molecular informatics
models – molecules – systems

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# Author Guidelines

## 1 Aims and Scope

*Molecular Informatics* (succeeding the journal *QSAR & Combinatorial Science* from 2010 onward) is a peer-reviewed, international forum for publication of high-quality, interdisciplinary research on all molecular aspects of bio/cheminformatics and computer-assisted molecular design. *Molecular Informatics* presents methodological innovations that will lead to a deeper understanding of ligand-receptor interactions, macromolecular complexes, molecular networks, design concepts and processes that demonstrate how ideas and design concepts lead to molecules with a desired structure or function, preferably including experimental validation. The journal's scope includes but is not limited to the fields of drug discovery and chemical biology, protein and nucleic acid engineering and design, the design of nanomolecular structures, strategies for modeling of macromolecular assemblies, molecular networks and systems, pharmaco- and chemogenomics, computer-assisted screening strategies, as well as novel technologies for the de novo design of biologically active molecules.

A purely theoretical study lacking any chemical, biochemical, pharmacological or biological application will be acceptable only when it complies with the most rigorous standards and presents research of outstanding novelty. Manuscripts describing the mere application of existing computational methods to a data set and conventional QSAR models will not be accepted. For QSAR/QSPR studies, please also refer to §5.2 and §5.3. Molecular structure and activity data of all studies must be fully disclosed (cf. §5.3). If not publicized otherwise, they should be made available as Supporting Information (cf. §5.4). Clinical studies will not be considered for publication.

## 2 General Information

*Molecular Informatics* publishes **Reviews**, **Full Papers** and **Communications**. The journal will also publish so-called "Methods Corner" review-type articles which will feature important technological concepts and advances within the scope of the journal. Except for original research papers, Reviews and **Methods Corner Reviews** are usually written upon invitation. Unsolicited manuscripts, however, are welcome, as long as they fit into the scope of the journal.

Authors are solely responsible for the contents of their contribution. It is assumed that they have the necessary authority for publication. Authors must send or fax the completed and signed **Copyright Transfer Agreement** to the respective Editor after manuscript submission. The contents of manuscripts submitted to *Molecular Informatics* must not have been submitted to any other journal in parallel or published previously. Any manuscript already available on personal/group web pages will be considered by the Editors as already published and will not be accepted. **The authors must inform the Editors of manuscripts submitted, soon to be submitted, or in press at other journals that have a bearing on the manuscript being submitted to *Molecular Informatics***.

All submissions and publication issues must be in keeping with the **Ethical Guidelines for Publication in Journals and Reviews** of the European Association of Chemical and Molecular Sciences. In particular, authors should reveal all sources of funding for the work presented in the manuscript and should declare any **conflict of interest**.

All submitted manuscripts that are suitable for consideration will be peer-reviewed. Manuscripts which are clearly inappropriate for the journal can be rejected by the Editors without consulting referees. If accepted for publication, all manuscripts will be edited with a view to clarity, brevity, and consistency. Authors are encouraged to suggest suitable referees (full names and affiliations). However, not necessarily those referees nominated by the authors will be contacted.

On behalf of our authors who are also **US National Institutes of Health (NIH) grantees**, we will deposit in PubMed Central (PMC) and make public after 12 months the accepted, peer-reviewed version of the author's manuscript. By assuming this responsibility, we will ensure our authors are in compliance with the NIH request, as well as make certain the appropriate version of the manuscript is deposited. We reserve the right to change or rescind this policy. For more information, please go to http://www.wiley.com/go/funderstatement.

## 3 Manuscript Submission

*Molecular Informatics* offers web-based manuscript submission and peer-review via Manuscript Central. This service guarantees fast and safe submission of manuscripts and rapid assessment processes. **Online submission is mandatory** – conventional submission of manuscripts via courier service or e-mail is not accepted. Please prepare your manuscript in keeping with the guidelines given below (§5).

- For the submission of **new manuscripts**, a single Word DOC file needs to be uploaded as "Main Document" on the File Upload screen (for use of the *Molecular Informatics* manuscript templates, please refer to §5.1). Tables and all graphics should be embedded in the DOC file in the text where they belong (not collected at the end). Do not choose the file designation "Image" when uploading new manuscripts. Supporting Information can be uploaded, e.g., as a single, separate Word DOC or PDF file with all graphics embedded by choosing the file designation "Supporting Information".
- For the submission of **revised manuscripts and final manuscript files for production**, text, tables and graphics prepared with ChemDraw, ISIS Draw and Excel need to be uploaded as a single Word DOC file; the graphics need to be linked to those programs within the Word file. Upload this file as "Main Document". All other graphics need to be uploaded as separate files in a graphic format such as TIFF or JPG with a resolution of 300 dpi or higher; for these graphic files choose the designation "Image" on the File Upload screen. Figure and Scheme captions should not be embedded into the graphic files, but rather included at the end of the text file of the manuscript. Supporting Information is uploaded as a single, separate Word DOC or PDF file with all graphics embedded by choosing the file designation "Supporting Information".

Steps for using the *Molecular Informatics* online submission system:

- Go to **http://mc.manuscriptcentral.com/minf**.
- If you use the system for the first time, you need to click on the "Create Account" link. If you have been an author or referee for *Molecular Informatics* recently, your e-mail address will already be in the database. In that case, enter your e-mail address under "Password Help" on the Log In screen. You will receive an automatically generated e-mail, providing you with the details to access your personal homepage (login and password).
- Once logged in, please click on "Authoring Center" and let the system guide you through the submission process. Online help is available at all times. It will be possible to exit and reenter the system without losing any information at any stage of the submission process. All submissions are kept strictly confidential.

- If applicable, please choose a Special Issue to which you have been invited to contribute.
- Authors can follow the progress of their manuscripts on their personal homepage: All manuscripts of the authors submitted to and all review reports written for *Molecular Informatics* are archived here. This homepage should also be used to upload the revised and final manuscript versions.

Note that when multiple files are uploaded as "Main Document" or "Image", the system generates a single PDF file. **IMPORTANT:** only Word DOC, TIFF and JPG files are included in the PDF file generated. File formats **not included** are Excel XLS, PowerPoint PPT, ChemDraw CDX, ISIS Draw SKC, GIF, PCT, PSD, BMP, 123, RAR, SIT and ZIP.

## 4 Types of Contribution

### 4.1 Reviews

Reviews deal with topics of current interest in any of the areas covered by *Molecular Informatics*. Rather than an assemblage of detailed information with a complete literature survey, they should give a critical overview of a particular field, providing the reader with an appreciation of the importance of the work, a summary of recent developments, a balanced discussion of problems and progress, and well selected literature coverage. Although Reviews are generally written on **invitation**, unsolicited manuscripts are also welcome provided their contents are in keeping with the character of the journal. Prospective authors should submit topic proposals to the Editors or discuss the article with them at an early stage. All Reviews will be peer-reviewed.

Reviews should be divided into numbered sections. Cross-references in the text refer to these section numbers. The review starts with a **Lead-in** (1000–1500 characters). This text should not be a mere summary; rather, it should arouse the readers' interest. The **Introduction** should introduce the non-specialist to the subject as clearly as possible. A Review should conclude with a **Summary** and **Outlook** section, in which the achievements and new challenges for the subject are presented succinctly. In addition, a biographical sketch (500–700 characters) and a portrait-quality black-and-white photograph of each author, as well as a graphical suggestion for a full-page picture (**Frontispiece**) to face the first page, should be submitted. Please note that a color frontispiece carries a charge of €495 (including tax). A Review should consist of a maximum of 40 pages (approximately 65,000 characters) of main text, footnotes, literature citations, tables, and legends.

### 4.2 Methods Corner Reviews

Methods Corner Reviews introduce the reader to a particular method or technology that lies within the scope of the journal. Starting with a brief outline of the method and presentation of one or two selected authoritative applications, the focus is on presenting current developments and up-to-date information. The content should balance scope with depth, and references to important works from others which are significant to the topic should be included. Authors of Methods Corner Reviews are encouraged to express explicit expert opinion about the applicability and limitations of the method or technique presented (i.e.: "What works, what does not work, dos and don'ts"). Authors of Methods Corner Reviews are usually invited by the Editors. Suggestions for potential topics of interest and authors are welcome and may be sent to the Editors. All Methods Corner Reviews will be peer-reviewed.

Methods Corner Reviews should have an **Abstract** and be organized in meaningful and numbered sections:

**1. Method/Technique Background** (description and historical evolution);
**2. State-of-the-art** (including details on applications to drug discovery or chemical biology);
**3. Current Limitations**;
**4. Outlook**.

As for Reviews, a biographical sketch (500–700 characters) and a portrait-quality black-and-white photograph of each author, as well as a graphical suggestion for a full-page picture (**Frontispiece**) to face the first page, should be submitted. Please note that a color frontispiece carries a charge of €495 (including tax). Inclusive of main text, footnotes, literature citations, tables, and legends, a Methods Corner Review should be no longer than six pages (approximately 10,000 characters).

### 4.3 Communications and Full Papers

Communications and Full Papers present results of experimental or theoretical studies of general interest or great importance to the development of a specific area of research. A short text justifying why the manuscript should appear in *Molecular Informatics* should be submitted. The quality of original research contributions is usually assessed by two or more independent referees. All contributions will be judged on the criteria of originality, quality and novelty. Detailed information that could be of importance to the referees, but that is unlikely to be of interest to the reader can be submitted as an enclosure or clearly marked as Supporting Information. Only articles that have already been published in a scientific journal should be cited. The citation should be fair and informative but not excessive. Copies of cited publications not yet available publicly should be submitted along with the manuscript. Unpublished results and lectures should only be cited in exceptional circumstances.

Inclusive of all references, footnotes, and tables, a **Communication** should be no longer than six manuscript pages (approximately 10,000 characters). Chemical formulae, figures, and schemes may also be added. Longer Communications will be accepted only if their quality warrants special consideration, and a written justification of their length is provided. Communications should not be divided into sections. However, experimental details can be succinctly summarized separately under the heading **Computational Methods** or **Experimental Section**. Please note, only pertinent experimental information should be included in this section, and any additional experimental data should be detailed in the Supporting Information. The first paragraph of a Communication should give an introduction to enable readers unfamiliar with the subject to become acquainted with the importance of the results presented. In the final paragraph the results should be summarized succinctly, and one sentence should be devoted to their significance and, if appropriate, to remaining challenges.

**Full Papers**, which generally contain a **Computational Methods** or **Experimental Section**, have no length restrictions. However, the Editors request that space be used thoughtfully and economically. *Molecular Informatics* will not publish Full Papers that consist mainly of results reported in previous Communications with an added Experimental Section. Full Papers contain an **Abstract**, which should be brief (600–1000 characters) and not too technical, and an **Introduction** including relevant references. The presentation of **Results and Discussion** may be combined or kept separate. These sections may be further divided by subheadings.

## 5 Preparation of Manuscripts

### 5.1 General Remarks

The following remarks aim to assist you in preparing your manuscript for submission to *Molecular Informatics*, and can also be found on the journal's homepage (www.molinf.com) under "For Authors". We strongly encourage our authors to adhere closely to these guidelines as it facilitates both the peer-review and the editorial process.

Printing of **Figures and Schemes in color** is expensive, and we request that part of the additional costs be carried by the author. If color printing is essential and the author does not have access to funds for color printing, the Editors can make an exception so that figures and schemes within an article are printed in color.

We recommend the use of the *Molecular Informatics* manuscript templates (MS Word for Win/Mac), which are available on the journal homepage at www.molinf.com under "For Authors". Each template can be downloaded and saved as a DOC file, in which the positions for inserting the parts of the text

and graphics of the manuscript have been clearly indicated. Supporting Information should be submitted as a separate file. In the revised or final accepted manuscript, graphics prepared with ChemDraw, ISIS Draw or Excel need to be embedded into the Word file and linked to those programs. All other graphics need to be supplied as separate files in a graphic format such as TIFF or JPG with a resolution of 300 dpi or higher.

**Spelling** may be either UK or US standard English, but consistency should be maintained within a manuscript. Authors less familiar with the English language should seek assistance from proficient colleagues in order to produce grammatically and semantically correct manuscripts. Authors are asked to make their manuscripts suitable for a heterogeneous readership of biologists and chemists and to be considerate to our many readers for whom English is a foreign language—please use a simple, clear style and avoid jargon.

**Abbreviations** and **acronyms** should be used sparingly and consistently, following the system of abbreviations and symbols recommended by the International Union of Pure and Applied Chemistry (IUPAC) and the International Union of Biochemistry and Molecular Biology (IUBMB). Where they first appear in the text, they should—apart from the most common ones such as NMR, IR, or UV—be defined. You may prefer to explain large numbers of abbreviations and acronyms in a **Glossary** at the end of the text. Names of organisms should comply with genetic conventions, with genus and species names written in italics and spelled out in full on first appearance. Abbreviations for genes should be written in lower-case letters and italicized, those of the corresponding protein products should start with a capital letter and should not be italicized (e.g., *hsp70* and Hsp70, respectively). Enzyme names should be accompanied by the respective Enzyme Commission (EC) numbers.

For all types of contribution described in §4, a suitable graphic (formula or part of a figure) for the **Table of Contents** should be included. Color pictures will be reproduced free of charge in the online version of the Table of Contents; the corresponding print version will be reproduced in black & white. Please make sure to submit color graphics that are viable for black & white print reproduction. Otherwise please submit both a color and black & white version of the graphic. Pictures should be kept small with minimum detail, as the maximum final width is 5 cm.

Detailed facts of importance to specialist readers can be submitted as **Supporting Information** and will be made accessible on the Internet. Color and animated multimedia applications are welcome (cf. §5.4).

If a **crystal structure analysis** or **sequence determination** is not an essential part of a manuscript, only a footnote is required indicating where the detailed results can be found. This can be a separate publication or a freely accessible database.

Authors are encouraged to submit suggestions for the *Molecular Informatics* cover page, together with an explanatory text (up to 500 characters) beginning with "The cover picture shows...". A template of the cover page to help you visualize the final effect of your design can be downloaded from the *Molecular Informatics* homepage at www.molinf.com under “For Authors”. Space available: 15 cm high × 20 cm wide. Part of the additional costs for color printing must be paid by the author. Details will be provided upon selection of the cover picture. The author of a Cover Picture will receive a complimentary PDF of his/her contribution containing the Cover Page. The Cover Page may be used, e.g., for presentations, on homepages or other promotional activities.

The correspondence author will receive page proofs as compressed PDF files. They should be returned within three days. Issue copies, reprints and high-resolution PDFs can be ordered for a reasonable price when the corrected proofs are returned.

### 5.2 Manuscript Styling

Your manuscript can be processed more rapidly if it is arranged as described below. Unless stated otherwise, the following instructions apply to all categories of contributions.

**Title page (in order)**: title; authors names with academic titles, alphabetical footnotes ([a], [b],...) referring to addresses, and an asterisk to denote the correspondence author; footnotes containing affiliations of all authors including the full postal address, fax number, and e-mail address of the correspondence author; series title, number, and reference to the previous paper in the series, if applicable; dedication, if applicable.

**QSAR/QSPR Manuscripts**: topics in quantitative structure–activity relationships occasionally appear in *Molecular Informatics*, and in light of the recent broadening of this field, it is important that prospective authors are aware of our editorial policy toward QSAR/QSPR manuscripts. First, the novelty of the QSAR/QSPR study should be clearly stated, preferably in the article's Abstract and Introduction. Second, if a new method or theory is reported, it should be validated against at least one other published dataset using at least one other commonly used method or theory; all QSAR/QSPR models must be validated using external data, and not data that were used for the development of the model. Finally, all data used in performing the QSAR study should be reported in the manuscript itself, provided in the Supporting Information, or otherwise readily available without restriction.

**Keywords**: A maximum of five keywords should be given in alphabetical order. In order to aid online searching, at least two keywords should be taken from the Keyword Catalog.

**Experimental Section** (applicable to Full Papers and Communications only) should be given in sufficient detail to enable others to repeat your work.

**Minimum spectral requirements:** Communications and Full Papers: $^{1}$H NMR and MS data are required for compounds used in biological testing.

In so far as is practical, authors should use a systematic name for each title compound in the Experimental Section (as suggested by IUPAC, IUBMB, or Chemical Abstracts) followed by the compound number in **bold**; parentheses for the compound number should be used *only* if the name identifies the compound uniquely and unambiguously (for example: "...2-ethyl-4-cyanobenzoate (**7**) was used..." or: "...cyanobenzoate **7** was used..."). Please do not use computer programs to generate elaborate systematic names or use extremely long compound names. For the sake of clarity general descriptors such as compound **1**, dendrimer **2**, or alcohol **3** should be used.

Equipment (including make, model, and software version) and conditions used for the measurement of physical data, as well as any organisms, proteins, or nucleic acids used, should be described at the beginning of the Experimental Section. Sources of less-common starting materials must be given, and solvent details should also be described.

Quantities of reactants, solvents, etc. should be included in parentheses rather than in the running text (e.g., "Triphenylstannyl chloride (0.964 g, 2.5 mmol) in toluene (20 mL)..."). Physical data (in SI units whenever possible) should be quoted with decimal points and negative exponents (e.g., 25.8 $JK^{-1}mol^{-1}$). Products should be described, and yields should be given as both a quantity (mol or g) and in percent (e.g., "...compound **7** as a white powder (34 mg, 89%)...").

Data in the Experimental Section should be **carefully and consistently formatted** according to the journal style. **Examples**: "...gave compound **7** as a white powder (34 mg, 89%): $R_f$=0.38 ($CHCl_3$/MeOH 9:1); mp: 70–71°C; [$\alpha$]$D_2$0=−13.5 (*c*=0.2 in acetone); $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$=1.35 (q, *J*=8.1 Hz, 2H), 0.97 ppm (t, *J*=8.2 Hz, 3H); $^{13}$C NMR (75 MHz, [$D_6$]DMSO): $\delta$=8.9, 27.3, 56.8, 64.2, 170.3 ppm; IR (KBr): $\tilde{\nu}$=3248, 3056, 1790, 1780, 1506, 1493 $cm^{-1}$; UV/Vis ($CH_2Cl_2$): $\lambda_{max}$ ($\varepsilon$)=320 (5000), 270 nm (12000); MS (EI, 70 eV) *m/z* (%): 173 (32), 171 (100) $[M+H]^+$; HRMS-FAB *m/z* $[M+H]^+$ calcd for $C_8H_7ClO_2$: 171.0135, found: 171.0142; Anal. calcd for $C_8H_7ClO_2$: C 56.32, H 4.14, O 18.76, found: C 56.35, H 4.11, O 18.79. ***Please give data in this order.***

**Compound Purity**: Those compounds used in biological testing should possess **purity of no less than 95%** as determined by elemental analysis (to an accuracy of within ±0.4%), HRMS or HPLC analysis. Data should be included in the Experimental Section or Supporting Information.

*We understand the associated limitations involved in chemical synthesis, these requirements are flexible within reason; please contact the* Editors *with any questions.*

**Computer-aided image enhancement** is often unavoidable. However, such manipulation cannot result in data that are less relevant or unrepresentative being shown and/or genuine and significant signals being lost. A clear relationship must remain between the original data and the electronic images that result from those data. If an image has been electronically modified, the form of the modification shall be given in the Figure caption. If computer-aided processing or modification of an image is a fundamental part of the experimental work, then the form that this processing takes must be clearly described in the Experimental Section.

Manuscripts containing **animal experiments** must include a statement in the Experimental Section to state that permission was obtained from the relevant national or local authorities. The institutional committees that have approved the experiments must be identified and the accreditation number of the laboratory or of the investigator given where applicable. If no such rules or permissions are in place in the country where the experiments were performed, then this must also be clearly stated.

Manuscripts containing experiments with **human subjects** or **tissue samples** from human subjects must contain a disclaimer in the Experimental Section to state that informed signed consent was obtained from either the patient or from next of kin.

**References**: In the text numbers corresponding to the appropriate reference should be typed in square brackets as superscript (e.g., Blobel[3]) and after any punctuation, where applicable. References must be listed in order of their appearance in the text. Please do not format the references section with the Numbering function on your word-processing program. If you use the automatic reference collation system of your word-processing program (Footnotes, EndNote), please convert the references into normal, typed text before submission of the final manuscript, otherwise they may disappear when typeset. Journal titles should be abbreviated according to the Chemical Abstracts Service Source Index (CASSI). Unpublished results and lectures should only be cited for exceptional reasons. Please follow the examples below. The page range is optional but its presence or absence should be consistent throughout any given manuscript.

*Journals*: [1] a) J. A. Pitcher, N. J. Freedman, R. J. Lefkowitz, *Annu. Rev. Biochem.* **1998**, *67*, 653–692; b) P. Sears, C.-H. Wong, *Angew. Chem*. **1999**, *111*, 2446–2471; *Angew. Chem. Int. Ed.* **1999**, *38*, 2300–2324.

[2] a) W. D. Wagner, *Ann. N.Y. Acad. Sci.* **1985**, *454*, 52–68, and references therein; b) J. C. Wang, *Sci. Am.* **1982**, *247*(1), 94–97.

*Books (Without editor)*: [3] E. Wingender, *Gene Regulation in Eukaryotes*, VCH, Weinheim, **1993**, p. 215.

*Books (With editor)*: [4] T. D. Tullius in *Comprehensive Supramolecular Chemistry*, *Vol. 5* (Eds.: J. L. Atwood, J. E. D. Davies, D. D. MacNicol, F. Vögtle, K. S. Suslick), Pergamon, Oxford, **1996**, pp. 317–343.

*Miscellaneous*: [5] a) C. R. A. Botta (Bayer AG), DE-B 2235093, **1973** [*Chem. Abstr.* **1974**, *80*, 55356 c]; b) A. Student, PhD thesis, University of Newcastle (UK), **1991**; c) "Synthesis in Biochemistry": R. Robinson, *J. Chem. Soc.* **1936**, 1079.

**Legends**: each figure and scheme should have a legend. These should be listed together at the end of the reference section of the text file rather than being included with the drawings in the graphics files.

**Tables** must have a brief title and should only be subdivided by three horizontal lines (head rule, neck rule, foot rule). Footnotes in tables are denoted [a], [b], [c], etc. Tables should not be created as graphics files or contain line brakes within single cells.

**Illustrations** (structural formulae, figures, schemes) should, if possible, be designed for reduction to a one-column format (8.5 cm wide). The maximum width is the two-column format (17.5 cm wide). For optimum reproduction, illustrations should be larger than the desired final size. We recommend: Helvetica font for script; size of lettering, 3–3.5 mm; total maximum width, 14 cm (or 28 cm for two-column width) for 60% reduction. Please use only one size of writing in any one diagram. Writing above the arrow in a scheme may be a little smaller. Good quality graphics should be submitted for referees and editors. For high quality reproduction, high resolution graphics must be supplied.

Please ***italicize*** symbols of physical quantities in both graphics and the text, but not their units (e.g., *T* for temperature, in contrast to T for the unit Tesla; *J*, but Hz; *a*, but nm). Stereochemical information

(*cis*, *Z*, *R*, etc.), locants (*N*-methyl, *α*-amino), and symmetry designations ($C_{2v}$) should also be italicized. Chemical formulae should be numbered with boldface Arabic numerals (e.g., **1**). Labels of axes should be separated from their units by a slash (e.g., *T*/K). Abbreviations such as Me, Et, *n*Bu, *i*Pr, *s*Bu, *t*Bu, and Ph (not ϕ) may be used. General substituents should be indicated by $R^1$, $R^2$ (not $R_2$, which means 2R), or R, R′. The spatial arrangement of the substituents should be indicated by hatched lines or a wedge. A minus sign must be as long as the crossbar of a plus sign.

**Mathematical formulae** should not be incorporated into the text as graphic files. Please type mathematical formulae as normal text in the body of the text, as far as is possible.

### 5.3 Structure and Sequence Data

Prior to manuscript submission, the author(s) must deposit the following information in the appropriate databases: the data of X-ray structure analyses of inorganic and organic compounds, proteins, or nucleic acids; structure determination of proteins and nucleic acids by NMR spectroscopy (together with a list of NEOs), and sequence determinations of proteins or nucleic acids. Authors of QSAR/QSPR studies have to take care that all data and compound data sets needed to understand and reproduce their study is made freely available. The name of the database and the deposition number(s) assigned by this database must be stated in the part of the manuscript where the respective structure or sequence determination(s) are described so that referees can retrieve the information electronically. Detailed instructions for data submission can be found on the WWW homepages of the databases listed below.

**Structure Data**
**Organic and organometallic compounds**: *Cambridge Crystallographic Data Centre* (CCDC; WWW: http://www.ccdc.cam.ac.uk).
**Inorganic compounds**: *Fachinformationszentrum Karlsruhe* (FIZ; WWW: http://www.fiz-karlsruhe.de).
**Proteins** and **nucleic acids**: *Protein Data Bank* (WWW: http://www.rcsb.org/pdb).
**NMR spectroscopy data**: *BioMagResBank* (WWW: http://www.bmrb.wisc.edu).

**Sequence Data**
**Nucleic acids**: *GenBank* (WWW: http://www.ncbi.nlm.nih.gov/) or *EMBL Nucleotide Sequence Database* (WWW: http://www.ebi.ac.uk/embl/index.html).
**Proteins**: *Protein Information Resource* (PIR; WWW: http://pir.georgetown.edu/) or SWISS-PROT (WWW: http://www.expasy.ch/sprot/sprot-top.html).
**Please note that the data in databanks must be released, at the latest, upon publication of your manuscript.**

### 5.4 Supporting Information

Supporting Information may be included for deposition on the internet. The author must keep a copy to make available to readers who do not have internet access. This material is peer-reviewed and must therefore be included with the original submission. After acceptance, succinct text and the necessary graphics should then be sent as a separately saved single MS Word (preferably Word 7) or MS Word for Macintosh file, with the final revised version of the manuscript. Only in this case should the graphics be present as imports in the file and not as separate files. Supporting Information should not include crystallographic or sequence data that are available from the relevant databases. Molecular structures may be included in PDB, FASTA, or SDF file format, the latter being preferred if activity data is to be made available. Color and animated multimedia applications are welcome for Supporting Information.

**We look forward to the ONLINE submission of your next excellent manuscript!**