Skysong Innovations
Advancing the Arizona State University Knowledge Enterprise

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FRODA: Framework Rigidity Optimized Dynamics Algorithm

The FRODA (Framework Rigidity Optimized Dynamics Algorithm) software was developed by researchers at Arizona State University for analyzing conformations of proteins and other biomolecules.

This software uses novel algorithms that are optimized to rapidly determine conformational changes in macromolecules, especially proteins. Knowledge of the conformational changes in a molecule is important for understanding the function of the molecule. A key example is the case of protein-ligand binding. For example, this software can lead to a better understanding of the conformational change in a deleterious enzyme when it binds to a substrate or another molecule. Having this knowledge, it may be easier to design a non-natural ligand to block the action of this enzyme.

This software in particular is faster than competing technologies (in the general category of "molecular dynamics"), allowing many more protein-ligand interactions to be probed in a given time.

Potential Applications

- Pharmaceutical research (e.g., searching for possible ligands to inactivate HIV protease)
- Understanding cellular metabolism
- Cancer and autoimmune disease research

Benefits and Advantages

- Novel algorithms are faster than competing software products