Guide to Scientific Writing and Publishing

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Chemical Abstracts Service, Columbus, OH

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“Guide to Scientific Writing and Publishing”
ASP Younger Members Working Luncheon
Crystal Gateway Marriott
August 6, 2006
Topics

- A. Douglas Kinghorn (Manuscript Reviewing; Ethical Aspects)
- Debora Bittaker (Production Aspects)
- Matt Price (Journal Marketing Aspects)
Manuscript Reviewing; Ethical Aspects

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Why Publish and When?

- Publication provides a permanent record of important, significant, and novel laboratory research results.
- This avoids unnecessary duplication of effort.
- Authors should normally present the results of a complete investigation, even if of quite limited scope (unless submitting a Rapid Communication).
Publish with Pride!

- A well-crafted manuscript is an author’s “window to the world”, and serves as an advertisement as to the quality of the work being performed in his or her lab.
- Publication should always be done with pride, since a bad paper will be widely accessed electronically with minimal effort by the reader. This can haunt an investigator for years!
Criteria for Peer Reviewers of Technical Manuscripts

- Being asked to serve as peer reviewer by a journal editor is a significant professional function for a scientist.
- To participate in this manner, referees should normally have a terminal degree in the discipline concerned.
- Reviewers should have relevant expertise in the sub-discipline covered by the paper being reviewed.
- Reviewers must be willing to spend the necessary personal time to perform a thorough review.
Some Attributes of a Well-Prepared Manuscript

- Scientific manuscripts should be logical, factually accurate, concisely written, and afford adequate attribution to previous work on the same topic.
- Papers should conform to the technical scope of a selected journal, and be presented in the correct journal format.
- The rationale for the study being conducted should be explained.
- The submitted manuscript should be seen and approved by all co-authors.
- Internal “peer review” of the paper is highly desirable prior to formal submission.
Some Common Problems with Submitted Manuscripts

- The work described is only of marginal significance (representing the “least publishable unit”)
- Factual inaccuracies evident
- Represents fragmentation of effort on same topic (e.g., the constituents of the same organism)
- Contains unnecessary components (e.g., unneeded compound trivial names or biological activity of threadbare significance)
- Poorly written (e.g., repetitive, meandering, expressed in “lab language”; lack of adhesion to required journal format)
Reviewing of Manuscripts

- Reviews should be impartial and offer constructive criticism
- A thorough check for the novel aspects (e.g., whether a structure is really new) is needed
- The correctness of the chemical and biological components of a paper should be checked
- The literature review should be specifically examined for completeness
- Suggestions for the improvement of rigor of the methodology used are very valuable
The Most Important Aspect of a Manuscript Review

- A decisive recommendation on only one of the following is the most helpful aspect of a review for an editor:
  - Accept without change
  - Minor revision
  - Major revision
  - Reconsider after major revision (this requires additional peer review)
  - Reject
  - Inappropriate/Publish elsewhere
Examples of Less Important Aspects to Be Addressed by Reviewers

- English grammar and manuscript construction
- Typographical errors
- Adherence to journal format
- Perception of how well the paper conforms to the technical scope of the journal
- Other factors (e.g., the peer review of previously published papers by the author currently being evaluated; evaluation of the scientific reputation of the manuscript co-authors)
How to Avoid Ever Being Invited to Review for a Given Journal Again

Provide a one line review such as:

“An excellent study for which no revision is needed” (!)
Issues of Integrity and Scientific Publishing

- Unfortunately, in recent years we have seen examples of the following negative aspects in scientific publishing:

  - **Fabrication** (inventing information where none previously existed)
  - **Falsification** (altering truthful information)
  - **Plagiarism** (the intentional or unintentional use of another person’s words or ideas)
  - “Self-plagiarism” is a variant in which authors attempt to publish verbatim the same information in two or more manuscripts
  - **Inclusion of “Guest Authors”** (persons who do not fulfill authorship criteria)
  - **Omission of “Ghost Authors”** (individuals who should have been included)

Progression of Honest Errors to Intentional Fraud

(Adapted from Nylenha and Simonsen, Lancet, 2006, 367, 1882-1884)
Who Should Be Included as a Co-Author?

- They should: (a) make a substantial and new contribution to the research; (b) take responsibility for some of the content of the manuscript; (c) read and agree to the manuscript before submission; and (d) agree to be named as a co-author.

- In practice, great reliance is placed on the integrity of the corresponding author to deal with the inclusion and ordering of co-author names.

- The corresponding (lead) author (designated with an asterisk) is usually head of a lab or a project, with a permanent or stable address (this is needed in case of queries about the paper).
Other Examples of Scientific Integrity Problems in Submitted Manuscripts

- Submission of paper by inappropriate corresponding author, without appropriate permission (e.g., an ex-graduate student or postdoctoral)
- An institution where the work is performed (in part or in full) is not included in the list of addresses (as well as the reverse situation)
- Submission of same paper to two different journals
- No permission obtained for exporting and importing organisms from the country of collection to the country where the laboratory work is conducted
Actions that Journal Editors May Take in Cases of Ethics Violations

- In cases of minor infractions, explain problem(s) to corresponding authors.
- For blatant or repeated violations, the editor can forbid the author in question from submitting to the journal for a specified period.
- In the United States, in cases of disputed coauthorship, fraud, or plagiarism, the matter may be turned over to the institutional Office of Research Integrity of the institution of the lead author, in order to set up an inquiry.
- For overseas authors, the President of an institute or other organization to which the lead author belongs may be informed of the breach of ethics.
Relevant Resources of the Journal of Natural Products

- For prospective reviewers, we have a questionnaire covering topics of expertise. For interested postdoctorals, please contact Rebecca Johnson at jnatprod@osu.edu

- Each year, “Ethical Guidelines to Publication of Chemical Research” is published in our January issue (J. Nat. Prod. 2006, 69, 16A-18A). Note in particular the ethical obligations of authors and reviewers.
Post-Peer-Review Journal Production: Transforming a Manuscript for Publication

Debora Bittaker
Young Members Working Luncheon
ASP Meeting

Adapted from a presentation by
Terri K. Lewandowski, Anne C. O’Melia, and Joseph E. Yurvati
CINF Presentation, ACS National Meeting, March 26, 2006

“Guide to Scientific Writing and Publishing”
ASP Younger Members Working Luncheon
Crystal Gateway Marriott
August 6, 2006
Manuscript Lifecycle

Author ↔ Editor ↔ Reviewer ↔ Editorial & Production

Electronic Journal
Printed Journal

Columbus Staff
Journal Leader: Diane Black, Associate Editor
Journals Editing Manager: Debora Bittaker
ACS Journals Statistics (2005)

All ACS Journals
- 34 titles
- 658 print issues
- 29,302 research articles
- 226,114 published pages

Journal of Natural Products
- 1 title
- 12 print issues
- 385 research articles
- 1956 published pages
- 2% of the ACS’ volume
- 100% of ACS’ publishing expertise!
Key Editorial Production Objectives

- Assist authors through publication process
- Ensure rapid time to publication
- Support Journal Editors
- Provide a uniform reader experience
- Improve discoverability
- Ensure archivability
- Minimize production costs
How ACS Assists Authors through the Publication Process

- Author guidelines for preparation of text and graphics
- Templates for manuscript preparation
- Manuscript content redaction and validation
- Author interface for galley review and comments
- Publication status information on author homepage of Paragon
Information for Authors on Paragon Submission Website

The *Journal of Natural Products* provides Document Templates for preparing manuscripts for submission as well as for preparing final, accepted manuscripts. The journal now requires a Table of Contents graphic that will be published on the Web only. Instructions for submitting the TOC graphic are below.

- **Scope of the Journal** [PDF]
- **Guidelines for Authors** [PDF]
- **Instructions for submitting a Table of Contents (TOC) graphic** [PDF]
- **Ethical Guidelines**

**General Submission Instructions**

Author instructions vary somewhat for each journal. However, there are general instructions for all journals that include the following:

- **How to Submit Online**
- **Preferred Software**
- **Preparing Manuscripts Using TeX/LaTeX**
- **Preparing Graphics and Illustrations**
- **Specifications for Web Enhanced Objects**
- **Submitting a Hardcopy Manuscript**
- **Completing a Media Description Form** [PDF]

**Copyright Forms and Information**

The *Journal of Natural Products* requires the use of a special **Copyright Status Form** [PDF].

Where to send the signed ACS Copyright Status Form

Information on Permissions Requests and other copyright information can be found here.

Additional information on the *Journal of Natural Products* can be found at the **Journal Home Page**.
Information for Authors on Preparing Graphics and Illustrations

- Illustrations must fit a one- or two-column format on the journal page: For efficient use of journal space, single column illustrations are preferred.
  - Single column (preferred)
    - Minimum width 10.50 cm (4.13 in.)
    - Maximum width 8.25 cm (3.25 in.) 17.78 cm (7 in.)
  - Double column
    - Maximum height 24.00 cm (9.5 in.) 24.00 cm (9.5 in.)
- Digital graphics should be saved as TIFF images with the following minimum resolution requirements:
  - Black and white line art: 1200 dpi
  - Grayscale art: 600 dpi
  - Color art 300: dpi
- For structure drawings, follow ChemDraw instructions in Guidelines for Authors
How ACS Ensures Rapid Time to Publication and Minimizes Production Costs

- Automate standard processes whenever possible, conserving staff time for editing and other tasks that require scientific knowledge.
  - Document management/workflow system
  - Automated background workflow tools
  - Automated tracking and reporting
  - On-demand reports

How Authors can help themselves:
Automated tools run best when standard software and document structures are used.
- Use suggested software for manuscript and graphic preparation.
- Use ACS reference style.
- Ensure all parts of paper are in final version.
# On-line Manuscript Workflow System Speeds Production

<table>
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<tr>
<th>File preparation</th>
<th>Technical editing</th>
<th>Page proof production</th>
<th>Page proof correction</th>
<th>Manuscript publication</th>
</tr>
</thead>
</table>

Manuscript workflow/tracking system
File Preparation

- Conversion to standard format
  - Text
  - Graphics
- Text tags applied for basic formatting
- Pre-editor applied to routine, standard editing changes:
  - For example: change ml to mL
Technical Editing: How ACS Provides a Uniform Reader Experience

- Standard presentation within a journal
- Appropriate file formats for SI
- Appropriate use of ACS style
- Defines nonstandard terminology
- Content validation
- Manuscript editing by scientists
Technical Editing of Text

- Grammar scrutinized
- Syntax polished
- ACS style applied
- Additional tags applied for page formatting, linking on Web, and discoverability
- Tabular material reviewed and format standardized
- Content checked for completeness:
  - missing figures
  - incomplete references
  - uncited references
Technical Editing: Improve Author’s Words without Losing the Author’s Voice

Author's original:

These above researches concentrated either in structure and orientations of crystals in mollusk shells or in polymorphs of SM/IM induced calcium carbonate. In this paper, we mimicked the biomineralization process to fabricate calcite crystals but mainly to analyze morphologies and orientation relationships.

Edited version:

The above research concentrated either on structure and orientations of crystals in mollusk shells or on polymorphs of SM/IM-induced calcium carbonate. In this paper, we mimicked the biomineralization process to fabricate calcite crystals but mainly to analyze morphologies and orientation relationships.
Technical Editing: Improve Author’s Words without Losing the Author’s Voice

Author's original:

Resonance of the latter could be the signal observed. But we have been surprised it was not easy to find literature data on chemical shift for such easiest molecule. Only in one of the later issues of JACS we found resonance of ortho-hydrogen (o-H₂) in polar solvents observed around G = 4.6.$^{15}$

Edited version:

The resonance of the latter could be the signal observed. However, we were surprised that it was not easy to find literature data on the chemical shift for such a simple molecule. Only in a recent issue of J. Am. Chem. Soc. did we find a resonance for o-hydrogen (o-H₂) in polar solvents that was observed to be around δ 4.6.$^{15}$
Table 2. Comparisons of ALR1 and ALR2 inhibitor binding constants IC$_{50}$ (µM) and ∆H (kcal/mol).

<table>
<thead>
<tr>
<th>Inhibitor</th>
<th>IC$_{50}$ porcine ALR1</th>
<th>IC$_{50}$ human ALR1</th>
<th>IC$_{50}$ human ALR2</th>
<th>IC$_{50}$ rat ALR2</th>
<th>∆H porcine ALR1</th>
<th>∆H human ALR2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fidarestat</td>
<td>2.5</td>
<td>1.2$^a$</td>
<td>0.009$^a$</td>
<td>0.035$^c$</td>
<td>-12</td>
<td>-15</td>
</tr>
<tr>
<td>Sorbinil</td>
<td>4.0</td>
<td>5.4$^b$</td>
<td>2.0$^b$</td>
<td>0.90$^c$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2R4S</td>
<td>17.8</td>
<td></td>
<td></td>
<td>0.57$^c$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

IC$_{50}$ values reported by $^a$Mizuno et al.,$^{57}$ $^b$Barski et al.$^{58}$ and $^c$Yamaguchi et al.$^{59}$
Figure 1. A schematic diagram of the T7 tail fiber. The relative locations of putative rod-domain, the recombinant truncated rod-domain fragment (residues 147-220) and the p17 synthetic peptides MC892 and MC917 are indicated.
Page Proof Production

- Text and graphics merged and formatted to journal specifications
- Format adjusted as needed
- Content checked for completeness
- Proof package forwarded to author: usually on the Web
  - Formatted page proofs
  - Manuscript with edit trace
  - Proof review instructions
The proof of your paper, manuscript number joxxxxxxx, entitled Synthesis of the Most Novel Compound Ever Conceived is now available electronically for your review and approval at the following URL:

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Page Proof Correction

Introduction

Discovery of novel lead compounds through virtual screening of chemical databases against protein structures is well established, but there is still much room for improvement in key aspects of algorithm performance. Many methods have been published that vary primarily in two components: scoring functions and search methods (for a more complete review, see Bissantz et al. and John). The primary criteria for evaluating docking strategies are geometric docking accuracy, screening utility, scoring accuracy, and speed. Geometric docking accuracy measures a dock's ability to generate and recognize the native conformation and alignment (pose) of a ligand bound to its cognate protein beginning from an arbitrary initial pose. This is typically reported as the fraction of cases where the dock's top-scoring ligand pose is within 2.0 Å rmsd from the experimentally determined binding geometry. Screening utility measures a dock's ability to rank cognate ligands of a protein above random ligands, as is desired in typical virtual screening applications. Methods for quantifying screening utility varies, but most frequently it is characterized by constructing virtual screening libraries that contain some small number of known active molecules for a protein under study along with a large number of randomly selected compounds typical of a screening library. Following docking of a such a virtual library to a protein, the resulting ranking of the ligands is used to compute the observed true positive rates (percentage of known ligands found determined values. This can be very important in focused medicinal chemistry exercises, but the thrust of this paper is on large-scale virtual screening, so that methodological evaluation focused most strongly on screening utility. One important recent trend in the docking literature has been the use of publicly available benchmarks for assessing the performance of methods. Rogman's group has been at the forefront of this trend, and others have made use of the benchmarks developed there, both for docking accuracy and for screening utility. In particular, reports on Surflex and GLIDE have made direct use of these benchmarks. In addition, reports of the performance of GOLD have been very important in establishing benchmarks of docking accuracy.

The issue of docking accuracy has been extensively tested by many groups, and the data sets are sufficiently large that the reports of different groups largely agree as to performance of the most widely used methods. The broadest recent study directly compared eight methods: DOCK, FlexX, FRED, Glide, GOLD, SLIDE, Surflex, and QXP. The four most successful methods achieved very similar results, ranging from 50% to 55% success in returning top-ranked poses within 2.0 Å rmsd of the experimental results: FlexX, GLIDE, GOLD, and Surflex. Recent methods that are focused on GOLD, Surflex, and GLIDE contained benchmarking information on docking accuracy as well, and these results largely agreed with the independent work of Rogman's group, suggesting comparable accuracy among these methods. Additional details of these benchmark results can be found in recent review studies.

How Authors can help themselves: Use line numbers when requesting changes via e-mail.
Page Proof Correction

- Author changes arrive via e-mail to ACSProof
- Author changes validated
- Revised page proofs created
- Corrections proofed
Manuscript Publication

- Published ASAP on the Web
- Print issues planned, paginated, printed.
- Metadata and abstracts sent to secondary services
- Publication status to author
- Final print version posted on the Web
Manuscript Publication:
Print Issue Planned
How ACS Improves Discoverability

- Tag manuscript components for Web products such as ASAP Alerts and TOC Alerts
- Tag manuscript components for discovery by search engines
- Provide data feeds to secondary services
How ACS Ensures Archivability

- Provide industry standard formats (PDF, HTML)
- Provide field specific file formats for Supporting Information and Web Enhanced Objects
Acknowledgement: Linda Hart, Teresa Schleifer, and Ram Ravi from the ACS Journals Manufacturing Group are thanked for their help in providing the material used in this presentation.
Journal Marketing Aspects

Matthew Price
Director, Sales & Marketing
ACS PUBLICATIONS

“Guide to Scientific Writing and Publishing”
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August 6, 2006
ACS Journals
The MOST Cited Journals in the Chemical and Related Sciences

ACS Journals:
- Rank #1 in citations and/or ISI® Impact factor in all 7 ISI® core chemistry categories:
  - analytical, applied, inorganic & nuclear, medicinal, multidisciplinary, organic, and physical chemistry
- Rank #1 in citations and/or ISI® Impact factor in 7 additional ISI® categories – from agriculture and environmental science to materials and polymer sciences, including the all-new ISI subject category of nanoscience and nanotechnology
- Overall exceeded 1.13 Million citations in 2005 AND 1 Million Article Downloads PER WEEK each and every week
ACS Journals
Biological & Medicinal Chemistry

- 12 ACS Journals in BIO/MED program
- Nearly 100,000 peer-reviewed articles published in these titles alone
- Long-established presence – and growing
  - Journal of Natural Products (Volume 69)
  - Journal of Medicinal Chemistry (Volume 49)
  - Biochemistry (Volume 45)
  - Biotechnology Progress (Volume 22)
  - Introduced ACS Chemical Biology in 2006
Marketing by the Numbers

Journal of Natural Products

- Co-published monthly by the ACS & ASP
- 2006, Volume 69, 12 Issues
- A Premier Arena for Natural Products Research
- More than 8,800 peer-reviewed articles published since 1979
- More than 4,000 articles in ACS Legacy Archives—all volumes published from 1979 to 1995 recently added
2005 ISI® Journal Citation Reports

- Recorded nearly 10,000 citations in 2005
- 13% increase in citations in 2005 over 2004
- Has nearly doubled # of citations in last 5 years
- ISI® Impact Factor of 2.267 is highest in its history
JNP is indexed in four ISI® subject categories:

- Plant Sciences
- Applied Chemistry
- Medicinal Chemistry
- Pharmacology & Pharmacy

That’s the most categories of any journal published or co-published by the ACS.
Journals that cited J Nat Prod the most include:

1. Natural Product Reports (582)
2. Tetrahedron (305)
3. Phytochemistry (258)
4. Organic Letters (255)
5. Tetrahedron Letters (254)
6. Chemical and Pharmaceutical Bulletin (245)
7. Planta Medica (209)
8. J Agricultural and Food Chemistry (202)

Overall, J Nat Prod was cited by 482 journals in 2005 – up from 297 citing journals in 2001, when only three journals cited articles in J Nat Prod 200 times or more.
2005 ISI® Journal Citation Reports

With nearly 10,000 total citations in 2005, *J Nat Prod* is:

- The most-cited journal published or co-published by the ACS in both Plant Sciences and Pharmacology & Pharmacy—ranking #13 overall out of 144 journals in Plant Sciences and #16 overall out of 193 journals in Pharmacology & Pharmacy -- *in the top 10% of both categories.*
Additionally, *J Nat Prod* is ranked by ISI® as:

- The #2 most-cited ACS journal in Medicinal Chemistry, after *J Med Chem*, ranking #4 overall out of 34 journals in the category.
- The #2 most-cited ACS journal in Applied Chemistry, after *J Agric & Food Chem*, ranking #4 overall out of 59 journals in the category.

*J Nat Prod* is among the most cited and most relevant journals in its respective fields.
A Premier Arena for Natural Products Research

The top three most-accessed articles in the Journal of Natural Products are available to all researchers for free via the journal's homepage!

The Journal of Natural Products is an international forum for the latest research on the chemistry and biochemicals of naturally occurring compounds and the biology of living systems from which these compounds are obtained. Topics include secondary metabolites of microorganisms, including antibiotics and mycotoxins; pharmaceutically active compounds from higher plants and animals; biochemical studies, including biosynthesis and microbiological transformations; fermentation and plant tissue culture; the isotopic, structural elucidation, and chemical synthesis of novel compounds from nature; and the pharmacology of compounds of natural origin.

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A. Douglas Steynberg, Editor-in-Chief
Jill L. Inouye Professor and Chair
Department of Natural Chemistry & Pharmaceutical Sciences
University College of Pharmacy

2006 / Volume 69 / 12 issues

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ACS PUBLICATIONS
HIGH QUALITY. HIGH IMPACT.
J Nat Prod periodically publishes Special Issues to highlight and honor significant, lasting contributions by leading figures in natural products research

- Volume 69, Issue 3, March 2006
  Special Issue honoring Norman R. Farnsworth

- Volume 67 issue 8, August 2004
  Special Issue honoring D. John Faulkner and Paul J. Scheuer

- Volume 67 issue 2, February 2004
  Special Issue honoring Monroe E. Wall and Mansukh C. Wani
The American Chemical Society designated the discovery of camptothecin and Taxol® at the Research Triangle Institute a National Historic Chemical Landmark on April 23, 2003.

The Discovery of Camptothecin and Taxol®

"Taxol is arguably the most celebrated, talked about and controversial natural product in recent years..."


Monroe Wall, Mansukh Wani, and colleagues at the Natural Products Laboratory of the Research Triangle Institute discovered and elucidated the structure Taxol® and camptothecin, two life-saving compounds for the treatment of cancer. These natural products kill cancer cells via unique mechanisms of action and in ways scientists had not previously imagined. The work of this research team led to the eventual development and marketing of drugs that have been approved for treatment of ovarian, breast, lung, and colon cancer and Kaposi’s sarcoma.


Note: Taxol® is a registered trademark of Bristol-Myers Squibb and camptothecin™ is a trademark of the Research Triangle Institute.
Most-Cited Articles

1. Pietta PG
   Flavonoids as antioxidants
   JOURNAL OF NATURAL PRODUCTS 63 (7): 1035-1042 JUL 2000
   Times Cited: 314

2. Alali FQ, Liu XX, McLaughlin JL
   Annonaceous acetogenins: Recent progress
   JOURNAL OF NATURAL PRODUCTS 62 (3): 504-540 MAR 1999
   Times Cited: 232

3. Cragg GM, Newman DJ, Snader KM
   Natural products in drug discovery and development
   JOURNAL OF NATURAL PRODUCTS 60 (1): 52-60 JAN 1997
   Times Cited: 222

4. Haslam E
   Natural polyphenols (vegetable tannins) as drugs: Possible modes of action
   Times Cited: 213

   Natural products as sources of new drugs over the period 1981-2002
   JOURNAL OF NATURAL PRODUCTS 66 (7): 1022-1037 JUL 2003
   Times Cited: 179
Structure-activity relationship and classification of flavonoids as inhibitors of xanthine oxidase and superoxide scavengers  
Times Cited: 162

7. Baloglu E, Kingston DGI  
The taxane diterpenoids  
JOURNAL OF NATURAL PRODUCTS 62 (10): 1448-1472 OCT 1999  
Times Cited: 124

Antioxidant and antiinflammatory activities of anthocyanins and their aglycon, cyanidin, from tart cherries  
Times Cited: 121

DNA polymerase and topoisomerase II inhibitors from Psoralea corylifolia  
Times Cited: 109

10. Shu YZ  
Recent natural products based drug development: A pharmaceutical industry perspective  
Times Cited: 104