



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. These studies 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.
- 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.
- Sample preparation for NMR experiments (biosynthetic and chemical methods for isotope labeling, preparation of nutrients for biosynthetic isotope labeling, etc.).

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.

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For the purpose of refereeing, papers for publication should initially be submitted in hardcopy (fourfold) and on diskette to any of the Associate Editors (see above).

MANUSCRIPT PRESENTATION

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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 'accelerate publication', with the same priority 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.

Assignment Notes

An *Assignment Note* announces NMR assignments for a new protein. To be acceptable, the assignments must be for a natural protein of size 100 amino acids or larger. 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. An *Assignment Note* 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 Note* (without figure and references) and the chemical shift list in the format of the data bank.

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First-, second-, third- and fourth-order headings should be clearly distinguishable.

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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 followed by 'et al.' should be used. In the event that the author has had two or more works published during the same year, the citation and the reference should contain a lower case letter like a and b after the date to distinguish the works.

Examples:

Winograd (1986, p. 204)
 (Winograd, 1986a)
 (Winograd, 1986b)
 (Winograd, 1986; Flores et al., 1988)
 (Bullen and Bennett, 1990)

References

References to books, journal papers, articles in collections and conference or workshop proceedings, and technical reports should be collected in an alphabetized list at the end of the paper, following the Harvard style.

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

Kubinyi, H. (Ed.) (1993) *3D QSAR in Drug Design: Theory, Methods and Applications*, ESCOM, Leiden.

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Kuramochi, H. and Singh, U.C. (1997) In *Computer Simulation of Biomolecular Systems: Theoretical and Experimental Applications*, Vol. 3 (Eds, Van Gunsteren, W.F., Weiner, P.K. and Wilkinson, A.J.), Kluwer, Dordrecht, pp. 563–600.

References to essays in conference proceedings should include the author's name(s); year of publication in parentheses; title of proceedings; editor's name(s); place and date of conference; publisher and/or organization from whom the proceedings can be obtained; place of publication; first and last page numbers. For example:

Hsieh, Y.F., Verentchikov, A., Gabeler, S., Vestal, M. and Martin, S.A. (1996), HPLC '96 – 20th International Symposium on High Performance Liquid Phase Separation and Related Techniques, San Francisco, CA, U.S.A., June 16–21, 1996.

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

Baleja, J.D., Thanabal, V. and Wagner, G. (1997) *J. Biomol. NMR*, **10**, 397–401.

References to technical reports or doctoral dissertations should include the author's name; year of publication in parentheses; institution; location of institution. For example:

Aslam Noor, M. (1996) Lecture Notes, Mathematics Department, King Sand University, Riyadh.

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.

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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