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ISSN: 1093-3263

DESCRIPTION

The *Journal of Molecular Graphics and Modelling* is devoted to the publication of papers on the uses of **computers** in theoretical investigations of molecular structure, function, interaction, and design. The scope of the journal includes all aspects of **molecular modeling** and **computational chemistry**, including, for instance, the study of molecular shape and properties, molecular simulations, protein and polymer engineering, drug design, materials design, structure-activity and structure-property relationships, database mining, and compound library design.

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AUDIENCE

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The *Journal of Molecular Graphics and Modelling* is devoted to the publication of papers on the uses of computers in theoretical investigations of molecular structure, function, interaction, and design. The scope of the journal includes all aspects of molecular modeling and computational chemistry, including, for instance, the study of molecular shape and properties, molecular simulations, protein and polymer engineering, drug design, materials design, structure-activity and structure-property relationships, database mining, and compound library design.

As a primary research journal, *JMGM* seeks to bring new knowledge to the attention of our readers. As such, submissions to the journal need to not only report results, but must draw conclusions and explore implications of the work presented. Authors are strongly encouraged to bear this in mind when preparing manuscripts.

JMGM is published in association with two of the largest and most active professional societies in the field: the Molecular Graphics and Modelling Society (MGMS) and the Computers in Chemistry (COMP) Division of the American Chemical Society. Several thousand computational chemists worldwide belong to these two societies and any research topic that may of interest to the membership is within the wide scope of the journal. It is not necessary to be a member of these professional societies to publish in the journal.

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