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A REVIEW

Molecular mechanics and dynamics

HEMANT U. CHIKHALE, POORVASHREE P. JOSHI, AMIT G. NERKAR AND SANJAY D. SAWANT

ABSTRACT

Computational chemistry is a branch of chemistry that uses principles of computer science to assist in solving chemical problems. It uses the results of theoretical chemistry, incorporated into efficient computer programs, to calculate the structures and properties of molecules and solids. It is widely used in the design of new drugs and materials. Because of the complexity of biological systems, computer methods have become increasingly important in the life sciences. With faster and more powerful computers larger and more complex systems may be explored using computer modelling or computer simulations. Various simulation techniques such as molecular mechanics (MM) and molecular dynamics (MD), Monte Carlo, and Brownian dynamics, as well as hybrids of these methods, have emerged as simplifications of the exact quantum mechanical description for large molecules.

Key words : Molecular mechanics (MM), Molecular dynamics (MD), Monte carlo (MC)

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MEMBERS OF THE RESEARCH FORUM

Address for correspondence :
HEMANT U. CHIKHALE, Post Graduate Department of Pharmaceutical and Medicinal Chemistry, STES's Smt. Kashibai Navale College of Pharmacy, Kondhwa, PUNE (M.S.) INDIA

Coopted auhors :
POORVASHREE P. JOSHI, AMIT G. NERKAR AND SANJAY D. SAWANT, Post Graduate Department of Pharmaceutical and Medicinal Chemistry, STES's Smt. Kashibai Navale College of Pharmacy, Kondhwa, PUNE (M.S.) INDIA