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conformational analysis

in drug design

Conformational analysis consists of the exploration of energetically favourable spatial arrangements (shapes) of a molecule (conformations) using molecular mechanics, molecular dynamics, quantum chemical calculations or analysis of experimentally-determined structural data, *e.g.*, NMR or crystal structures.
Molecular mechanics and quantum chemical methods are employed to compute conformational energies, whereas systematic and random searches, Monte Carlo, molecular dynamics, and distance geometry are methods (often combined with energy minimization procedures) used to explore the conformational space.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1141

