JOURNAL OF CHEMICAL INFORMATION AND MODELING

Editorial

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Letter from the Editors

Dear JCIM Community,

First, we want to thank everyone for the continued support of *Journal of Chemical Information and Modeling* (JCIM) through article submission and providing timely and detailed referee reports! We strive to publish the best the computational chemistry/biology field has to offer, and we thank you for your continued strong support.

JCIM has undergone a significant transition over the past year. First, Kennie Merz took over as Editor-in-Chief (EIC) at the start of 2014 from Bill Jorgensen who had been the EIC for the previous decade. Bill instituted a broad range of changes to the journal as documented by several editorials he published (e.g., http://pubs.acs.org/doi/pdf/10.1021/ci200046r and http://pubs.acs.org/doi/pdf/10.1021/ci0680079) during his tenure. We have largely strived to follow many of these modifications, which we discuss further below. At the same time of the EIC transition, Wendy Warr retired from the journal in her role as an Associate Editor (AE), and Matthias Rarey stepped in as a new AE in early 2014. Over the course of 2014, both Dušanka Janežič and Tony Hopfinger retired. Habibah Wahab and Alexander Tropsha came on board to serve as AEs. Wendy, Dušanka, and Tony together served JCIM for many years. The tremendous effort they expended, together with Bill, over more than a decade made JCIM the successful journal it is today. We, as the new team, are grateful for their work, and we hope to continue their success in the future. With significant transitions like the one experienced by JCIM in 2014, there are challenges to overcome, but also new opportunities emerge.

NEW OPPORTUNITIES

The Editor, AEs, and Editorial Board Advisory (EAB) all enthusiastically supported the creation of a new article category called the Application Note. This 5000 word article type is aimed at supporting the ongoing development of new software tools and web services giving them an outlet for publication. The details of this manuscript type can be found in this link (http://pubs.acs.org/doi/pdf/10.1021/ci500685s) for those interested in considering this publication mechanism. We have already had a few submissions using the manuscript type, and we look forward to further submissions in the coming years.

JCIM is also now on Twitter (@JCIM_ACS), which gives us an outlet to highlight the exciting articles published in the journal. Please follow the account so you can get the latest news from JCIM!

JOURNAL SNAPSHOT FOR 2014

At JCIM, we take great pride in the speed to publication. Typically, most manuscripts that are accepted are published online within 2−3 months of submission. The latest Thomson Reuters ISI Impact Factor of the journal (2013) is 4.068, and the journal garnered over 11,000 citations. The importance of the Impact Factor is hotly debated, but for the present, they are a ubiquitous metric, often used by authors in deciding where to submit.

UPDATE ON RETURN AFTER EDITORIAL REVIEW

Due to many journals being overwhelmed with submissions, coupled with a desire to not further stretch already overburdened referees, most high-quality journals return a number of submissions (deemed unlikely to succeed in peer review) after editorial review.

At JCIM, we consider every paper very carefully with regard to a number of factors, which are discussed below. RAERing an article is not taken lightly, and we strive to do the very best we can in making this very important decision. Typically, we now carry a two-editor review. If both editors are in agreement, the manuscript is returned after editorial review (RAER), and if there is a split vote, the paper is sent out for review. We hope this approach will further improve the quality and efficiency of our overall decision-making process.

In a previous editorial (http://pubs.acs.org/doi/pdf/10.1021/ci200046r), many of the reasons for RAERing a manuscript were given, and we recapitulate these reasons herein with some contemporary additions. Overarching reasons include "(a) the content does not fit well with the scope of JCIM such that submission to an alternative journal is more appropriate, (b) the content is narrow in scope such that many similar submissions could be envisioned with minor change in the systems studied, and (c) the content is routine or does not represent a significant advance in the field. More specific examples that are problematic for JCIM include (i) straightforward, retrospective QSAR or QSPR studies that do not advance the modeling of specific end points of interest, (ii) routine applications of quantum mechanics with little justification through contact with related experimental studies or conceptual debates, (iii) reports of virtual screening exercises that identify potentially active compounds without any subsequent experimental validation, and (iv) purely retrospective computational studies of structure−activity data that do not provide significant novel insights and testable prospective hypotheses."

Many of the above reasons specifically singled out problematic QSAR/QSPR publications. However, since the publication of the above-quoted policy, it has become clear that some of the papers using other methodologies (e.g., docking or molecular simulations) suffer from similar deficiencies concerning model utility, reproducibility, or accuracy as many QSAR papers did. Thus, to help JCIM authors prepare high-quality manuscripts, we propose the extended guidelines listed in Table 1, on which we are seeking community feedback.

Another aspect we want to emphasize during reviewing is the reproducibility of results. A method, which is not disclosed in detail or a data set, that is unavailable to the readership causes a lack of reproducibility. Not every software described has to be open source, but every interested scientist should be able to comprehend the methods published. Not every data set has to be disclosed, but a least one data set used should be in the public domain or made available upon publication. This information allows for the comparison of computational approaches in a fair

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Table 1. Criteria for Assessing Manuscripts

More Likely To Succeed in Review	Less Likely To Succeed in Review
Modeling study leading to a design that enables new and successful experiments (e.g., new potent compounds) irrespective of the modeling technique.	Routine modeling studies or modeling of thoroughly explored biological endpoints (LogP or well-studied inhibitor classes such as ACE inhibitors)
Models (with clearly outlined availability, e.g., implemented as a web service) of important new endpoints and demonstrably better models (e.g., larger and/or much higher quality) than any other existing models. Models for a known endpoint but a new biological target (e.g., human vs rodent data) confirmatory vs primary assay that leads to clearly outlined design strategies.	Models for a known endpoint, or an old data set, that do not show any advantage over existing models or models that are not OECD-compliant viz (1) a defined endpoint, (2) an unambiguous algorithm, (3) a defined domain of applicability, (4) appropriate measures of goodness-of-fit, robustness, and predictivity, or (5) a mechanistic interpretation, if possible
	Any paper without a section on data curation.
	Any paper containing proprietary data without making an explicit argument why the data should be protected and yet why in the absence of the data the manuscript is still valuable.
Provocative papers criticizing/rejecting existing paradigms; should be very well grounded and preferably must provide the reader some idea(s) how to solve the problem. Methodological papers summarizing best practices.	
New approaches for modeling, clustering, similarity estimation, etc. Must be benchmarked against multiple different tasks and consistently show superiority. These approaches could be developed and tested using simulated data sets but applied to several real tasks, and actual compounds should be designed using them.	New approaches for modeling, clustering, similarity estimation, etc. without benchmarking, or if benchmarked, showed results similar to existing methods.
Manuscripts describing databases/data sets; should contain some unique features—the biggest existing data set, user-friendly database, etc.	
Perspectives on "hot" or important topics.	
New nontrivial analyses/concepts of all related fields including med chem, drug design, tox, etc., approached from the molecular modeling point of view.	
Papers describing innovative application of existing cheminformatics techniques to new types of substances (nanomaterials, materials, mixtures, polymers, macromolecules, texts) that lead to new testable hypotheses.	Papers with innovative applications but not demonstrating predictive or instructional value (e.g., application of chemical graph-based descriptors to proteins without a clear indication of their value to structural biology).

and transparent fashion allowing for the advancement of the scientific endeavor.

UPDATE ON "ACS IS OPEN"

During the last year, the American Chemical Society expanded open access options available for authors publishing in ACS journals, including JCIM. For all peer-reviewed articles, the corresponding author is presented with the option to purchase an open access license immediately after acceptance under the umbrella of *ACS AuthorChoice*. Authors can also purchase open access at any time using the *ACS AuthorChoice* app in the freely available *ACS ChemWorx*. Licensing options include immediate open access and a lower-cost 12-month embargoed option with prices starting at $750. Creative commons license add-ons are available to meet some funder mandates. ACS also gives the corresponding author of all peer-reviewed articles published during 2014, including JCIM authors, two $750 ACS Author Rewards. These rewards can be used anytime between now and December 31, 2017 for any ACS open access option. Read more details of the four-pillar *ACS Is Open* initiative by clicking on the *ACS Is Open* link.

GENERAL PUBLISHING TIPS

With all the modern conveniences of electronic submission, authors sometimes ignore some basic publishing Publishing 101 concerns. Many cover letters are perfunctory at best and are not helpful in setting the stage for your article. Many of the RAER issues listed above can be addressed in the cover letter to help you, the authors, establish the context of your work in a concise and clear manner.

Stylistic issues nowadays are becoming less and less excusable given the availability of modestly priced editorial services worldwide. For those who struggle with stylistic issues, we highly encourage you to avail yourself of these services.

Journals now have access to many programs that rapidly identify plagiarism issues, which can result in a manuscript being held up in the publication process. Please take this into consideration when submitting your work to any journal. Proper attribution and requests for permission to reuse figures and schemes are essential.

IN SUMMARY

JCIM continues to prosper with ongoing contributions from our readers and authors. To even better support the community we serve, we have introduced Application Notes, and we continue to discuss modifications of the types of articles we support. Please feel free to contact any of us with your suggestions about how to further improve any aspect of the journal.

Sincerely,

The Editors of JCIM

Kenneth M. Merz, Jr.
Matthias Rarey
Alexander Tropsha
Habibah A. Wahab

AUTHOR INFORMATION

Notes

Views expressed in this editorial are those of the authors and not necessarily the views of the ACS.

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