

molecular dynamics

in drug design

Molecular dynamics is a simulation procedure consisting of the computation of the motion of atoms in a molecule or of individual atoms or molecules in solids, liquids and gases, according to Newton's laws of motion. The forces acting on the atoms, required to simulate their motions, are generally calculated using molecular mechanics force fields.

Source:

PAC, 1997, 69, 1137 (*Glossary of terms used in computational drug design (IUPAC Recommendations 1997)*) on page 1146