Journal of Medicinal Chemistry

Editorial

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Progress in Computational Medicinal Chemistry

The *Journal of Medicinal Chemistry* (JMC) is the leading international journal for publication of state-of-the-art research in medicinal chemistry including computational studies. As emphasized in the recent Editorial by the Editors-in-Chief, Professors Gunda I. Georg and Shaomeng Wang, JMC continues to strive for scientific excellence at all levels with a strong focus on publishing new experimental and computational methodologies that further advance the field of medicinal chemistry.[1] In the computational area, JMC has made significant efforts over the past years to establish high publication standards. As a central part of these efforts, JMC announced the introduction of an internal prereview process for computational manuscripts in 2008 that involved members of the Editorial Advisory Board.[2] The prereview process was designed with a dual purpose: first, to ensure high quality standards and a high level of consistency in evaluating computational studies; second, to further refine guidelines and acceptance criteria for computational manuscripts. As a consequence of the prereview procedures conducted over the past few years, JMC has achieved a high level of consistency in evaluating computational studies and established clearly defined acceptance criteria for the publication of computational research.[3] Full details are provided in the Guidelines for Authors of JMC, sections 2.3.5 and 2.3.6 (current revision, January 2012). Achieving and maintaining these high standards would not have been possible without the dedicated efforts of our Editorial Advisory Board members and their continued support, which JMC gratefully acknowledges. Furthermore, these guidelines and acceptance criteria have been implemented in close alignment with the *Journal of Chemical Information and Modeling*. As pointed out by Professor William L. Jorgensen, Editor-in-Chief of the *Journal of Chemical Information and Modeling*, the two journals share common philosophy in this area.[4]

Having reached the stage where desired quality standards and acceptance criteria for computational studies have been implemented, JMC will no longer subject computational manuscripts to prereviews, in keeping with the intentions of the Journal to further streamline the editorial and publication process going forward.[1] As before, the editors will internally evaluate submissions in all areas prior to peer review to ensure that manuscripts meet the requirements specified in the Guidelines for Authors.

In the computational area, positive trends can currently be observed. For example, many of the computational studies submitted to JMC have traditionally been predictions of compound binding modes in the context of SAR investigations. We are pleased to note that the scientific quality and relevance of these types of modeling studies have notably increased over the past years. Consequently, rejection rates for combined experimental and computational investigations have decreased. However, we also note that there continues to be room for improvement of prospective virtual screening investigations. JMC has implemented stringent criteria for virtual screening applications reporting new active compounds. For publication in JMC, such studies must be of a high scientific rigor, concerning both computational and experimental procedures, and reported active compounds should be novel and have the potential to further advance medicinal chemistry.[3] We currently observe that many virtual screening applications submitted to JMC do not meet one or more of the acceptance criteria specified below. In these cases, manuscripts are returned to the authors with a revision and resubmission request.

Prospective virtual screening studies submitted to JMC must meet all of the following criteria (as specified in the current version of the Guidelines for Authors):

1. To validate virtual screening hits obtained from any source (e.g., in-house, commercial, public domain repositories), the following data must be provided:
   - 1.1. Proof of dose–response behavior.
   - 1.2. Confirmation of IC_{50} or K_i values.
   - 1.3. Controls for nonspecific or artificial inhibition (i.e., proof of reversibility, detergent controls, etc.).
   - 1.4. For target-directed virtual screens, evidence for direct binding/inhibition must be provided; the exclusive use of cell-based/functional/reporter assays is insufficient.
2. For virtual screening hits from any source, identity and purity data consistent with the Scope and Editorial Policy must be submitted. For active compounds obtained from external sources, ^{1}H NMR and MS data should also be provided.
3. Please provide explicit support in the manuscript for the significance of the experimental findings. Identifying weakly potent inhibitors or antagonists of a given target is no longer considered a significant advance if many potent compounds acting by the same mechanism are already available.
4. For virtual screens that produce compound rankings, the total number of compounds that were screened and the ranks of identified hits before application of any further manual or other subjective selection steps must be provided as Supporting Information.
5. Complex virtual screening protocols are not per se validated by identifying active compounds. In such cases, evidence must be provided in the manuscript that much simpler approaches such as 2D similarity or substructure searching would not have yielded comparable results.
6. For prospective virtual screening applications using previously reported methods, calculations must be limited to those that were essential for the identification of novel active compounds. Retrospective computational studies such as standard benchmarking or similar in silico validation attempts should not be reported. All computational studies that do not directly contribute to the identification of novel active compounds should be omitted.

Giving careful consideration to these acceptance criteria prior to submission of virtual screening applications will save authors

Published: April 9, 2012

dx.doi.org/10.1021/jm300429z | *J. Med. Chem.* 2012, 55, 3593–3594

and editors considerable time and effort and also help to further speed up the review process. Publications of prospective virtual screening studies in JMC are highly encouraged and well recognized in the field.

Going forward, JMC also specifically encourages the submission of manuscripts describing new computational methodologies that have the potential to directly impact the practice of medicinal chemistry.[1] Over the years, some of the most cited publications in the Journal have been computational methods papers, and we look forward to receiving manuscripts describing new and exciting computational developments.

Jürgen Bajorath, Associate Editor

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