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process modeling through a better understanding of the fundamental physical and chemical interactions, by forming the basis for predicting thermodynamic properties of materials that are difficult to calculate using experimental procedures, and enabling the development of new theories, models, processes, and products. Molecular modeling is now available from within process simulation software tools.

Molecular Modeling - an overview | ScienceDirect Topics

Molecular modelling is a collection of (computer based) techniques for deriving, representing and manipulating the structures and reactions of molecules, and those properties that are dependent on these three dimensional structures.

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Molecular Modelling

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Guidebook on Molecular Modeling in Drug Design | ScienceDirect

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

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design, computational biology and materials science to study molecular systems ranging from small chemical systems to large biological molecules and material assemblies. The simplest calculations can be performed by hand, but inevitably computers are required to perform molecular modelling of any reasona

Molecular modelling - Wikipedia

Molecular modeling has become a valuable and essential tool to medicinal chemists in the drug design process. Molecular modeling describes the generation, manipulation or representation of three-dimensional structures of molecules and associated physico-chemical properties.

Molecular modeling: A powerful tool for drug design and ...

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