Arizona State University

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FIRST software (Floppy Inclusions and Rigid Substructure Topography) for analyzing conformations of proteins and other biomolecules

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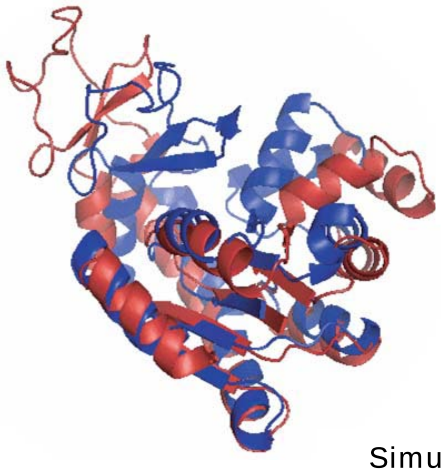
Invention Description

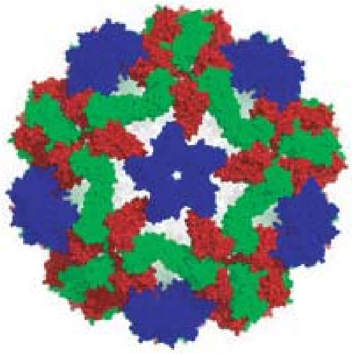
The FIRST software (Floppy Inclusions and Rigid Substructure Topography) was developed by researchers at Arizona State University for analyzing conformations of proteins and other biomolecules.

This software uses patented algorithms for identifying rigid and flexible regions within proteins and other biomolecules of thousands of residues in a few seconds.

The FRODA module (Framework Rigidity-Optimized Dynamics Algorithm) within the FIRST software uses geometric simulation algorithms to quickly explore the “clash free” conformational space in proteins or other biomolecules. FRODA is capable of generating thousand of distinct conformations within minutes on a single-processor computer.



Conformational change in ADK protein is produced in five minutes using FRODA dynamics



Simulating the motion in large structures is not a problem. This virus capsid structure contains ~450,000 atoms. Different colors identify rigid clusters.

flexibility and motion in biomolecules

The on-line freeware version is available at: http:/flexweb.asu.edu

Easy to work with and easy to analyze!

Inventors

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