

Data Structures

Project proposal

Theme:

Bioinformatics

Title:

Calculation of protein energetics

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Abstract:

Implementing a source program in object oriented c++ language that is capable of computing energies of protein structures. This program is also capable of manipulating protein structures within the Rotamer space instead of Cartesian space. This approach simplifies the calculation.

Introduction:

Proteins play a critical role in maintaining the functions of biological cells. Therefore, protein must be folded into its proper structure to carry out a specific function. Otherwise it results in certain diseases. For proper protein folding there is an important concept of energy. This program allows the user to recreate structure and calculate energy potentials for those structures.

Brief Description:

The class structure starts from the ATOM class and through compositional inheritance constructs AMINO ACID class and finally polypeptide objects.

Conclusion:

This program might results in refinement of computationally modelled structure. This program uses only structure and angle files to reconstruct proteins and output energy analysis of the newly created structure.