



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 of biological macromolecules (polypeptides/proteins, DNA, RNA, oligosaccharides) by NMR. New approaches for primary structure determination by NMR (e.g., cyclopeptides, oligosaccharides) may also be considered.
- 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.

A broad spectrum of papers dealing with both the theory and application of nuclear magnetic resonance spectroscopy in the study of the structure and dynamics of biological macromolecules will be considered for publication.

MANUSCRIPT SUBMISSION

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For the purpose of reviewing, articles for publication should be submitted as hard-copy printout (fourfold) and on diskette to one of the Associate Editors (see above).

MANUSCRIPT PRESENTATION

The journal's language is English. British English or American English spelling and terminology may be used, but either one should be followed consistently throughout the article. Manuscripts should be printed or typewritten on A4 or US Letter bond paper, one side only, leaving adequate margins on all sides to allow reviewers' remarks. Please double-space all material, including notes and references. Quotations of more than 40 words should be set off clearly, either by indenting the left-hand margin or by using a smaller typeface. Use double quotation marks for direct quotations and single quotation marks for quotations within quotations and for words or phrases used in a special sense.

Number the pages consecutively with the first page containing **the article type, title, author(s), affiliation, full address for correspondence, including phone, fax and e-mail number, 5 to 10 key words in alphabetical order, a short summary of 100 to 250 words, and abbreviations if applicable**. Since the summary and the key words will be used to select appropriate reviewers, it is essential to make them as informative as possible.

Article types

Full-length papers, short communications, and assignment notes.

Articles

Full-length papers should conform to a sectional format, usually including Title, Summary, Key words, Introduction, Materials and Methods, Results, Discussion, 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 describing computer programs should include a statement how access to this software can be obtained. Articles of outstanding quality and interest may be processed as 'accelerated publication', with the same priority for rapid publication as *Short Communications*.

Communications

Communications are restricted to reports of unusual urgency, significance, and interest, and must fit on 4 printed pages, including figures, tables and references. Each short communication should be accompanied by a summary identifying in 100 words or less the major observation reported, and 4–6 key words. Communications should not be sectionalized. The authors should point out in their cover letter why they believe the manuscript meets the criteria of unusual urgency, significance or interest. Sizing guide: The first page with the heading contains about 4400

characters, including spaces. A full page of text contains about 5800 characters. A character count must be given on the title page. Please allow for the space used for figures and tables when estimating the length.

Letters to the Editor: New NMR assignments

An assignment for a new protein (i.e., a natural protein of size 100 amino acids or larger in the native state, for which no solution structure has as yet been reported) can be published in the section *Letters to the Editor: New NMR assignments*. Complete backbone assignments and complete or nearly complete side chain assignments are expected. The manuscript must follow the layout of *J. Biomol. NMR*, **9**, 445–446 (1997), with the three subtitles *Biological Context*, *Methods and Results*, and *Extent of Assignments and Data Deposition*, and a list of chemical shifts must be deposited with the BioMagResBank (BMRB; <http://www.bmrb.wisc.edu>). The text may be supplemented by at most 1 figure and 10 references. A ‘Letter to the Editor’ must fit on two printed pages. The manuscript submitted for review must include the BMRB accession number. BMRB accepts deposits consisting of the text of the assignment (without figure and references) and the chemical shift list in the format of the data bank.

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.

Figures and Tables

Submission of electronic figures

In addition to hard-copy printouts of figures, authors are encouraged to supply the electronic versions of figures in either Encapsulated PostScript (EPS) or TIFF format. Many other formats, e.g., Microsoft Postscript, PiCT (Macintosh) and WMF (Windows), cannot be used and the hard copy will be scanned instead.

Figures should be saved in separate files *without* their captions, which should be included with the text of the article. Files should be named according to DOS conventions, e.g., ‘figure1.eps’. For vector graphics, EPS is the preferred format. Lines should not be thinner than 0.25 pts and in-fill patterns and screens should have a density of at least 10%. Font-related problems can be avoided by using standard fonts such as Times Roman and Helvetica. For bitmapped graphics, TIFF is the preferred format but EPS is also acceptable. The following resolutions are optimal: black-and-white line figures – 600–1200 dpi; line figures with some grey or coloured lines – 600 dpi; photographs – 300 dpi; screen dumps – leave as is. Higher resolutions will not improve output quality but will only increase file size, which may cause problems with printing; lower resolutions may compromise output quality. Please try to provide artwork that approximately fits within the typeset area of the journal. Especially screened originals, i.e. originals with grey areas, may suffer badly from reduction by more than 10–15%.

AVOIDING PROBLEMS WITH EPS GRAPHICS

Please always check whether the figures print correctly to a PostScript printer in a reasonable amount of time. If they do not, simplify your figures or use a different graphics program.

If EPS export does not produce acceptable output, try to create an EPS file with the printer driver (see below). This option is unavailable with the Microsoft driver for Windows NT, so if you run Windows NT, get the Adobe driver from the Adobe site (www.adobe.com).

If EPS export is not an option, e.g., because you rely on OLE and cannot create separate files for your graphics, it may help us if you simply provide a PostScript dump of the entire document.

HOW TO SET UP FOR EPS AND POSTSCRIPT DUMPS UNDER WINDOWS

Create a printer entry specifically for this purpose: install the printer 'Apple Laserwriter Plus' and specify 'FILE': as printer port. Each time you send something to the 'printer' you will be asked for a filename. This file will be the EPS file or PostScript dump that we can use.

The EPS export option can be found under the PostScript tab. EPS export should be used only for single-page documents. For printing a document of several pages, select 'Optimise for portability' instead. The option 'Download header with each job' should be checked.

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If no electronic versions of figures are available, submit only high-quality artwork that can be reproduced as is, i.e., without any part having to be redrawn or re-typeset. The letter size of any text in the figures must be large enough to allow for reduction. Photographs should be in black-and-white on glossy paper. If a figure contains colour, make absolutely clear whether it should be printed in black-and-white or in colour. Figures that are to be printed in black-and-white should not be submitted in colour. Authors will be charged for reproducing figures in colour.

Each figure and table should be numbered and mentioned in the text. The approximate position of figures and tables should be indicated in the margin of the manuscript. On the reverse side of each figure, the name of the (first) author and the figure number should be written in pencil; the top of the figure should be clearly indicated. Figures and tables should be placed at the end of the manuscript following the Reference section. Each figure and table should be accompanied by an explanatory legend. The figure legends should be grouped and placed on a separate page. Figures are not returned to the author unless specifically requested.

In tables, 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.

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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* (Eds., Kubinyi, H., Folkers, G. and Martin, Y.C.), 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* (Eds., Tam, J.P. and Kaumaya, P.T.P.), Proceedings of the Fifteenth American Peptide Symposium, Nashville, TN, June 14–19, 1997, Kluwer, 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; institution; location of institution, in the order given in the example below.

Gippert, G. (1995) Ph.D. Thesis, The Scripps Research Institute, La Jolla, CA.

Special instructions for reports on protein structure determination by NMR

Acceptance of papers will be based primarily on two criteria, i.e., the biological interest of the structure, and the use of innovative technical approaches.

Normally, a report on a structure determination is expected to describe the complete three-dimensional structure, which is based on extensive collection of conformational constraints and structure calculations, for example, using distance geometry or molecular dynamics techniques. The material covered should include a brief account of the resonance assignments, a statistical analysis of the residual errors, a quantitative comparison of the conformers used to describe the solution structure, and a discussion on the biological relevance of the structure. A tabulation of the chemical shifts can also be included. The input list for the structure calculation and the atomic coordinates will not be published, but need to be deposited in a databank, such as the Brookhaven Protein Databank or the BioMagResBank. For further guidance to the presentation, 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.

Supplementary material. In an effort to keep the length of articles 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 from the corresponding author who agrees to provide this material on request to interested individuals for a period of at least 3 years following the date of publication.

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