

Bioorganic & Medicinal Chemistry

Instructions to Contributors

Bioorganic & Medicinal Chemistry seeks to publish review articles and experimental or theoretical research results of outstanding significance and timeliness in the fields of chemical biology, medicinal chemistry, bioinorganic chemistry, and related disciplines. *Articles* should describe original research of high quality and timeliness.

Reviews of topical importance and current relevance are specially commissioned in appropriate fields. Authors wishing to submit a non-solicited review article are requested to first contact the Editor-in-Chief, Professor C.-H. Wong.

Perspectives briefly review (in 1–4 printed pages) specific subjects which already have or are likely to have major impact in areas related to chemical biology and drug discovery. Authors of perspectives are those who have made the original contribution or have extended the original research to new breakthroughs. Perspectives are generally specially commissioned by the Editors, however, suggestions for topics and authors are welcomed. Individuals interested in contributing should contact the Editor-in-Chief, Professor C.-H. Wong.

Symposia-in-Print comprise collections of original research papers (including experimental sections) covering specific topics. Topics for forthcoming symposia are announced in the Journal from time to time. A Guest Editor will invite authors active in the field to submit papers, which are then reviewed and processed for publication by the Guest Editor under the usual refereeing system. Opportunity is also provided for other active investigators to submit contributions.

Journal policy

Publications will be typeset. The language of submission is English.

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), 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and tacitly or explicitly by the responsible authorities where the work was carried out, and that, if accepted, it will not be published elsewhere in the same form, in English or in any other language, without the written consent of the Publisher. Authors accept full responsibility for the factual accuracy of the data presented and should obtain any authorization necessary for publication. **As such the contents of the papers are the sole responsibility of the authors and publication shall not imply the concurrence of the Editors or Publisher.**

All papers are submitted to referees who advise the Editor on the matter of acceptance in accordance with the high standards required, on the understanding that the subject matter has not been previously published and is not under consideration elsewhere. Referees will be asked to distinguish contributions meeting the above requirements and having an element of novelty, timeliness, and urgency that merits publication in the Journal. We ask referees to help in the selection of articles that have this breadth and suggest that papers covering narrower aspects of the field be sent to journals specializing in those areas. Referee names are not disclosed, but their views are forwarded by the Editor to the authors for consideration. Authors are **strongly** encouraged to suggest names of several experts in the field when papers are first submitted or at any time in the evaluation process.

Preparation of manuscripts

General requirements: Manuscripts should be printed, double line spaced, one side only, using black type on good quality white paper in a manner that ensures a clean, clear impression on the letters. The corresponding author's full mailing address, including mail codes, phone number, fax number, and e-mail address should be included. Authors are asked to provide four key words, which will be used for indexing purposes. The manuscript should be compiled in the following order: Graphical Abstract, Title, Authors, Affiliations, Abstract, Keywords, Introduction, Results, Discussion, Conclusion, Experimental, References and Notes, Tables, Figures, Schemes, and Legends. Any author who is not fluent in idiomatic English are urged to gain

assistance with manuscript preparation. Reviewers are not expected to correct grammatical errors and any deficiency in this area may detract from the scientific content of the paper.

Graphical abstracts: Authors must supply a graphical abstract at the time the paper is first submitted. The abstract should summarise the contents of the paper in a concise, pictorial form designed to capture the attention of a wide readership and for compilation of databases. Carefully drawn chemical structures are desired that serve to illustrate the theme of the paper. Authors may also provide appropriate text, not exceeding 50 words.

The content of the graphical abstract will be typeset and should be kept within an area of 5cm by 17cm. Authors must supply the graphical abstract on disk as well as in printed form, or if using online submission include the graphical abstract in the main article file and then attach the graphic separately.

For examples of graphical abstracts, please consult a recent issue of the journal or visit the journal page on ScienceDirect at: <http://www.sciencedirect.com/science/journal/00404039> and click 'Sample Issue Online'.

Title: The title should be brief, specific, and rich in informative words, it should not contain any literature references or compound numbers.

Authors and affiliations: Where possible, supply given names, middle initials and family names for complete identification. Use superscript lowercase letters to indicate different addresses, which should be as detailed as possible, and must include the country name. The corresponding author should be indicated with an asterisk, and contact details (fax, e-mail) may be placed in a footnote. Information relating to other authors (e.g. present addresses) should be placed in footnotes indicated by the appropriate symbols (see below).

Abstract: Authors must include a short abstract of approximately four to six lines that states briefly the purpose of the research, the principal results, and major conclusion(s). References and compound numbers should not be mentioned in the abstract unless full details are given.

Text: Text should be subdivided in the simplest possible way consistent with clarity. Headings and subheadings should reflect the relative importance of the sections, and all headings should be numbered. In the introductory section of the manuscript, the author should strive to define the significance of the work and the justification for its publication. Any background discussion should be brief and restricted to pertinent material. Ensure that all tables, figures and schemes are cited in the text in numerical order. The preferred position for chemical structures should be indicated. Trade names should have an initial capital letter, and trademark protection should be acknowledged in the standard fashion, using the superscripted letters TM and R for trademarks and registered trademarks respectively. All measurements and data should be given in SI units where possible, or other internationally accepted units. Abbreviations should be used consistently throughout the text, and all nonstandard abbreviations should be defined on first usage. Authors are requested to draw attention to hazardous materials or procedures by adding the word **CAUTION** followed by a brief descriptive phrase and literature references if appropriate. The experimental section should be as concise as possible, while containing all the information necessary to guarantee reproducibility (see also, Experimental section).

Reviews: When submitting a review article, authors should submit biographical information for each author as well as a black and white photograph. It should be one paragraph (approximately 150–200 words) and should include: date and place of birth, universities attended, degrees obtained, principal professional posts held, present title, a line or

two about the major research interests, and anything else professionally relevant that is of special interest.

Experimental section: Authors should be as concise as possible in experimental descriptions. The Experimental section must contain all the information necessary to guarantee reproducibility. An introductory paragraph containing information concerning solvents, sources of less common starting materials, special equipment, etc. should be provided. The procedures should be written in the past tense and include the weight, mmol, volume, etc. in brackets after the names of the substances or solvents. General reaction conditions should be given only once. The title of an experiment should include the chemical name and compound number of the product prepared; subsequently, this compound should be identified by its number. Details of the workup procedure must be included. Physical and spectroscopic data, including NMR, high-resolution mass analysis, and elemental analysis can be included in the experimental section or presented in tables.

Acknowledgment: An acknowledgment section may be included, it should be placed after the manuscript text and before the references.

References and notes: In the text, references should be indicated by superscript Arabic numerals which run consecutively through the paper and appear after any punctuation. Please ensure that all references are cited in the text and vice versa. The reference list should preferably contain only literature references though other information (e.g. experimental details) can be placed in this section. Preferably, each reference should contain only one literature citation. Authors are expected to check the original source reference for accuracy. Journal titles should be abbreviated according to American Chemical Society guidelines (The ACS Style Guide; Dodd, J. S., Ed.: American Chemical Society: Washington DC, 1997). Formatting for common references are shown below.

Scientific Articles:

1. Barton, D. H. R.; Yadav-Bhatnagar, N.; Finet, J.-P.; Khamsi, J. *Tetrahedron Lett.* **1987**, 28, 3111.

Books:

2. Doe, J. S.; Smith, J. In *Medicinal Chemistry*; Roe, P., Ed.; Pergamon Press: Oxford, 1990; Vol. 1, pp. 301–383.

Footnotes: Footnotes should appear at the bottom of the appropriate page and be indicated by the following symbols *, †, ‡, §, ¶, ||.

Abbreviations: Standard ACS abbreviations should be used throughout the manuscript and are employed without periods. The preferred forms for some of the more commonly used abbreviations are mp, bp, °C, °K, min, h, mL, µL, g, mg, µg, cm, mm, nm, mol, mmol, µmol, M, mM, µM, ppm, HPLC, TLC, GC, ¹H NMR, GC–MS, HRMS, FABHRMS, UV, IR, EPR, ESR, DNase, ED₅₀, ID₅₀, IC₅₀, LD₅₀, im, ip, iv, mRNA, RNase, rRNA, tRNA, cpm, Ci, dpm, $V_{\max}$, K_m , k , $t_{1/2}$. All nonstandard abbreviations should be defined following the first use of the abbreviation. For a detailed listing of standard abbreviations, see: *The ACS Style Guide*; American Chemical Society: Washington, DC, 1997.

Tables: All tables should be cited in the text, and numbered in order of appearance with Arabic numerals. All table columns should have a brief explanatory heading and where appropriate, units of measurement. Vertical lines should not be used. Footnotes to tables should be typed below the table and should be referred to by superscript letters. Each table should be provided with a descriptive heading, which, together with the individual column headings, should make the table, as nearly as possible, self-explanatory. In setting up tabulations, authors are requested to keep in mind the column widths (8.4 cm and 17.7 cm), and to make the table conform to the limitations of these dimensions.

Captions: Captions for figures and schemes should be grouped together separately.

Artwork: Figures, schemes and equations must be cited in the text and numbered in order of appearance with Arabic numerals. Other graphics, such as structures, do not need to be numbered, but please indicate in the text where these are to appear. All graphics (including chemical structures) must be provided at the actual size that they are to appear (single-column width is 8.4 cm, double-column width is 17.7 cm). Please arrange schematics so that they fill the column space (either single or double), so as not to leave a lot of unused white space. Please ensure that all illustrations within a paper are consistent in type, quality and size. Captions should not be included as part of the graphic; instead all captions should be supplied at the end of the text. Reagents and conditions (unless incorporated into the actual schematic) should also be labelled with the figure or scheme number, and the corresponding author's name.

To help author's provide actual size graphics, it is suggested that the following settings be used with CSC ChemDraw™ and ISIS DRAW™: font 10 pt Helvetica, chain angle 120°, bond spacing 18% of length, fixed length 14.4 pt (0.508 cm), bold width 2.0 pt (0.071 cm), line width 0.6 pt (0.021 cm), margin width 1.6 pt (0.056 cm), and hash spacing 2.5 pt (0.888 cm). Compound numbers should be in boldface. With these settings, to ensure a proper size, the graphic must be printed at 70%. In order to accurately design schematics to print out at the proper width with the reduction, the original drawing cannot exceed a column width of 8.4 cm (for single column) and 17.7 cm (for double column). To produce a double column width landscape mode will need to be used. Layout design is facilitated if authors submit their original artwork in the actual size to be published. Please save graphics as an Encapsulated PostScript file (EPS) or a Tagged Image File Format (TIFF), as well as the program the graphic was originally drawn in. For more details on the preparation and submission of artwork, please visit <http://www.authors.elsevier.com>

Photographs: High quality glossy prints of black and white photographs (i.e., high contrast gels) can be directly reproduced with inclusion in the manuscript. Four sets of originals should be supplied. Photocopies of photographs are unacceptable.

Colour: Colour figures may be printed in the journal at no charge to the author, provided that the Editor considers the colour necessary to convey scientific information. Colour figures should be supplied in electronic format as JPEG files (minimum 300 dots per inch) and if possible also in hard copy format.

Journal conventions

Nomenclature: It is the responsibility of the authors to provide correct nomenclature. Chemical names for drugs are preferred. If these are not practical, generic names, names approved by the U.S. Adopted Names Council, or those approved by the World Health Organization may be used. If a generic name is used, its chemical name or structure should be provided at the point of first citation. Authors will find the following as useful reference books for recommended nomenclature.

IUPAC Nomenclature of Organic Chemistry; Rigaudy, J.; Klesney, S. P., Eds; Pergamon: Oxford, 1979.

Enzyme Nomenclature; Webb, E. C., Ed.; Academic Press; Orlando, 1984.

Biochemical Nomenclature and Related Documents; The Biochemistry Society; London, 1978.

The ACS Style Guide; Dodd, J. S., Ed.; American Chemical Society: Washington, DC, 1986.

Characterization of new compounds: All new compounds should be fully characterized with relevant spectroscopic data. Microanalyses should be included whenever possible. Under appropriate circumstances, high resolution mass spectra may serve in lieu of microanalysis, if accompanied by suitable NMR criteria for sample homogeneity.

Biological data: Biological test methods must be referenced or described in sufficient detail to permit the experiments to be repeated by others.

Standard compounds and established drugs/agents should be tested in the same system for comparison. Statistical limits (statistical significance) for the biological data are usually required. If statistical limits cannot be provided, the number of determinations and an indication of the variability and reliability of the results should be given. References to statistical methods of calculation should be included. Doses and concentrations should be expressed in molar quantities when comparisons of potencies are made with compounds having substantial differences in molecular weights. For inactive agents, the highest concentration or dose level tested should be indicated. Detailed descriptions of biological methods should be placed in the Experimental section.

Structural data: Atomic coordinates for structures of biological macromolecules determined by X-ray, NMR, or other methods should be deposited with the Protein Data Bank (PDB), Chemistry Department, Brookhaven National Laboratories, Upton, Long Island, New York 11973. It is the responsibility of the author to obtain a file name for the macromolecule; the file name must be referenced in the manuscript. Manuscripts will be sent out for review only after receiving a written statement from the author that the coordinates will be deposited. If a manuscript is accepted for publication, and the PDB file name has not yet been obtained, it must be added in the proof prior to publication. Upon written request by the author the PDB will refer requests for coordinates to the originating author, but one year after publication, they will be made generally available upon request. Please address all inquiries about depositing to the PDB.

X-Ray crystallographic data: Prior to submission of the manuscript, the author should deposit crystallographic data for organic and metal-organic structures with the Cambridge Crystallographic Data Centre. The data, without structure factors, should be sent by e-mail to: deposit@ccdc.cam.ac.uk, as an ASCII file, preferably in CIF format. Hard copy data should be sent to CCDC, 12 Union Road, Cambridge, CB2 1EZ. A checklist of data items for deposition can be obtained from the CCDC Home Page on the World Wide Web (<http://www.ccdc.cam.ac.uk/>) or by e-mail to: fileserv@ccdc.cam.ac.uk, with the one-line message, sendme checklist. The data will be acknowledged, within three working days, with one CCDC deposition number per structure deposited. These numbers should be included with the following standard text in the manuscript: Crystallographic data (excluding structure factors) for the structures in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication nos. CCDC.....Copies of the data can be obtained, free of charge, on application to CCDC, 12 Union Road, Cambridge, CB2 1EZ, UK, (fax: +44-(0)1223-336033 or e-mail: deposit@ccdc.cam.ac.uk). Deposited data may be accessed by the journal and checked as part of the refereeing process. If data are revised prior to publication, a replacement file should be sent to CCDC.

Software: Software used as part of computer-aided drug/agent design (e.g. molecular modeling, QSAR, conformational analysis, molecular dynamics) should be readily available from accepted sources and the authors may specify where the software can be obtained. Assurance of the quality of the parameters employed for the relevant potential functions should be detailed in the manuscript.

Supplementary material: Elsevier now accepts electronic supplementary material to support and enhance your scientific research. Supplementary files offer the author additional possibilities to publish supporting applications, movies, animation sequences, high-resolution images, background datasets, 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>. The presence of these files will be signified by a footnote to the article, and within the text of the paper.

In order to ensure that your submitted material is directly usable, please ensure that data is provided in one of our recommended file formats. Supplementary data must be saved in files separate from those

for the manuscript and figures, and all file names must be supplied. For more detailed instructions please visit Elsevier's Author Gateway at <http://authors.elsevier.com>, and click on [Artwork instructions](#), then [Multimedia files](#).

Authors should also supply a concise and descriptive caption for each file of data, and at the end of the manuscript add a paragraph entitled Supplementary Data, in which they detail what data is supplied.

When supplying supplementary data files with their article, authors must state whether they wish to have these files published online alongside their article (some authors may choose to submit supplementary data as an aid to the referees only). All supplementary data will be subject to peer-review.

Copyright guidelines

All authors must sign the "Transfer of Copyright" agreement before the article can be published. This transfer agreement enables Elsevier Ltd to protect the copyrighted material for the authors, but does not relinquish the author's proprietary rights. The copyright transfer covers the exclusive rights to reproduce and distribute the article, including reprints, photographic reproductions, microform, or any other reproductions of similar nature and translations, and includes the right to adapt the article for use in conjunction with computer systems and programs, including reproduction or publication in machine-readable form and incorporation into retrieval systems. Authors are responsible for obtaining from the copyright holder permission to reproduce any figures for which copyright exists. Please note that photocopied signatures are not acceptable. Transfer of copyright agreement forms will be sent to the Corresponding author following acceptance of the manuscript.

Manuscript submission

Online submission of manuscripts: *Bioorganic & Medicinal Chemistry* manuscripts can be submitted using the TetSubmit online submission and review environment. Authors are required to go to the website and upload their article and its associated artwork. A PDF is generated and the reviewing process is carried out using that PDF. All correspondence between editor and author is performed by e-mail. Authors are, however, legally obliged to sign and return a physical transfer of copyright form by conventional mail. To submit your paper online, please go to: <http://www.tetsubmit.com>.

Please ensure that the graphical abstract is included as page 1 of your manuscript when submitting online.

For detailed instructions on the preparation of electronic artwork, consult the Author Gateway from Elsevier at <http://authors.elsevier.com>

Templates are provided in order to allow authors to view their paper in a style close to the final printed form. Their use is optional.

All manuscripts will be fully typeset from the author's electronic files. It should be noted that due to defined typesetting standards and the complex requirements of electronic publishing, the Publisher will not always be able to exactly match the layout the author has submitted. In particular, in the finished journal article, figures and tables are usually placed at the top or bottom of pages. The template is only intended to be used in assisting with the preparation and submission of manuscripts.

It should be noted that use of the journal template is not a requirement and its adoption will neither speed nor delay publication. Elsevier can handle most major word processing packages and in general most formatting applied by authors for style and layout is replaced when the article is being typeset.

These templates contain a large number of macros. To ensure successful PDF conversion in TetSubmit, it is important that the author saves a new document based on the template, rather than saving the template itself. To use the template, the author should save the final document as a Word file with a '.doc' extension (rather than the '.dot' extension).

Mail submission of manuscripts: The original and three copies of the manuscript, including the graphical abstract, should be sent to the

appropriate editorial office (see below). To achieve rapid publication authors are encouraged to fax or preferably e-mail their submission to the Editor at the time that they mail the manuscript; the date of submission will be taken as the date of fax or e-mail. The corresponding author's full mailing address, phone and fax numbers, and e-mail address should be supplied to aid rapid communication. Papers sent to the wrong Regional Editor will be forwarded to the appropriate Editor as determined by the permanent address of the corresponding author.

Disk submission: When a manuscript has been accepted for publication by the editorial office, authors are requested to also supply their paper and graphical abstracts in electronic format on disk. Please give full details of operating system, programs used, number of files sent, and information contained in each file. It is essential that the file on disk and the accepted printout are identical.

Text: We can accept most word-processing formats but prefer Microsoft Word: IBM or Macintosh. Most formatting codes will be removed or replaced on processing the article so there is no need to use excessive layout styling. In addition, do not use options such as automatic word breaking, justified layout, double-columns, automatic paragraph numbering (especially for numbered references) or End-Note. However, do use bold face, italic, subscripts, superscripts, etc. Do not embed the figures into the text file.

Graphics: Computer-generated illustrations, halftones and line/tones should also be provided where possible. The following points should be taken into consideration when preparing electronic graphic files: Tagged Image File Format (TIFF) or Encapsulated PostScript (EPS) files are preferred. Suggested packages for line graphics are ChemDraw, Adobe Illustrator (version 3.0 or above), Freehand and Corel Draw. Graphics created in WordPerfect and Word generally have too low a resolution for our requirements. Files of scanned line graphics can be accepted at a minimum resolution of 1000 dpi, for scanned halftones, 300 dpi, and scanned line/tones, 500 dpi. Colour should be scanned at 300 dpi (500 dpi for colour line/tones).

Since we cannot guarantee the usability of graphic files, hardcopies of all illustrations must accompany the accepted printout of the manuscript in all cases.

Submissions from Japan and other Asian countries:

Professor Y. Hashimoto
Institute of Molecular & Cellular Biosciences
The University of Tokyo
1-1-1 Yayoi, Bunkyo-ku
Tokyo 113-0032
Japan
FAX: (81) 3 5841 8495
E-mail: bmcyfh@iam.u-tokyo.ac.jp

Submissions from Europe:

Professor H. Waldmann
Department of Chemical Biology
Max-Planck-Institut für Molekulare Physiologie
Otto-Hahn-Strasse 11
44227 Dortmund
Germany

FAX: (49) 231 133 2499
Telephone: (49) 231 133 2400
E-mail: bmc@mpi-dortmund.mpg.de

Submissions from USA, Canada and all others:

Professor Chi-Huey Wong
The Scripps Research Institute
Department of Chemistry, BCC 483A
10550 North Torrey Pines Road
La Jolla, California 92037
USA
FAX: (858) 784 7550 or (800) 410 1557 toll-free within the USA or Canada
Telephone: (858) 784 7525
E-mail: bmc-bmcl@scripps.edu

Corrections

If there are errors of consequence in a published paper, a correction of the error should be sent to the Editor for publication in an "Additions and Corrections" section.

Proofs

Proofs will be despatched via e-mail by the Publisher and should be returned with corrections as quickly as possible, normally within 48 hours of receipt. Authors should ensure that corrections are returned in one communication and are complete, as subsequent corrections will not be possible. Any amendments will be incorporated and the final article will then be published online as an Article in Press on ScienceDirect www.sciencedirect.com.

Articles in Press take full advantage of the enhanced ScienceDirect functionality, including the ability to be cited. This is possible due to the innovative use of the DOI article identifier, which enables the citation of a paper before volume, issue and page numbers are allocated. The Article in Press will be removed once the paper has been assigned to an issue and the issue has been compiled.

Offprints

The corresponding author will be sent 25 free offprints. Additional reprints can be ordered when the paper is accepted. Correspondence regarding offprints should be directed to: Global Author Support, Elsevier Ireland Ltd, Elsevier House, Brookvale Plaza, East Park, Shannon, Co. Clare, Ireland; e-mail: authorsupport@elsevier.com

Page charges

None.

Author benefits

Contributors to Elsevier journals are entitled to a 30% discount on all Elsevier books.

Other enquiries

Visit the Author Gateway from Elsevier Science at (<http://authors.elsevier.com>) for the facility to track accepted articles and set up e-mail alerts to inform you of when an article's status has changed. The Author Gateway also provides detailed artwork guidelines, copyright information, frequently asked questions and more.

Contact details for questions arising after acceptance of an article, especially those relating to proofs, are provided after registration of an article for publication.