

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 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 theory, methods and application of nuclear magnetic resonance spectroscopy in the study of the structure and dynamics of biological macromolecules will be considered for publication.

MANUSCRIPT TYPES

Article

Full-length papers 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 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 a *Communication*.

Communication

Communications are restricted to reports of unusual urgency, significance, and interest, and must fit on 6 printed pages, including figures, tables and references (see Sizing guide section). Each *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.

Letter to the Editor: New NMR structure

A structure determination that yields a high quality NMR structure but may not warrant description in an *Article* or *Communication* can be published as a *Letter to the Editor: New NMR structure*. 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 manuscript must follow the layout of *J. Biomol. NMR*, **19**, 75–78 (2001), with the 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 *Letter to the Editor: New NMR structure* must fit on 4 printed pages (see Sizing guide section).

Letter to the Editor: New NMR assignment

An assignment for a new, well-structured protein 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. A protein is considered 'new' if no NMR structure or resonance assignments have yet been published for any protein that is more than 70% identical in sequence. Assignments for proteins that are part of an intermolecular complex cannot be considered if either the NMR structure or assignments for the free protein or for the protein as part of another complex have been published. In case of doubt, authors are advised to contact an Associate Editor prior to preparation of the manuscript. Complete backbone assignments and complete or nearly complete side chain assignments are required. Partial assignments may be considered for publication if the authors present, in the *Biological context* section, a *convincing reason* for publication of this data in view of its biological interest. For example, assignments only for the polypeptide backbone in proteins for which a crystal structure is available could provide a basis for functional studies of the protein. In each individual case the decision on whether or not an assignment letter is accepted for review, and hence given a chance for acceptance, is with the Associate Editor to whom the manuscript has been submitted. The manuscript must follow the layout of *J. Biomol. NMR*, **19**, 79–80 (2001), with the three subtitles *Biological context*, *Methods and experiments*, and *Extent of assignments and data deposition*. The text must be supplemented by one figure, illustrating the quality of annotated spectral data

underlying the assignments, and at most 10 references. A *Letter to the Editor: New NMR Assignment* must fit on two printed pages (see Sizing guide section).

MANUSCRIPT PRESENTATION

The *Journal of Biomolecular NMR*'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, up to 6 keywords in alphabetical order, and abbreviations if applicable.**

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. A character count must be given on the title page of each manuscript submitted. Please allow for the space used for figures and tables when estimating the overall length.

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). New structures may be published either as an *Article* a *Communication* or as a *Letter to the Editor: New NMR structure*. The principal criteria for deciding about the appropriate format for the publication are novelty of the structure, and the biological interest of the work presented. At the discretion of the Associate Editor to whom the manuscript has been submitted, the authors may be asked to change the format from that of an *Article* or *Communication* to a *Letter to the Editor: New NMR structure*, or *vice versa*. Such a decision may be made either before the manuscript is accepted for review, or after the initial review in view of the referee's comments.

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.bmrb.wisc.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.

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

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, 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

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