

Journal of Biomolecular NMR

INSTRUCTIONS FOR AUTHORS

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AIMS AND SCOPE

The *Journal of Biomolecular NMR* provides a forum for publishing research on technical developments and innovative applications of nuclear magnetic resonance spectroscopy for the study of structure and dynamic properties of biopolymers in solution, liquid crystals, solids and mixed environments, e.g., attached to membranes. This may include:

- Three-dimensional structure determination and studies of dynamic and interactions of biological macromolecules (polypeptides/proteins, DNA, RNA, oligosaccharides) by NMR.
- NMR applications in structural genomics and proteomics.
- New NMR techniques for studies of biological macromolecules.
- Novel approaches to computer-aided automated analysis of multidimensional NMR spectra.
- Computational methods for the structural interpretation of NMR data, including structure refinement.
- Comparisons of structures determined by NMR with those obtained by other methods, e.g., by diffraction techniques with protein single crystals.
- New techniques of sample preparation for NMR experiments (biosynthetic and chemical methods for isotope labeling, preparation of nutrients for biosynthetic isotope labeling, etc.). An NMR characterization of the products must be included.

MANUSCRIPT TYPES

Article

Articles are full-length papers that should conform to a sectional format, usually including Title, Summary, Key words, Introduction, Materials and methods, Results, Discussion and conclusions, Acknowledgements and References. Descriptions of novel experimental or computational procedures should include sufficient detail to enable others to repeat these procedures. Use of published procedures should merely be referred to by literature citation of both the original experiment and any published modifications. Manuscripts that primarily describe computer programs should present new algorithms or novel implementations of existing ones. In the latter case, the paper must provide evidence for the improvements offered. The computer programs should be readily available, with information given on how to access the software, and include adequate documentation and manuals. *Articles* of outstanding quality and interest may be processed as '*accelerated publication*', with guaranteed publication within 8 weeks after acceptance.

NMR structure note

A structure determination that yields a high quality NMR structure but may not warrant description in an *Article* can be published as *NMR structure note*. Possible examples for such submissions are high quality structures of biologically interesting molecules that are homologous to previously published structures, of gene products with unknown function, etc. Preliminary reports on incomplete or unrefined structures are not acceptable and will be returned to the authors without being reviewed. The title must have the format 'NMR structure note: name and origin of the protein', and the manuscript must follow the layout with an Abstract and three subtitles *Biological context*, *Methods and results*, and *Discussion and conclusions*. The text may be supplemented by up to four items of documentation, for example, one table and three figures. One of the figures must illustrate the NMR data on which the structure determination is based, and the presentation of the structure must include a stereo view that contains the side chains. Up to 20 references may be cited. A *NMR structure note* must fit on 6 printed pages (see 'Sizing guide').

Letter to the Editor: New NMR assignment

An assignment for a new, functional protein or protein domain of at least 100 amino acid residues in size (i.e., data collected under non-denaturing conditions for the active form of the protein) can be published as a *Letter to the Editor: New NMR assignment*. Residues added in the cloning process that are not part of the native sequence are not to be included in the residue count, and the size of a homo-oligomeric protein is evaluated on the basis of its monomer chain length. Complete backbone assignments and complete or nearly complete side chain assignments are required. Assignments only for the polypeptide backbone in large proteins may in exceptional cases be accepted, provided that the authors present a convincing reason for publication of the data in their cover letter. The manuscript must follow the layout of *J. Biomol. NMR* **30**, 97 (2004), which includes at most two references in short format, and has an all-inclusive size limit of 1,500 characters. The assignment data must be deposited in the BioMagResBank (<http://www.bmrb.wisc.edu>) and manuscript submission must be accompanied by a character count and the BMRB entry processing letter together with the author's response to any issues raised. The processing letter is typically provided by the BMRB within 10 days of submission, provided that authors indicate *J. Biomol. NMR* as the journal citation. The short printed version may be accompanied by supplementary material, which should follow the layout of *J. Biomol. NMR* **19**, 79–80 (2001). The text may be supplemented by one figure and at most ten additional references, and it must fit on two printed pages (see sizing guide section). The Editors encourage authors of assignment data that do not qualify for publication as a 'Letter to the Editor' to document their work by submission to the BMRB and, if applicable, include a description of the work in a manuscript describing the project for which the assignments were used.

Perspectives

Perspectives will be by invitation only.

MANUSCRIPT PRESENTATION

The *Journal of Biomolecular NMR*'s language is English. Manuscripts should be printed or typewritten on A4 or US Letter bond paper, one side only, leaving adequate margins on all sides to allow reviewer's remarks. All

material, including notes and references must be double-spaced. Number the page consecutively, with the first page containing the article type, title, author(s), affiliation, full address for correspondence, including phone, fax and e-mail number, up to 6 keywords in alphabetical order, abbreviations if applicable, and a character count of the entire text including spaces.

Sizing guide

The first printed manuscript page with the heading contains about 4400 characters, including spaces. A full page of text contains about 5500 characters. Allow for the space used for figures and tables when estimating the overall length of *NMR structure notes*.

Special comment on manuscripts describing new NMR structures

For guidance to the preparation of manuscripts describing the determination of new NMR structures of biological macromolecules with the use of established methodology, authors are referred to *Recommendations for the Presentation of NMR Structures of Proteins and Nucleic Acids* (Markley, J.L. et al. (1998) *J. Biomol. NMR*, **12**, 1–23).

Requirements for deposition of data

For new NMR structures, atomic coordinates must be deposited in the Protein Data Bank (PDB) and, unless presented elsewhere previously, the resonance assignments must be deposited with the BioMagResBank (BMRB; <http://www.bmrwisc.edu>). All manuscripts submitted for review describing either new structures or new assignments must include the PDB and/or BMRB accession numbers, and on a separate sheet the acknowledgement of receipt by the database, including the hidden access code (BMRB). Deposited data must be released at the latest on the date of publication. The Editors further recommend that additional data, such as the input for a structure calculation, relaxation times, and similar should be either included as supplementary material or deposited in a publicly accessible database.

Symbols and Units

SI units should be used.

Nomenclature

All nomenclature should be consistent, conforming to the recommendations of the International Union of Pure and Applied Chemistry, International Union of Biochemistry, and other appropriate bodies.

Section Headings

In articles first-, second-, third- and fourth-order headings should be clearly distinguishable but not numbered.

Notes

Please use footnotes rather than endnotes. Notes should be indicated by consecutive superscript numbers in the text. A source reference note should be indicated by means of an asterisk after the title. This note should be placed at the bottom of the first page.

Cross-Referencing

In the text, a reference identified by means of an author's name should be followed by the date of the reference in parentheses and page number(s) where appropriate. When there are more than two authors, only the first author's name should be mentioned, followed by 'et al.'. In the event that an author cited has had two or more works published during the same year, the reference, both in the text and in the reference list, should be identified by a lower case letter like 'a' and 'b' after the date to distinguish the works.

Examples:

Winograd (1986, p. 204)

(Winograd, 1986a, b)

(Winograd, 1986; Flores et al., 1988)

(Bullen and Bennett, 1990)

Acknowledgements

Acknowledgements of people, grants, funds, etc. should be placed in a separate section before the References.

References

References to books, journal articles, articles in collections and conference or workshop proceedings, and technical reports should be listed at the end of the article in alphabetical order following the Harvard style (see examples below). Articles in preparation or articles submitted for publication, unpublished observations, personal communications, etc. should not be included in the reference list but should only be mentioned in the article text (e.g., T. Moore, personal communication).

References to books should include the author's name(s); year of publication in parentheses; title (in italics); page numbers where appropriate; publisher; place of publication, in the order given in the example below.

Wüthrich, K. (1986) *NMR of Proteins and Nucleic Acids*, Wiley, New York, NY.

References to articles in an edited collection should include the author's name(s); year of publication in parentheses; editor's name(s); title of collection (in italics); first and last page numbers; publisher; place of publication, in the order given in the example below.

Norinder, U. (1998) In *QSAR in Drug Design*, Vol. 3: Recent Advances, Kubinyi, H., Folkers, G. and Martin, Y.C. (Eds.), Kluwer, Dordrecht, pp. 25–39.

References to articles in conference proceedings should include the author's name(s); year of publication in parentheses; editor's name (if any); title of proceedings; first and last page numbers; place and date of conference; publisher and/or organization from which the proceedings can be obtained; place of publication, in the order given in the example below.

Mechnich, O., Hessler, G., Bernd, M., Kutscher, B. and Kessler, H. (1999) In *Peptides: Frontiers of Peptide Science*, Tam, J.P. and Kaumaya, P.T.P. (Eds.), *Proceedings of the Fifteenth American Peptide Symposium, Nashville, TN, June 14–19, 1997*, Kluwer Academic Publishers, Dordrecht, pp. 465–466.

References to articles in periodicals should include the author's name(s); year of publication in parentheses; abbreviated title of periodical (in italics); volume number (in bold); first and last page numbers, in the order given in the example below.

Mäler, L., Potts, B.C.M. and Chazin, W.J. (1999) *J. Biomol. NMR*, **13**, 233–247.

References to technical reports or doctoral dissertations should include the author's name; year of publication in parentheses; title; institution; location of institution, in the order given in the example below.

Burgering, M.J.M. (1994) *NMR Studies of Arc and Mnt Repressors*, Ph.D. Thesis, Utrecht University, Utrecht.

Figures

All photographs, graphs and diagrams should be referred to as a 'Figure' and they should be numbered consecutively (1, 2, etc.). Multi-part figures ought to be labelled with lower case letters (a, b, etc.). Please insert keys and scale bars directly in the figures. Small text sizes within figures should be avoided as figures are often reduced in size to fit within the column(s) of the journal. Provide a detailed legend (without abbreviations) to each figure, refer to the figure in the text and note its approximate location in the margin. In the manuscript the legends are placed after the references.

Tables

Each table should be numbered consecutively (1, 2, etc.). Footnotes are preferable to long explanatory material in either the heading or body of the table. Such explanatory footnotes, identified by superscript letters, should

be placed immediately below the table. Please provide a caption (without abbreviations) to each table, refer to the table in the text and note its approximate location in the margin. Finally, please place the tables after the figure legends in the manuscript.

Supplementary material

In an effort to keep the length of printed publications within reasonable limits, provision is made to submit supplementary material. This should be prepared in the same style as the article itself and submitted along with the manuscript for refereeing. If accepted for publication, such articles will contain a statement that supplementary material is available electronically.

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Manuscripts must be submitted electronically as a PDF format file (including figures) to one of the Associate Editors (see above). This electronic submission must be complemented by two hard copies with high-quality reproductions of the figures, and a compact disk containing a Word file of the text and original graphics files of all figures.

PROOFS

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