Technology Opportunity

Drug and Protein Design System Based on Advanced Free Energy Simulation Algorithms

Free energy simulation algorithms are designed to solve problems in protein and drug design. This software is more accurate than any other method at predicting binding free energy changes upon the modifications of ligands to allow for more efficient, accurate, and reliable samples for pharmaceutical and bio-technology research.

Applications

This software will allow pharmaceutical and bio-technology companies to create new drugs and products with more efficiency and accuracy.

Advantages

- Reduces cost and time spent discovering new medicines
- Helps identify lead ligands, the initial bottleneck step in research and development for new pharmaceuticals

Technology

The fundamentals of this algorithm are based on physical principles, various conformations of trial small molecules, or proteins are docked into the target proteins. Then binding affinity changes (scoring) are evaluated on each obtained docking mode. The combination of these two centerpieces in structure based rational drug/protein design can facilitate the drug discovery and protein engineering processes dramatically.