

# Instructions for Authors

## 1 General

*QSAR & Combinatorial Science* is an international journal that publishes contributions on aspects of computer-assisted design of biologically active compounds and high-quality information in combinatorial chemistry and related fields. Related scientific fields include computational, medicinal, pharmaceutical, bio-, bioorganic, organic, inorganic, environmental and analytical chemistry, chemical biology, spectroscopy and material science.

## 2 Language

Papers must be written in English. American spelling is preferred. Authors less familiar with English should seek assistance from proficient colleagues in order to produce grammatically and semantically correct manuscripts.

## 3 Types of manuscripts

- *Review articles* on subjects of current interest in the field. Authors wishing to submit a review article should send a brief outline of its content in duplicate to the Editor before the manuscript is drafted.
- *Full Papers* describing investigations that have come to a preliminary or final conclusion.
- *Short communications* describing results of such importance that rapid dissemination is warranted.

## 4 Submission of manuscripts

*Manuscripts on QSAR, Chemometrics and Molecular Modelling* should be submitted to

Prof. Dr. Michael Wiese  
Friedrich-Wilhelms-University  
Department of Pharmacy  
An der Immenburg 4  
53121 Bonn/Germany  
Telephone: Int. code + 228/735212  
Fax: Int. code + 228/737929  
e-mail: m.wiese@uni-bonn.de

*Manuscripts on Cheminformatics and Molecular Design* should be submitted to

Prof. Dr. Gisbert Schneider  
Johann Wolfgang-Goethe University  
Department of Organic Chemistry & Chemical Biology  
Marie-Curie-Str. 11  
60439 Frankfurt/Germany  
Telephone: Int. code + 69/79829821  
Fax: Int. code + 69/79829826  
e-mail: g.schneider@chemie.uni-frankfurt.de

*Manuscripts on Combinatorial Science* should be submitted to

Prof. Dr. Jean Martinez  
L.A.P.P., UMR 5810 CNRS  
University of Montpellier I & II  
Department of Pharmacy  
15, Avenue C. Flahault  
34095 Montpellier Cedex 5/France  
Telephone: Int. Code + 4/6754-8650  
Fax: Int. Code + 4/6714-2017  
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**All manuscripts should be submitted preferably by e-mail** in order to speed up the reviewing process. Upon notification of acceptance for publication, the **final** accepted version of the manuscript must be submitted not only in electronic format, but also as a printout. The electronic version **must** exactly match the final version accepted in hardcopy. Currently the following word processing packages for IBM and compatibles are supported: WordPerfect and Word for Windows. If a non-Western version of the supported word processing program was used, or this software is not available, rich-text format should be used to save the file.

## 5 Refereeing

Prior to publication, all contributions are evaluated by referees whose names are normally not disclosed to authors. Authors may suggest referees as well as name individuals whom they wish to be excluded from the review process.

## 6 Organization of manuscript

### 6.1 Introductory material

The first page of the manuscript should contain only the following:

- Title of the paper with as many meaningful terms as possible.
- Authors' names (with at least one forename spelled out in every case) and full **postal addresses** (without abbreviations) of the institutions where the work was done. If the publication originates from several institutions the affiliation of all authors must be clearly stated. An arrangement of the following kind is suggested:  
Author A<sup>1</sup>, Author B<sup>1</sup>, Author C<sup>2</sup> and Author D<sup>3</sup>  
Full address of institution 1  
Full address of institution 2  
Full address of institution 3

- The author who is to receive correspondence (including page proofs) is to be marked with an asterisk.
- The **footnote** **\*\*** To receive all correspondence".
- Up to five **keywords** characterizing the contents of the contribution are to be listed to facilitate the preparation of a subject index for the journal.
- A list of all **abbreviations** and symbols used in the paper.
- The line "Received on ..."

### 6.2 Abstract

The second page of the manuscript should contain the abstract. This must be self-explanatory and intelligible without reference to the text. It should not exceed 30 typeset lines. In addition, manuscripts should be subdivided for clarity into sections like Introduction, Materials and Methods, Results, Discussion, Conclusion, Experimental Section, and References. All sections and subsections must be provided with titles and numbered.

### 6.3 References

- References should be numbered sequentially, in the order in which they are cited in the text with numbers in square brackets, thus [2, 13]. They are to be collected in numerical order at the end of the manuscript under the heading "References". Responsibility for the accuracy of all bibliographic data rests with the authors. Titles of journals must be abbreviated according to the practice of Chemical Abstracts and references should follow the *Angewandte Chemie* format shown below.
- *Journal articles*: K. C. Nicolaou, S. A. Snyder, A. Bigot, J. A. Pfefferkorn, *Angew. Chem. Int. Ed.* **2000**, *39*, 1093–1096; S. Hannongbua, L. Lawtrakul, J. Limtrakul, *J. Comput.-Aided Mol. Design* **1996**, *10*, 145–153. Other serial publications such as *Advances in Protein Chemistry* should be cited in the same manner as journals.
- *Books*: K. C. Nicolaou, R. Hanco, W. Hartwig (Eds.), *Handbook of Combinatorial Chemistry, Drugs, Catalysis, Materials*, Wiley-VCH, Weinheim, **2002**, pp. 75–78.
- *Chapters from multi-author books*: U. Cruciani, S. Clementi, GOLPE: Philosophy and Applications in 3D QSAR un H. van de Waterbeemd (Ed.), *Advanced Computer-Assisted Techniques in Drug Discovery*, Wiley-VCH, Weinheim, **1995**, pp. 61–88.

### 6.4 Footnotes

Footnotes, i.e., explanations or comments on the text, should be avoided. If they are indispensable they should be indicated in the text by asterisks or similar symbols in parentheses and written at the bottom of the relevant text page.

### 6.5 Tables

Tables with suitable captions at the top and numbered with Arabic numerals should be collected at the end of the manuscript. Each table must be referred to in the text. Column headings should be kept as brief as possible and must indicate units unambiguously. Footnotes to tables should be indicated by (a) (b) (c) etc. and typed on the same page as the table.

### 6.6 Figures, Legends, Chemical Structures and Equations

*Diagrams* and *photographs* should be submitted on separate pages at the end of the article and electronically, if possible. They should be numbered consecutively with Arabic numerals in the order of their appearance. Photographs should be large, fine quality, glossy prints suitable for direct reproduction.

*Figures*: Each figure must be referred to in the text and is to be accompanied by a legend, which should be self-explanatory. The legends should not appear under the figures, but be collected and typewritten with double spacing on a separate page. Color figures can be printed free of charge, but only when necessary (the Editor of the journal will decide upon that). In addition, all diagrams and photographs should be submitted as TIFF or EPS files.

*Chemical Structures* should be produced with a graphics program (e.g. ChemDraw or ISIS Draw) and be submitted on separate printouts and electronically (soft- and hardware should be specified). They should be numbered in the order of their appearance with Arabic numerals in parentheses.

Chemical structures should be formatted according to the guidelines of *Angewandte Chemie* ([www.angewandte.com](http://www.angewandte.com)). A template for structure drawings in ChemDraw is available on this website.

*Mathematical equations* are to be written in the manuscript at the places they belong. Such equations must be labeled with Arabic numerals in parentheses in the right-hand margin in the order of their appearance.

### 7 Quantities, Units and Nomenclature

Authors are requested to quote quantities in SI units only. When a non-SI unit is still in use, it may be cited with the corresponding value in parentheses after the quantity expressed in SI units. Particular care is to be taken to use correct unit symbols.

Nomenclature must follow international rules, whenever they exist.

### 8 Page Proofs and Reprints

Correspondence authors will receive page proofs. One corrected set should be returned promptly to the Editor of the journal. The correspondence authors will receive a free copy of the issue. Additional reprints can be ordered at prices shown on the reprint order form which will be sent with the page proofs.