuriev, Monash University, Parkville, Victoria, Australia
GUIDE FOR AUTHORS

Your Paper Your Way
We now differentiate between the requirements for new and revised submissions. You may choose to submit your manuscript as a single Word or PDF file to be used in the refereeing process. Only when your paper is at the revision stage, will you be requested to put your paper in to a 'correct format' for acceptance and provide the items required for the publication of your article.
To find out more, please visit the Preparation section below.

INTRODUCTION
Published in Affiliation with the Molecular Graphics and Modelling Society and the ACS Division of Computers in Chemistry Former title: Journal of Molecular Graphics

Scope
The Journal of Molecular Graphics and Modelling is devoted to the publication of papers on the uses of computers in theoretical investigations of molecular structure, function, interaction, and design. The scope of the journal includes all aspects of molecular modeling and computational chemistry, including, for instance, the study of molecular shape and properties, molecular simulations, protein and polymer engineering, drug design, materials design, structure-activity and structure-property relationships, database mining, and compound library design.

As a primary research journal, JMGM seeks to bring new knowledge to the attention of our readers. As such, submissions to the journal need to not only report results, but must draw conclusions and explore implications of the work presented. Authors are strongly encouraged to bear this in mind when preparing manuscripts.

JMGM is published in association with two of the largest and most active professional societies in the field: the Molecular Graphics and Modelling Society (MGMS) and the Computers in Chemistry (COMP) Division of the American Chemical Society. Several thousand computational chemists worldwide belong to these two societies and any research topic that may of interest to the membership is within the wide scope of the journal. It is not necessary to be a member of these professional societies to publish in the journal.

Programs
Descriptions of programs will not be accepted for publication by JMGM, but descriptions of algorithms are acceptable.

Supplementary Information
Authors should carefully develop manuscripts with brevity and clarity in mind, and as much material as possible should be deposited online as Supplementary Information. Consider placing items that are not REQUIRED for understanding the main conclusions of the paper, but are necessary for the reasons of repeatability and more detailed analysis in this category.

Types of papers
The editors also welcome authoritative review articles or commentaries on any aspect of molecular modeling and computational chemistry. If you are interested in contributing such material, you should first contact one of the Editors.

Structural Data
For papers describing structures of biological macromolecules, the atomic coordinates and the related experimental data (structure factor amplitudes/intensities and/or NMR restraints) must be deposited at a member site of the Worldwide Protein Data Bank (http://www.wwpdb.org): RCSB PDB (http://www.pdb.org), MSD-EBI (http://www.ebi.ac.uk/pdbe/), PDBj (http://www.pdbj.org, or BMRB (http://www.bmrb.wisc.edu). Manuscripts must carry a statement that coordinates and structure factors (or NMR restraints) have been deposited in the Protein Data Bank. The accession number(s) must be cited in the manuscript at the end of the Materials and Methods section. Authors must agree to release the atomic coordinates and experimental data immediately upon publication.
It is increasingly common for coordinates to be deposited in the Protein Data Bank without an associated publication. Before submission to JSB, authors are expected to search the Protein Data Bank for related structures using one or more alignment programs and report the outcome. Prior deposition of related coordinates, without an associated publication, does not necessarily preclude publication in JMGM. The primary criteria for publication of a structure in JMGM are that it provides novel structural insights or important new functional and biological insights that are likely to be of general interest.

**Page Charges**
This journal has no page charges.

**Submission checklist**
You can use this list to carry out a final check of your submission before you send it to the journal for review. Please check the relevant section in this Guide for Authors for more details.

Ensure that the following items are present:

One author has been designated as the corresponding author with contact details:
- E-mail address
- Full postal address

All necessary files have been uploaded:
**Manuscript:**
- Include keywords
- All figures (include relevant captions)
- All tables (including titles, description, footnotes)
- Ensure all figure and table citations in the text match the files provided
- Indicate clearly if color should be used for any figures in print

**Graphical Abstracts / Highlights files** (where applicable)

**Supplemental files** (where applicable)

Further considerations:
- Manuscript has been 'spell checked' and 'grammar checked'
- All references mentioned in the Reference List are cited in the text, and vice versa
- Permission has been obtained for use of copyrighted material from other sources (including the Internet)
- A competing interests statement is provided, even if the authors have no competing interests to declare
- Journal policies detailed in this guide have been reviewed
- Referee suggestions and contact details provided, based on journal requirements

For further information, visit our Support Center.

**BEFORE YOU BEGIN**

**Ethics in publishing**
Please see our information pages on Ethics in publishing and Ethical guidelines for journal publication.

**Declaration of interest**
All authors must disclose any financial and personal relationships with other people or organizations that could inappropriately influence (bias) their work. Examples of potential conflicts of interest include employment, consultancies, stock ownership, honoraria, paid expert testimony, patent applications/registrations, and grants or other funding. If there are no conflicts of interest then please state this: 'Conflicts of interest: none'. More information.

**Submission declaration and verification**
Submission of an article implies that the work described has not been published previously (except in the form of an abstract or as part of a published lecture or academic thesis or as an electronic preprint, see 'Multiple, redundant or concurrent publication' section of our ethics policy for more information), that it is not under consideration for publication elsewhere, that its publication is approved by all authors and tacitly or explicitly by the responsible authorities where the work was...
carried out, and that, if accepted, it will not be published elsewhere in the same form, in English or in any other language, including electronically without the written consent of the copyright-holder. To verify originality, your article may be checked by the originality detection service CrossCheck.

**Changes to authorship**
Authors are expected to consider carefully the list and order of authors **before** submitting their manuscript and provide the definitive list of authors at the time of the original submission. Any addition, deletion or rearrangement of author names in the authorship list should be made only **before** the manuscript has been accepted and only if approved by the journal Editor. To request such a change, the Editor must receive the following from the **corresponding author**: (a) the reason for the change in author list and (b) written confirmation (e-mail, letter) from all authors that they agree with the addition, removal or rearrangement. In the case of addition or removal of authors, this includes confirmation from the author being added or removed.

Only in exceptional circumstances will the Editor consider the addition, deletion or rearrangement of authors **after** the manuscript has been accepted. While the Editor considers the request, publication of the manuscript will be suspended. If the manuscript has already been published in an online issue, any requests approved by the Editor will result in a corrigendum.

**Copyright**
Upon acceptance of an article, authors will be asked to complete a 'Journal Publishing Agreement' (see [more information](#) on this). An e-mail will be sent to the corresponding author confirming receipt of the manuscript together with a 'Journal Publishing Agreement' form or a link to the online version of this agreement.

Subscribers may reproduce tables of contents or prepare lists of articles including abstracts for internal circulation within their institutions. **Permission** of the Publisher is required for resale or distribution outside the institution and for all other derivative works, including compilations and translations. If excerpts from other copyrighted works are included, the author(s) must obtain written permission from the copyright owners and credit the source(s) in the article. Elsevier has [preprinted forms](#) for use by authors in these cases.

For open access articles: Upon acceptance of an article, authors will be asked to complete an 'Exclusive License Agreement' ([more information](#)). Permitted third party reuse of open access articles is determined by the author’s choice of [user license](#).

**Author rights**
As an author you (or your employer or institution) have certain rights to reuse your work. [More information](#).

Elsevier supports responsible sharing
Find out how you can [share your research](#) published in Elsevier journals.

**Role of the funding source**
You are requested to identify who provided financial support for the conduct of the research and/or preparation of the article and to briefly describe the role of the sponsor(s), if any, in study design; in the collection, analysis and interpretation of data; in the writing of the report; and in the decision to submit the article for publication. If the funding source(s) had no such involvement then this should be stated.

**Funding body agreements and policies**
Elsevier has established a number of agreements with funding bodies which allow authors to comply with their funder's open access policies. Some funding bodies will reimburse the author for the Open Access Publication Fee. Details of [existing agreements](#) are available online.

**Open access**
This journal offers authors a choice in publishing their research:

**Subscription**
- Articles are made available to subscribers as well as developing countries and patient groups through our [universal access programs](#).
- No open access publication fee payable by authors.

**Open access**
- Articles are freely available to both subscribers and the wider public with permitted reuse.
• An open access publication fee is payable by authors or on their behalf, e.g. by their research funder or institution.

Regardless of how you choose to publish your article, the journal will apply the same peer review criteria and acceptance standards.

For open access articles, permitted third party (re)use is defined by the following Creative Commons user licenses:

Creative Commons Attribution (CC BY)
Lets others distribute and copy the article, create extracts, abstracts, and other revised versions, adaptations or derivative works of or from an article (such as a translation), include in a collective work (such as an anthology), text or data mine the article, even for commercial purposes, as long as they credit the author(s), do not represent the author as endorsing their adaptation of the article, and do not modify the article in such a way as to damage the author's honor or reputation.

Creative Commons Attribution-NonCommercial-NoDerivs (CC BY-NC-ND)
For non-commercial purposes, lets others distribute and copy the article, and to include in a collective work (such as an anthology), as long as they credit the author(s) and provided they do not alter or modify the article.

The open access publication fee for this journal is USD 2600, excluding taxes. Learn more about Elsevier's pricing policy: http://www.elsevier.com/openaccesspricing.

Green open access
Authors can share their research in a variety of different ways and Elsevier has a number of green open access options available. We recommend authors see our green open access page for further information. Authors can also self-archive their manuscripts immediately and enable public access from their institution's repository after an embargo period. This is the version that has been accepted for publication and which typically includes author-incorporated changes suggested during submission, peer review and in editor-author communications. Embargo period: For subscription articles, an appropriate amount of time is needed for journals to deliver value to subscribing customers before an article becomes freely available to the public. This is the embargo period and it begins from the date the article is formally published online in its final and fully citable form. Find out more.

This journal has an embargo period of 24 months.

Elsevier Publishing Campus
The Elsevier Publishing Campus (www.publishingcampus.com) is an online platform offering free lectures, interactive training and professional advice to support you in publishing your research. The College of Skills training offers modules on how to prepare, write and structure your article and explains how editors will look at your paper when it is submitted for publication. Use these resources, and more, to ensure that your submission will be the best that you can make it.

Language (usage and editing services)
Please write your text in good English (American or British usage is accepted, but not a mixture of these). Authors who feel their English language manuscript may require editing to eliminate possible grammatical or spelling errors and to conform to correct scientific English may wish to use the English Language Editing service available from Elsevier's WebShop.

Submission
Our online submission system guides you stepwise through the process of entering your article details and uploading your files. The system converts your article files to a single PDF file used in the peer-review process. Editable files (e.g., Word, LaTeX) are required to typeset your article for final publication. All correspondence, including notification of the Editor's decision and requests for revision, is sent by e-mail.

Referees
The names, affiliation and email addresses of five potential Referees are required (no generic mail addresses such as gmail or hotmail are allowed). Appropriate Referees should be knowledgeable about the subject and have potential interest in the work. Referees should have no close connection with any of the authors and be from institutions other than (and preferably countries other than) those of any of the Authors. Articles will not be considered for publication if this requirement is not met.

PREPARATION

NEW SUBMISSIONS
Submission to this journal proceeds totally online and you will be guided stepwise through the creation and uploading of your files. The system automatically converts your files to a single PDF file, which is used in the peer-review process.
As part of the Your Paper Your Way service, you may choose to submit your manuscript as a single file to be used in the refereeing process. This can be a PDF file or a Word document, in any format or layout that can be used by referees to evaluate your manuscript. It should contain high enough quality figures for refereeing. If you prefer to do so, you may still provide all or some of the source files at the initial submission. Please note that individual figure files larger than 10 MB must be uploaded separately.

References
There are no strict requirements on reference formatting at submission. References can be in any style or format as long as the style is consistent. Where applicable, author(s) name(s), journal title/book title, chapter title/article title, year of publication, volume number/book chapter and the pagination must be present. Use of DOI is highly encouraged. The reference style used by the journal will be applied to the accepted article by Elsevier at the proof stage. Note that missing data will be highlighted at proof stage for the author to correct.

Formatting requirements
There are no strict formatting requirements but all manuscripts must contain the essential elements needed to convey your manuscript, for example Abstract, Keywords, Introduction, Materials and Methods, Results, Conclusions, Artwork and Tables with Captions.
If your article includes any Videos and/or other Supplementary material, this should be included in your initial submission for peer review purposes.
Divide the article into clearly defined sections.
Figures and tables embedded in text
Please ensure the figures and the tables included in the single file are placed next to the relevant text in the manuscript, rather than at the bottom or the top of the file. The corresponding caption should be placed directly below the figure or table.

Peer review
This journal operates a single blind review process. All contributions will be initially assessed by the editor for suitability for the journal. Papers deemed suitable are then typically sent to a minimum of two independent expert reviewers to assess the scientific quality of the paper. The Editor is responsible for the final decision regarding acceptance or rejection of articles. The Editor’s decision is final. More information on types of peer review.

REVISED SUBMISSIONS
Use of word processing software
Regardless of the file format of the original submission, at revision you must provide us with an editable file of the entire article. Keep the layout of the text as simple as possible. Most formatting codes will be removed and replaced on processing the article. The electronic text should be prepared in a way very similar to that of conventional manuscripts (see also the Guide to Publishing with Elsevier). See also the section on Electronic artwork.
To avoid unnecessary errors you are strongly advised to use the 'spell-check' and 'grammar-check' functions of your word processor.

LaTeX
You are recommended to use the Elsevier article class elsarticle.cls to prepare your manuscript and BibTeX to generate your bibliography.
Our LaTeX site has detailed submission instructions, templates and other information.
**Essential title page information**

- **Title.** Concise and informative. Titles are often used in information-retrieval systems. Avoid abbreviations and formulae where possible.
- **Author names and affiliations.** Please clearly indicate the given name(s) and family name(s) of each author and check that all names are accurately spelled. Present the authors’ affiliation addresses (where the actual work was done) below the names. Indicate all affiliations with a lower-case superscript letter immediately after the author’s name and in front of the appropriate address. Provide the full postal address of each affiliation, including the country name and, if available, the e-mail address of each author.
- **Corresponding author.** Clearly indicate who will handle correspondence at all stages of refereeing and publication, also post-publication. **Ensure that the e-mail address is given and that contact details are kept up to date by the corresponding author.**
- **Present/permanent address.** If an author has moved since the work described in the article was done, or was visiting at the time, a 'Present address' (or 'Permanent address') may be indicated as a footnote to that author’s name. The address at which the author actually did the work must be retained as the main, affiliation address. Superscript Arabic numerals are used for such footnotes.

**Graphical abstract**

A graphical abstract is mandatory for this journal. It should summarize the contents of the article in a concise, pictorial form designed to capture the attention of a wide readership online. Authors must provide images that clearly represent the work described in the article. Graphical abstracts should be submitted as a separate file in the online submission system. Image size: please provide an image with a minimum of 531 × 1328 pixels (h × w) or proportionally more. The image should be readable at a size of 5 × 13 cm using a regular screen resolution of 96 dpi. Preferred file types: TIFF, EPS, PDF or MS Office files. You can view Example Graphical Abstracts on our information site.

Authors can make use of Elsevier's Illustration Services to ensure the best presentation of their images also in accordance with all technical requirements.

**Highlights**

Highlights are mandatory for this journal. They consist of a short collection of bullet points that convey the core findings of the article and should be submitted in a separate editable file in the online submission system. Please use 'Highlights' in the file name and include 3 to 5 bullet points (maximum 85 characters, including spaces, per bullet point). You can view example Highlights on our information site.

**Keywords**

Immediately after the abstract provide a minimum of 5 keywords. These keywords will be used for indexing purposes.

**Formatting of funding sources**

List funding sources in this standard way to facilitate compliance to funder's requirements:

Funding: This work was supported by the National Institutes of Health [grant numbers xxxx, yyyy]; the Bill & Melinda Gates Foundation, Seattle, WA [grant number zzzz]; and the United States Institutes of Peace [grant number aaaa].

It is not necessary to include detailed descriptions on the program or type of grants and awards. When funding is from a block grant or other resources available to a university, college, or other research institution, submit the name of the institute or organization that provided the funding.

If no funding has been provided for the research, please include the following sentence:

This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

**Nomenclature and Units**

Use of Systeme Internationale (SI) units is encouraged; provide a conversion factor in parentheses at the first mention of non-SI units. Biochemical nomenclature should conform to that recommended by the IUPAC-IUB Commission, and enzymes should be referred to by their recommended names and numbers.
Mathematical and Technical Terms

Write mathematical, Greek and other symbols carefully using, for instance, a Symbol font. Explain the meaning of all symbols and acronyms in the text where they first occur. Identify Greek letters at their first mention by writing their names in English words in the margin. If you use several symbols, a list of definitions -- not necessarily for publication -- will be useful to and ensure the accuracy of the production editors. Identify all vectors, tensors, and matrices in bold. The journal is read by an international audience; therefore authors should attempt to make their work clear to diverse readers. Note the following points:

- Use a zero before decimal quantities less than one, e.g., 0.376, not .376.
- Group numbers consisting of more than three numerals in threes separated by spaces, rather than commas.
- Use fractional exponents instead of root signs, e.g., (3x + 9y)**1/2, not the square root symbol. (Here ** indicates that 1/2 is an exponent).
- Specify whether logarithms are to base 10 or base e.
- Write simple mathematical fractions in the text on one line, e.g., L(N - l)/L(l), not as a stacked fraction. If the fraction is complicated with superscripts and subscripts, then present it in a manner consistent with maximum clarity.

Footnotes

Footnotes should be used sparingly. Number them consecutively throughout the article. Many word processors build footnotes into the text, and this feature may be used. Should this not be the case, indicate the position of footnotes in the text and present the footnotes themselves separately at the end of the article.

Artwork

Electronic artwork

General points

- Make sure you use uniform lettering and sizing of your original artwork.
- Preferred fonts: Arial (or Helvetica), Times New Roman (or Times), Symbol, Courier.
- Number the illustrations according to their sequence in the text.
- Use a logical naming convention for your artwork files.
- Indicate per figure if it is a single, 1.5 or 2-column fitting image.
- For Word submissions only, you may still provide figures and their captions, and tables within a single file at the revision stage.
- Please note that individual figure files larger than 10 MB must be provided in separate source files.

You are urged to visit this site; some excerpts from the detailed information are given here.

Formats

Regardless of the application used, when your electronic artwork is finalized, please 'save as' or convert the images to one of the following formats (note the resolution requirements for line drawings, halftones, and line/halftone combinations given below):
- EPS (or PDF): Vector drawings. Embed the font or save the text as 'graphics'.
- TIFF (or JPEG): Color or grayscale photographs (halftones): always use a minimum of 300 dpi.
- TIFF (or JPEG): Bitmapped line drawings: use a minimum of 1000 dpi.
- TIFF (or JPEG): Combinations bitmapped line/half-tone (color or grayscale): a minimum of 500 dpi is required.

Please do not:

- Supply files that are optimized for screen use (e.g., GIF, BMP, PICT, WPG); the resolution is too low.
- Supply files that are too low in resolution.
- Submit graphics that are disproportionately large for the content.

Color artwork

Please make sure that artwork files are in an acceptable format (TIFF (or JPEG), EPS (or PDF) or MS Office files) and with the correct resolution. If, together with your accepted article, you submit usable color figures then Elsevier will ensure, at no additional charge, that these figures will appear in color online (e.g., ScienceDirect and other sites) in addition to color reproduction in print. Further information on the preparation of electronic artwork.
Figure captions
Ensure that each illustration has a caption. A caption should comprise a brief title (not on the figure itself) and a description of the illustration. Keep text in the illustrations themselves to a minimum but explain all symbols and abbreviations used.

Tables
Please submit tables as editable text and not as images. Tables can be placed either next to the relevant text in the article, or on separate page(s) at the end. Number tables consecutively in accordance with their appearance in the text and place any table notes below the table body. Be sparing in the use of tables and ensure that the data presented in them do not duplicate results described elsewhere in the article. Please avoid using vertical rules and shading in table cells.

References
Citation in text
Please ensure that every reference cited in the text is also present in the reference list (and vice versa). Any references cited in the abstract must be given in full. Unpublished results and personal communications are not recommended in the reference list, but may be mentioned in the text. If these references are included in the reference list they should follow the standard reference style of the journal and should include a substitution of the publication date with either 'Unpublished results' or 'Personal communication'. Citation of a reference as 'in press' implies that the item has been accepted for publication.

Reference links
Increased discoverability of research and high quality peer review are ensured by online links to the sources cited. In order to allow us to create links to abstracting and indexing services, such as Scopus, CrossRef and PubMed, please ensure that data provided in the references are correct. Please note that incorrect surnames, journal/book titles, publication year and pagination may prevent link creation. When copying references, please be careful as they may already contain errors. Use of the DOI is encouraged.

A DOI can be used to cite and link to electronic articles where an article is in-press and full citation details are not yet known, but the article is available online. A DOI is guaranteed never to change, so you can use it as a permanent link to any electronic article. An example of a citation using DOI for an article not yet in an issue is: VanDecar J.C., Russo R.M., James D.E., Ambeh W.B., Franke M. (2003). Aseismic continuation of the Lesser Antilles slab beneath northeastern Venezuela. Journal of Geophysical Research, https://doi.org/10.1029/2001JB000884. Please note the format of such citations should be in the same style as all other references in the paper.

Data references
This journal encourages you to cite underlying or relevant datasets in your manuscript by citing them in your text and including a data reference in your Reference List. Data references should include the following elements: author name(s), dataset title, data repository, version (where available), year, and global persistent identifier. Add [dataset] immediately before the reference so we can properly identify it as a data reference. The [dataset] identifier will not appear in your published article.


Reference management software
Most Elsevier journals have their reference template available in many of the most popular reference management software products. These include all products that support Citation Style Language styles, such as Mendeley and Zotero, as well as EndNote. Using the word processor plug-ins from these products, authors only need to select the appropriate journal template when preparing their article, after which citations and bibliographies will be automatically formatted in the journal's style. If no template is yet available for this journal, please follow the format of the sample references and citations as shown in this Guide.

Users of Mendeley Desktop can easily install the reference style for this journal by clicking the following link:
When preparing your manuscript, you will then be able to select this style using the Mendeley plug-ins for Microsoft Word or LibreOffice.
Reference formatting
There are no strict requirements on reference formatting at submission. References can be in any style or format as long as the style is consistent. Where applicable, author(s) name(s), journal title/book title, chapter title/article title, year of publication, volume number/book chapter and the pagination must be present. Use of DOI is highly encouraged. The reference style used by the journal will be applied to the accepted article by Elsevier at the proof stage. Note that missing data will be highlighted at proof stage for the author to correct. If you do wish to format the references yourself they should be arranged according to the following examples:

Reference Style


Commercial products, including computer programs, are to be mentioned in the text of the manuscript and not normally referenced. If required the reference should list the first author et al. only.

Video
Elsevier accepts video material and animation sequences to support and enhance your scientific research. Authors who have video or animation files that they wish to submit with their article are strongly encouraged to include links to these within the body of the article. This can be done in the same way as a figure or table by referring to the video or animation content and noting in the body text where it should be placed. All submitted files should be properly labeled so that they directly relate to the video file's content. In order to ensure that your video or animation material is directly usable, please provide the files in one of our recommended file formats with a preferred maximum size of 150 MB in total. Any single file should not exceed 50 MB. Video and animation files supplied will be published online in the electronic version of your article in Elsevier Web products, including ScienceDirect. Please supply 'stills' with your files: you can choose any frame from the video or animation or make a separate image. These will be used instead of standard icons and will personalize the link to your video data. For more detailed instructions please visit our video instruction pages. Note: since video and animation cannot be embedded in the print version of the journal, please provide text for both the electronic and the print version for the portions of the article that refer to this content.

Supplementary data
Elsevier accepts electronic supplementary material to support and enhance your scientific research. Supplementary files offer the author additional possibilities to publish supporting applications, high-resolution images, machine-readable files of datasets (especially compounds) sound clips and more. Supplementary files supplied will be published online alongside the electronic version of your article in Elsevier Web products, including ScienceDirect: http://www.sciencedirect.com. In order to ensure that your submitted material is directly usable, please provide the data in one of our recommended file formats. Authors should submit the material in electronic format together with the article and supply a concise and descriptive caption for each file. For more detailed instructions please visit our artwork instruction pages at http://www.elsevier.com/artworkinstructions.

RESEARCH DATA
This journal encourages and enables you to share data that supports your research publication where appropriate, and enables you to interlink the data with your published articles. Research data refers to the results of observations or experimentation that validate research findings. To facilitate reproducibility and data reuse, this journal also encourages you to share your software, code, models, algorithms, protocols, methods and other useful materials related to the project.
Below are a number of ways in which you can associate data with your article or make a statement about the availability of your data when submitting your manuscript. If you are sharing data in one of these ways, you are encouraged to cite the data in your manuscript and reference list. Please refer to the "References" section for more information about data citation. For more information on depositing, sharing and using research data and other relevant research materials, visit the research data page.

**Data linking**

If you have made your research data available in a data repository, you can link your article directly to the dataset. Elsevier collaborates with a number of repositories to link articles on ScienceDirect with relevant repositories, giving readers access to underlying data that gives them a better understanding of the research described.

There are different ways to link your datasets to your article. When available, you can directly link your dataset to your article by providing the relevant information in the submission system. For more information, visit the database linking page.

For supported data repositories a repository banner will automatically appear next to your published article on ScienceDirect.

In addition, you can link to relevant data or entities through identifiers within the text of your manuscript, using the following format: Database: xxxx (e.g., TAIR: AT1G01020; CCDC: 734053; PDB: 1XFN).

**Mendeley Data**

This journal supports Mendeley Data, enabling you to deposit any research data (including raw and processed data, video, code, software, algorithms, protocols, and methods) associated with your manuscript in a free-to-use, open access repository. During the submission process, after uploading your manuscript, you will have the opportunity to upload your relevant datasets directly to Mendeley Data. The datasets will be listed and directly accessible to readers next to your published article online.

For more information, visit the Mendeley Data for journals page.

**Data in Brief**

You have the option of converting any or all parts of your supplementary or additional raw data into one or multiple data articles, a new kind of article that houses and describes your data. Data articles ensure that your data is actively reviewed, curated, formatted, indexed, given a DOI and publicly available to all upon publication. You are encouraged to submit your article for Data in Brief as an additional item directly alongside the revised version of your manuscript. If your research article is accepted, your data article will automatically be transferred over to Data in Brief where it will be editorially reviewed and published in the open access data journal, Data in Brief. Please note an open access fee of 500 USD is payable for publication in Data in Brief. Full details can be found on the Data in Brief website. Please use this template to write your Data in Brief.

**MethodsX**

You have the option of converting relevant protocols and methods into one or multiple MethodsX articles, a new kind of article that describes the details of customized research methods. Many researchers spend a significant amount of time on developing methods to fit their specific needs or setting, but often without getting credit for this part of their work. MethodsX, an open access journal, now publishes this information in order to make it searchable, peer reviewed, citable and reproducible. Authors are encouraged to submit their MethodsX article as an additional item directly alongside the revised version of their manuscript. If your research article is accepted, your methods article will automatically be transferred over to MethodsX where it will be editorially reviewed. Please note an open access fee is payable for publication in MethodsX. Full details can be found on the MethodsX website. Please use this template to prepare your MethodsX article.

**Data statement**

To foster transparency, we encourage you to state the availability of your data in your submission. This may be a requirement of your funding body or institution. If your data is unavailable to access or unsuitable to post, you will have the opportunity to indicate why during the submission process, for example by stating that the research data is confidential. The statement will appear with your published article on ScienceDirect. For more information, visit the Data Statement page.
ARTICLE ENRICHMENTS

AudioSlides
The journal encourages authors to create an AudioSlides presentation with their published article. AudioSlides are brief, webinar-style presentations that are shown next to the online article on ScienceDirect. This gives authors the opportunity to summarize their research in their own words and to help readers understand what the paper is about. More information and examples are available. Authors of this journal will automatically receive an invitation e-mail to create an AudioSlides presentation after acceptance of their paper.

Chemical Compound Viewer (Reaxys)
You can enrich your article with visual representations, links and details for those chemical structures that you define as the main chemical compounds described. Please follow the instructions to learn how to do this.

3D molecular models
You can enrich your online articles by providing 3D molecular models (optional) in PDB, PSE or MOL/MOL2 format, which will be visualized using the interactive viewer embedded within the article. Using the viewer, it will be possible to zoom into the model, rotate and pan the model, and change display settings. Submitted models will also be available for downloading from your online article on ScienceDirect. Each molecular model will have to be uploaded to the online submission system separately, via the '3D molecular models' submission category. More information.

Interactive plots
This journal enables you to show an Interactive Plot with your article by simply submitting a data file. Full instructions.

Interactive Network Viewer
This journal enables you to enrich your online article by including interactive network diagrams created with the latest version of Cytoscape. Each network should be exported from Cytoscape as a ZIP file containing a pair of network (.cyjs) and visual style (.json) files, which is most easily done using the green "SD" button. The recommended maximum file size of a dataset is 150 MB or less. Once the article is accepted, your ZIP datasets will appear as supplementary material on ScienceDirect and will be visualized inside the Cytoscape application which is displayed alongside your article. Readers will then be able to interactively explore your networks while reading the article. Please note that you must use the latest available version of Cytoscape. More information.

AFTER ACCEPTANCE

Online proof correction
Corresponding authors will receive an e-mail with a link to our online proofing system, allowing annotation and correction of proofs online. The environment is similar to MS Word: in addition to editing text, you can also comment on figures/tables and answer questions from the Copy Editor. Web-based proofing provides a faster and less error-prone process by allowing you to directly type your corrections, eliminating the potential introduction of errors. If preferred, you can still choose to annotate and upload your edits on the PDF version. All instructions for proofing will be given in the e-mail we send to authors, including alternative methods to the online version and PDF.

We will do everything possible to get your article published quickly and accurately. Please use this proof only for checking the typesetting, editing, completeness and correctness of the text, tables and figures. Significant changes to the article as accepted for publication will only be considered at this stage with permission from the Editor. It is important to ensure that all corrections are sent back to us in one communication. Please check carefully before replying, as inclusion of any subsequent corrections cannot be guaranteed. Proofreading is solely your responsibility.

Offprints
The corresponding author will, at no cost, receive a customized Share Link providing 50 days free access to the final published version of the article on ScienceDirect. The Share Link can be used for sharing the article via any communication channel, including email and social media. For an extra charge, paper offprints can be ordered via the offprint order form which is sent once the article is accepted for publication. Both corresponding and co-authors may order offprints at any time via Elsevier's Webshop. Corresponding authors who have published their article open access do not receive a Share Link as their final published version of the article is available open access on ScienceDirect and can be shared through the article DOI link.
AUTHOR INQUIRIES

Visit the Elsevier Support Center to find the answers you need. Here you will find everything from Frequently Asked Questions to ways to get in touch.

You can also check the status of your submitted article or find out when your accepted article will be published.