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Molecular modelling - Wikipedia

Molecular modelling encompasses all methods, theoretical and computational, used to model or mimic the behaviour of molecules. The methods are used in the fields of computational chemistry, drug design, computational biology and materials science to study molecular systems ranging from small chemical systems to large biological molecules and material assemblies.

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Molecular Modeling - an overview | ScienceDirect Topics

Recently we have obtained a copy of a new molecular modeling program, MOBY, and a CD-ROM containing all of the structure files in the Brookhaven Protein Data Bank (both MOBY and the CD-ROM are available from Springer-Verlag NY, Inc., 175 Fifth Avenue, New York, NY 1 001 0). This year we used MOBY to teach protein structure in a senior biochemistry course.

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