



# CHEMOMETRICS AND INTELLIGENT LABORATORY SYSTEMS

An International Journal Sponsored by the Chemometrics Society

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ISSN: 0169-7439

### DESCRIPTION

*Chemometrics and Intelligent Laboratory Systems* publishes original research papers, short communications, reviews, tutorials and Original Software Publications reporting on development of novel **statistical, mathematical, or computer techniques in Chemistry** and related disciplines.

**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, -Omics, etc.)
- 2)** Novel applications of chemometrics to all branches of Chemistry and related fields (typical domains of interest are: process data analysis, experimental design, data mining, signal processing, supervised modelling, decision making, robust statistics, mixture analysis, multivariate calibration etc.) Routine applications of established chemometrical techniques will not be considered.
- 3)** Development of new software that provides novel tools or truly advances the use of chemometrical methods.
- 4)** Well characterized data sets to test performance for the new methods and software.

The journal complies with International Committee of Medical Journal Editors' Uniform requirements for manuscripts.

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## IMPACT FACTOR

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## ABSTRACTING AND INDEXING

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## GUIDE FOR AUTHORS

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### INTRODUCTION

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

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- 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.

#### *Types of paper*

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, Original Software Publications and reviews of software.

#### **a) 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.

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The journal invites Original Software Publications. 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

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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.

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## **PREPARATION**

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[2] J. van der Geer, J.A.J. Hanraads, R.A. Lupton, 2018. The art of writing a scientific article. *Heliyon.* 19, e00205. <https://doi.org/10.1016/j.heliyon.2018.e00205>.

Reference to a book:

[3] W. Strunk Jr., E.B. White, *The Elements of Style*, fourth ed., Longman, New York, 2000.

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[4] G.R. Mettam, L.B. Adams, How to prepare an electronic version of your article, in: B.S. Jones, R.Z. Smith (Eds.), *Introduction to the Electronic Age*, E-Publishing Inc., New York, 2009, pp. 281–304.

Reference to a website:

[5] Cancer Research UK, Cancer statistics reports for the UK. <http://www.cancerresearchuk.org/aboutcancer/statistics/cancerstatsreport/>, 2003 (accessed 13 March 2003).

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