Journal of Molecular Modeling

Computational Chemistry - Life Science - Advanced Materials - New Methods
Editor-in-Chief: T. Clark

- Covers all aspects of molecular modeling and its application
- Focuses on "hardcore" modeling, publishing high-quality research and reports
- Topics include life science modeling; materials modeling; new methods; and computational chemistry
- 100% of authors who answered a survey reported that they would definitely publish or probably publish in the journal again

The Journal of Molecular Modeling focuses on "hardcore" modeling, publishing high-quality research and reports. Founded in 1995 as a purely electronic journal, it has adapted its format to include a full-color print edition, and adjusted its aims and scope to fit the fast-changing field of molecular modeling, with a particular focus on three-dimensional modeling.

Today, the journal covers all aspects of molecular modeling including life science modeling; materials modeling; new methods; and computational chemistry.

Topics include computer-aided molecular design; rational drug design, de novo ligand design, receptor modeling and docking; cheminformatics, data analysis, visualization and mining; computational medicinal chemistry; homology modeling; simulation of peptides, DNA and other biopolymers; quantitative structure-activity relationships (QSAR) and ADME-modeling; modeling of biological reaction mechanisms; and combined experimental and computational studies in which calculations play a major role.

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