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Editorial

Computational Chemistry Publications in the *Journal of Medicinal Chemistry*

Computational methods are an integral part of medicinal chemistry and the *Journal of Medicinal Chemistry* has a long history of publishing computational studies. Currently, computational approaches are rapidly evolving at interfaces with chemistry and the life sciences and we are excited to see many new developments in this field.

The Journal strives to be the leading journal for first-class computational studies with significant relevance for medicinal chemistry. Criteria have been formulated that define the suitability of and required standards for computational manuscripts and are available in the Scope and Editorial Policy as well as the Guidelines for Authors (revised January 2008).

Given the continuous evolution of the computational chemistry field and its increasing scientific diversity, the Journal has taken the further step of assembling a panel of advisory board members who are experts in different areas of computational and medicinal chemistry. The panel supports the editor responsible for computational chemistry at the Journal in the initial evaluation of submissions and the selection of manuscripts that merit full peer review.

The editor solicits advice from the panel regarding the suitability of manuscripts. On the basis of the evaluation and recommendations of panel members and his own judgment, the editor decides whether to submit a manuscript to full peer review. Final decisions are subject to editorial discretion and are not made at the level of the panel. In general, panel members are not informed of the editor's decision and, in keeping with the confidential nature of the review process, opinions expressed by the panel will not be disclosed or discussed with authors. The editorial team and the panel members are, first and foremost, advocates of computational studies and will work to ensure the high quality standards and mission of the Journal.

The *Journal of Medicinal Chemistry* welcomes a broad range of computational studies that are relevant for medicinal chemistry including, for example, ligand- or structure-based design, chemoinformatics, and statistics. The Journal specifically encourages submission of manuscripts that fall into one or more of the following categories:

(1) Practical applications of computational methods including experimental data, in particular, experimental evaluation of computational predictions.

(2) Substantially novel methods along with evidence for utility in medicinal chemistry and significant potential for advancing the field. Methods must be described clearly and comprehensibly.

(3) Computational analyses of currently available data that provide unexpected or provocative insights into topical problems and advance medicinal chemistry knowledge.

QSAR/QSPR studies must adhere to the requirements stated in the Guidelines for Authors and the Editorial on QSAR/QSPR and Proprietary Data (June 15, 2006).

It is essential that computational manuscripts are presented in an accessible and lucid style that can be appreciated by a wide medicinal chemistry audience.

We look forward to receiving many excellent contributions that advance our field.

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Senior Editor

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