

Guide for Authors – Chemometrics and Intelligent Laboratory Systems

Chemometrics and Intelligent Laboratory Systems publishes original research papers, short communications, reviews, tutorials and software descriptions reporting on novel developments in techniques for chemistry and related disciplines that are characterised by the application of statistical and computer methods.

Chemometrics is the chemical discipline that uses mathematical and statistical methods to design or select optimal procedures and experiments, and to provide maximum chemical information by analysing chemical data

The journal deals with the following topics:

- 1) Development of new statistical, mathematical and chemometrical methods for Chemistry and related fields (Environmental Chemistry, Biochemistry, Toxicology, System Biology etc.)
- 2) Applications of chemometrics to all branches of Chemistry and related fields (typical domains of interest are: process control, experimental design, data mining, signal processing, supervised modelling, decision making, robust statistics, mixture analysis, multivariate calibration etc.)
- 3) Development of new software
- 4) Well characterized data sets to test performance for the new methods and software.

2. Types of contributions

The Journal publishes original research papers, short communications, tutorials and reviews. Tutorials and reviews are written by invitation of the Editors, who welcome suggestions for subjects. Short communications are usually complete descriptions of limited investigations, and should generally not exceed four printed pages. The Journal also participates actively in software dissemination through articles on software developments, software descriptions and reviews of software.

2.1. Mathematical papers

The Journal publishes papers from all areas of mathematics (including computer science, numerical methods, operations research, probability and statistics) that are clearly written and advance the fields of chemistry and chemometrics. The motivation and results of the paper must be understandable to chemists and chemometricians, but additional sections giving technical details are also welcomed. The level of the papers is expected to be comparable with that of existing professional mathematical science Journals.

2.2. Software descriptions

The journal invites for publication software descriptions. Emphasis should be laid on the quality, performance and relevance of the software to chemometrics, not on the novelty of the mathematics or the algorithms.

These descriptions should contain:

- a short description of the mathematical or chemical background (if relevant)
- a sample of the input (if relevant) and the output
- a description of the configurations on which the software runs
- key performance figures (number of variables treated, typical running times, etc.)

- details about how to access the software and its documentation, web page and internet addresses for download

No mention of costs or other commercial details may be made.

Details of the reviewing procedure:

The journal or its Editors cannot take on any responsibility for the functioning of the software. At least one review is, however, necessary. The authors must find at least one reviewer, outside their own institute, who will independently implement the software on his/her own computer. His/her declaration that he/she has been able to implement the program and his/her comments about it must be added to the manuscript and his name will be published under the heading "independently tested by". The Editors may require that the program is submitted to a second reviewer if they feel that this is necessary.

2.3. Software reviews

The Journal regularly publishes reviews of commercially available software.

2.4. Tutorials and reviews

If tutorials and reviews are submitted without prior consultation with the Editors, they will be refereed in the usual manner. However, to avoid duplication of material potential authors are advised to submit a synopsis in advance. Acceptance of the synopsis does not commit the Editors to acceptance of the article. It does, however, give the author priority in the subject area and assures the author that the subject area is relevant.

Tutorials do not involve original research nor should they present scientific results that have not yet been published. However, novel mathematical ways of approaching chemical problems, putting example data through improved algorithms, and example experiments are acceptable.

3. Submission of papers

3.1 Online Submission of Papers

Authors are encouraged to submit their manuscript online to one of the Journal Editors by using the online submission tool at www.ees.elsevier.com/chemolab. To submit a paper authors are required to go to this website and upload their manuscript article (with tables and figures inline) as a Microsoft (MS) Word, Word-Perfect, LaTeX or PostScript document and separately upload associated artwork files. An electronic Adobe Acrobat PDF version of the article is generated and the reviewing process is carried out using that PDF. Authors, Editors and Reviewers send and receive all correspondence by email via the website and no paper correspondence is performed.

Authors may suggest names of possible reviewers for their paper. They may also suggest the names of persons whom they do not want to review the paper. The Editors try to use at least one reviewer who has been suggested by the authors.

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4. Manuscripts

Manuscripts should be in double spacing on consecutively numbered pages of uniform size. The manuscript should be preceded by a sheet of manuscript paper carrying the title of the paper and the name, full postal address, telephone and fax number, and e-mail address of the person to whom the proofs are to be sent. As a rule, papers should be divided into numbered sections, headed by a caption (e.g., Abstract, Introduction, Experimental, Results, Discussion). All illustrations, photographs, tables, etc., should be on separate pages.

4.1. Title and authors

All manuscripts should be headed by a concise but informative title, since titles are widely used in information retrieval systems. The title is followed by the names of the authors, and the address where the work was carried out. The author to whom correspondence should be addressed must be indicated. If the present address of an author is different from that mentioned, it should be given in a footnote. Acknowledgements of financial support should not be made in a footnote, but should be included in the Acknowledgements at the end of the paper.

4.2. Abstract

All papers must include an abstract (50-250 words) which should comprise a brief factual account of the contents of the paper, with emphasis on new information. Abbreviations, jargon and reference numbers must not be used. The abstract should be suitable for use by abstracting services without rewriting. To facilitate the insertion of the paper in information retrieval systems, a listing of 5-6 subject keywords should be given below the abstract section.

4.3. Introduction

Every paper must have a concise introduction mentioning what has been done before on the topic described, and stating clearly what is new in the paper now submitted.

4.4. Experimental

The experimental methods and the materials used should be described after the introductory paragraphs. Detailed technical descriptions should be restricted to one section of the paper, and not scattered throughout the text. Sufficient information should be given to allow any reasonably experienced worker to carry out the procedure. Detailed descriptions of well-known techniques and equipment are unnecessary, as are simple preparations of reagents or solutions, and lists of common chemicals. In writing, complete sentences should be used.

4.5. Results and discussion

Preferably these should be treated together to avoid unnecessary repetition. Unsupported elaboration of hypotheses, and verbose exposition of ideas should be avoided. Chemical formulae should not be used in the text unless confusion is likely to arise from the use of names. Formulae may, however, be used for brevity in tables and figures.

4.6. Conclusions

The significance of the results should be presented here.

4.7. Acknowledgements

Acknowledgements should be kept as short as possible, and placed at the conclusion of the text.

4.8. References

The references should be collected at the end of the paper, numbered in order of their appearance in the text, and typed on a separate sheet. References given in tables should be numbered according to the position of the table in the text. Every reference listed must be cited in the text. Reference numbers in the text are set in square brackets on the line.

In the list of references, periodicals [1], books [2], and proceedings [3] should be cited in accordance with the following examples:

[1] V. Kvasnicka and J. Phospichal, *J. Math. Chem.*, 9 (1992) 181-196.

[2] E.D. Sontag, in R.P. Lippmann, J.E. Moody and D.S. Touretzky (Eds.), *Advances in Neural Information Processing Systems*, Vol. III, Morgan Kaufmann, San Mateo, CA, 1991, p. 153.

[3] P.J. Lewi, J. van Hoof and K. Andries, in E.J. Karjalainen (Ed.), *Scientific Computing and Automation (Europe) 1990*. Proceedings of the Conference, 12-15 June 1990, Maastricht, The Netherlands, Elsevier, Amsterdam, 1990, pp. 97-103.

Articles not yet published should be given as 'in press' only if accepted for publication, otherwise unpublished articles should be referred to as 'submitted for publication', 'in preparation' or 'personal communication+year', as appropriate.

4.9. Tables

The tables should be typed (in double spacing) on separate pages, and numbered in Arabic numerals according to their sequence in the text. A brief descriptive heading should be given above each table. Below the table the experimental conditions should be described. The layout of the tables should be given serious thought, so that the reader can grasp quickly the significance of the results.

4.10. Illustrations

Number illustrations consecutively in the order in which they are referred to in the text. Each illustration should have a descriptive legend, which should be understandable without reference to the text. Original line drawings and chemical formulae should be in a form suitable for direct reproduction, prepared with a good contrast (i.e. black on a white background). Photographs should be black and white glossy prints and as rich in contrast as possible. Care should be taken when submitting graphs to ensure that line thickness and labelling is of sufficient size and quality; any lettering should be a minimum height of 3-5mm. Axes on a graph should be clearly labelled, along the axes, and outside the graph itself. The preferred positions for all illustrations should be indicated in the manuscript by the authors. Please make sure that artwork files are in an acceptable format (TIFF, EPS or MS Office files) and with the correct resolution (see <http://authors.elsevier.com/artwork>). Electronic submission: please include your figures in their preferred positions in your article and also submit these as separate high resolution files. Electronic submission of your artwork helps us to produce your work to the best possible standards. For a detailed guide on electronic artwork please visit: <http://authors.elsevier.com/artwork> Print submission: All illustrations should be placed at the end of the manuscript as separate high-quality original printouts, suitable for reproduction. Mark the appropriate position of each illustrations in the article. The written permission of the author and publisher must be obtained for the use of any figure already published. Its source must be indicated in the legend. The written permission of the author and publisher must be obtained for the use of any figure already published. Its source must be indicated in the legend.

4.10.1. Colour Illustrations

Colour in print - please submit colour illustrations as original photographs, high-quality computer prints, transparencies or high resolution electronic files close to the size expected in publication, or as 35mm slides. Polaroid colour prints are not suitable. For colour reproduction in print, you will receive information regarding the costs from Elsevier after receipt of your accepted article. For further information on the preparation of electronic artwork, please see <http://authors.elsevier.com/artwork> Free colour on the web - if, together with your accepted article, you submit usable colour figures then Elsevier will ensure, at no additional charge, that these figures will appear in colour on the web (e.g., ScienceDirect and other sites) regardless of whether or not these illustrations are reproduced in colour in the printed version. Please note that if you do not opt for colour in print, you should submit relevant figures in both colour (for the web) and black and white (for print).

4.11. Software and data

Technical details of software should preferably be given in table format. Statements on the availability of the software to interested readers and on its price and storage medium should be given. In some cases the author may want to make the data or software discussed in a paper available on diskette. If so, the author should inform the Editor. The symbol for a diskette will then be printed with the article, so that the reader can contact the author directly. An example of the output may be given provided it is not too large. In some cases, the Editors may, however, accept publication of a program or, preferably, of its key subroutines.

4.12. Supplementary data

To support and enhance your scientific research the Journal can publish supporting datasets, applications, animation sequences, high-resolution images and more. Supplementary files supplied will, subject to peer review, be published online alongside the electronic version of your article in Elsevier web products, including Science- Direct (www.sciencedirect.com). The presence of these files will be signified by a footnote to the article title, and by a description included in a 'Supplementary Data' section at the end 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 and supply a concise and descriptive caption for each file. Please also clearly indicate whether data files are either i) for publication online or ii) only to be used as an aid for the refereeing of the paper. For more detailed instructions please visit our Author Gateway at <http://authors.elsevier.com>.

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