



CHEMOMETRICS AND INTELLIGENT LABORATORY SYSTEMS

An International Journal Sponsored by the Chemometrics Society

AUTHOR INFORMATION PACK

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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.

AUDIENCE

Chemists and Physical and Life Scientists as well as Statisticians and Information Specialists working in a variety of fields of chemistry, including Analytical Chemistry, Organic Chemistry and Synthesis, Environmental Chemistry, Food Chemistry, Industrial Chemistry, Pharmaceutical Chemistry and Pharmacy.

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GUIDE FOR AUTHORS

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

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.

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.

b) Original Software Publications

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:

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

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[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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