Scope of the Journal

*Journal of the American Society for Mass Spectrometry* is a monthly, peer-reviewed journal that covers all aspects of mass spectrometry, including fields of scientific inquiry in which mass spectrometry can play a role. These fields include chemistry, physics, geology, and environmental science as well as the biological, health and life sciences. The journal publishes papers on both fundamentals and applications of mass spectrometry.

In addition to full papers, the journal offers Short Communications, Application Notes, Letters to the Editor, Accounts and Perspectives, and Critical Insights.

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**Research Article:** Fundamental subjects include, but are not restricted to, instrumentation principles, design, and demonstration, structures and chemical properties of gas-phase ions, studies of thermodynamic properties, ion spectroscopy, chemical kinetics, mechanisms of ionization, theories of ion fragmentation, cluster ions, potential energy surfaces, and modeling.

Papers that report on an application should have as a principal focus the use of mass spectrometry to solve a qualitative or quantitative problem. Application subjects include, but are not limited to, structural elucidation, biopolymer sequencing, development or validation of new methodology, proteomics and other ‘omics related research, and environmental and forensic measurements. Papers describing development of new software and its applications will be considered, but details and compilations of programs will not be published. A report of a routine application of mass spectrometry is likely to be better suited to a journal specializing in the subject of the application.

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Communications will be published in separate sections at the beginning of each issue. Application Notes will be published at the end of an issue. Both will, insofar as possible, receive expedited handling. They may contain up to three single-column figures or tables (up to one page, total) and up to 2,300 words, including references and abstract. Space allocated to figures and tables may be replaced by text (~250 words per figure or table). Submissions exceeding these guidelines will be treated as Regular Articles.

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Manuscript Preparation

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- Submissions must be complete with clearly identified standard sections used to report original research, free of annotations or highlights, and include all numbered and labeled components.
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**Main Body Text:** Organize the text as Introduction, Experimental or Methods, Theory (if applicable), Results and Discussion, and Conclusions. Conclusions should not be a repetition of the abstract or a summary of the paper.

In the experimental section of the manuscript, all special safety considerations should be described in sufficient detail so that appropriate safety measures can be taken by those repeating the experiments (see below).

Refer to illustrations and tables in numerical order in the text.

Spell out, or define in parentheses, all abbreviations, even if they are commonly employed, the first time they are used in the text. Non-standard abbreviations should be used sparingly and must be defined at their first appearance.


Give all measurements and weights in SI units, using standard abbreviations (see IUPAC Quantities, Units and Symbols in Physical Chemistry). Daltons (Da) or mass units (u) may be used, but amu should not be used.

Consult articles in recent issues of the Journal for the recommended style for headings and subheadings.

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Supporting Information. Brief descriptions in nonsentence format listing the contents of the files supplied as Supporting Information.

When including supporting information for review only, include copies of references that are unpublished or in-press. These files are available only to editors and reviewers.

Data Requirements

The Use of High Resolution Mass Spectral Data for Formula Confirmation: For publication of exact- mass data that are used to confirm identities of synthetic and natural products, report the uncertainty in the accurate-mass measurement used for formula verification along with the result. The acceptable uncertainty in a measurement by any analytical method must be adequate for the intended use of the data.

Evaluate the uncertainty of accurate mass measurement by any statistically valid method. Determine, for example, the precision and accuracy of replicate measurements or evaluate the performance characteristics of the mass spectrometer (see, for example, Sack, T. M., Lapp, R. L., Gross, M. L., and Kimble, B. J. Int. J. Mass Spectrom. Ion Proc. 1984, 61, 191-213).

Consider all candidates fitting the experimentally determined value and its reported uncertainty when the result of accurate mass measurement is used for formula confirmation. Do not set fixed acceptable error limits for exact mass measurement. Consider the following when using accurate mass data.

When valence rules and candidate compositions encompassing C0-100, H3-74, O0-4, and N0-4 are considered at nominal parent m/z of 118, there are no candidate formulae within 34 ppm of each other. When the ion is of m/z 750.4 and the formulae are in the range C0-100, H25-110, O0-15, and N0-15, there are 626 candidate formulae that are possible within 5 ppm. Thus, for a measurement at m/z 118, an error of only 34 ppm uniquely defines a particular formula, whereas at m/z 750, an error (and precision) of 0.018 ppm would be required to eliminate all extraneous possibilities.

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ACS editors have provided Ethical Guidelines for persons engaged in the publication of chemical research—specifically, for editors, authors, and reviewers. Each journal also has a specific policy on prior publication.

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Authors must emphasize any unexpected, new, and/or significant hazards or risks associated with the reported work. This information should be in the Experimental Section of the full article and included in the main text of a letter.

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Appendix 2: Preparing Graphics

Resolution

Digital graphics pasted into manuscripts should have the following minimum resolutions:

- Black and white line art, 1200 dpi
- Grayscale art, 600 dpi
- Color art, 300 dpi

Size

Graphics must fit a one- or two-column format. Single-column graphics can be sized up to 240 points wide (3.33 in.) and double-column graphics must be sized between 300 and 504 points (4.167 in. and 7 in.). The maximum depth for all graphics is 660 points (9.167 in.) including the caption (allow 12 pts. For each line of caption text). Lettering should be no smaller than 4.5 points in the final published format. The text should be legible when the graphic is viewed full-size. Helvetica or Arial fonts work well for lettering. Lines should be no thinner than 0.5 point.

Color

Color may be used to enhance the clarity of complex structures, figures, spectra, and schemes, etc., and color reproduction of graphics is provided at no cost to the author. Graphics intended to appear in black and white or grayscale should not be submitted in color.
**Type of Graphics**

**Table of Contents (TOC)/Abstract Graphic**

Consult the Guidelines for Table of Contents/Abstract Graphics for specifications.

**Figures**

A caption giving the figure number and a brief description must be included below each figure. The caption should be understandable without reference to the text. It is preferable to place any key to symbols used in the artwork itself, not in the caption. Ensure that any symbols and abbreviations used in the text agree with those in the artwork.

**Charts**

Charts (groups of structures that do not show reactions) may have a brief caption describing their contents.

**Tables**

Each table must have a brief (one phrase or sentence) title that describes the contents. The title should be understandable without reference to the text. Details should be put in footnotes, not in the title. Tables should be used when the data cannot be presented clearly in the narrative, when many numbers must be presented, or when more meaningful inter-relationships can be conveyed by the tabular format. Tables should supplement, not duplicate, information presented in the text and figures. Tables should be simple and concise.

**Schemes**

Each scheme (sequences of reactions) may have a brief caption describing its contents.

**Chemical Structures**

Chemical structures should be produced with the use of a drawing program such as ChemDraw.

**Cover Art**

The Editorial Office for the *Journal of the American Society for Mass Spectrometry* selects papers to be featured on the front cover. Additional details on these requirements will be provided by the Editorial Office if selected. If your art is selected for front cover, ACS will send you information about how to request one complimentary 18” by 24” printed poster featuring your work.

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