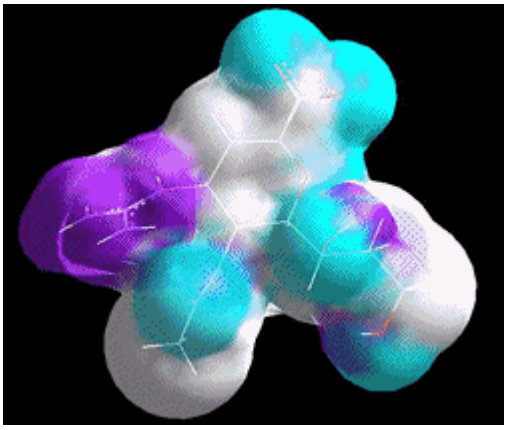
Computational Chemistry: Introduction

Computational chemistry allows pharmaceutical chemists to predict the structures of compounds that might have activity as drugs. It uses computers to model the shapes of molecules and the ways in which molecules bond together. This enables chemists to predict what sort of molecule might fit the active site of an enzyme, or bond to a receptor molecule on the surface of a cell, for example. Molecules that are predicted to be effective can then be made in the laboratory for actual testing. The modelling process cuts down the number of molecules that have to be made in the laboratory.



Some background

The key to molecular modelling is calculating the energy of different possible shapes for a molecule. The molecule will tend to adopt the shape that has the lowest energy. Computers can rapidly calculate the energies of millions of possible shapes for a particular molecular formula and select the one with lowest energy. So the rapid growth of computing power and speed over recent years has made computational chemistry practical. The first calculations of molecular shape were done on paper or by hand cranked calculators.

Did you know?

About 10,000 compounds are made for every one that is eventually marketed.

One of the first molecules to be 'designed by computer' is a treatment for 'flu.

The actual shapes of molecules can be found by a method called x-ray diffraction.