Skysong Innovations
Advancing the Arizona State University Knowledge Enterprise

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Software Package for the Solvation Thermodynamics of Biomolecules

Models of molecular dynamics are important tools in the study of biological molecules. Understanding how molecules interact can lead to better predictions of conformational transitions and protein folding, substrate (drug) binding, and binding of proteins to DNA. Current models, however, lack sufficient computational load to efficiently study properties of biopolymers.

Researchers at Arizona State University have designed an efficient algorithm for calculating the thermodynamics of biopolymers in aqueous solution. SolvMol performs calculations of the free energy of polar solvation of a molecule defined by coordinates of its atoms or atomic groups and a set of partial charges. In this way, the program provides results in better agreement with the known biomolecular database.

Potential Applications

- Protein discovery
- Drug interactions
- Gene expression

Benefits and Advantages

- Provides a more accurate model of biopolymer properties

For more information about the inventor(s) and their research, please see Dr. Matyushov's departmental webpageDr. Matyushov's laboratory webpage