



TABLE OF CONTENTS

●	Description	p.1
●	Audience	p.1
●	Impact Factor	p.2
●	Abstracting and Indexing	p.2
●	Editorial Board	p.2
●	Guide for Authors	p.3



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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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Scope

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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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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1. D.C. Spellmeyer, A.K. Wong, M.J.. Bower, and J.M. Blaney, Conformational analysis using distance geometry methods. *J. Mol. Graphics Modell.* 15 (1997) 18-36.
2. S.A. Best, K.M. Merz, Jr., and C.H. Reynolds, Free energy perturbation study of octanol/water partition coefficients: Comparison with continuum GB/SA calculations. *J. Phys. Chem. B* 103 (199) 714-726.
3. J. Gao, Methods and applications of combined quantum mechanical and molecular mechanical potentials. In: *Reviews in computational chemistry*, K.B. Lipkowitz and D.B. Boyd, Eds., VCH Publishers, New York, 1995, Vol. 7, pp. 119-185.
4. M.P. Allen and D.J. Tildesley, *Computer simulation of liquids*. Clarendon, Oxford, 1987.
5. Spartan, version 4.1.1, 1993, Wavefunction, Inc., Irvine, Calif.

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