

Structure Simulation of Pentapeptide with Real Valued Genetic Algorithm

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Introduction

The problem of predicting the 3D native conformation of a polypeptide, given the primary sequence, is one of the greatest challenges of contemporary structural biology. In order to solve this problem, we designed a new method: "Real valued Genetic algorithm".

Unlike other genetic algorithms, which are constrained to operate on bit strings, real valued Genetic Algorithm operates on real values

Complexity of the problem:

- Search space of the protein conformation is very large and complex.
- This makes the problem difficult to be solved in polynomial time even with an optimized algorithm.
- Thus this problem turns out to be "NP Complete".

Filters used to reduce the complexity:

The algorithm used Ramachandran plot statistics and secondary structure prediction method (Effective for longer polypeptides) to reduce conformation search space.

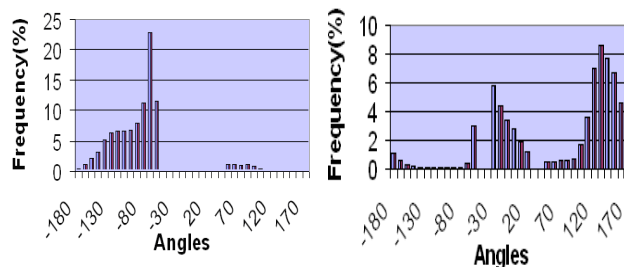
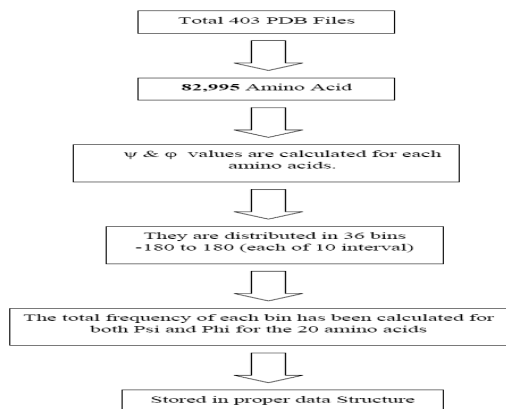
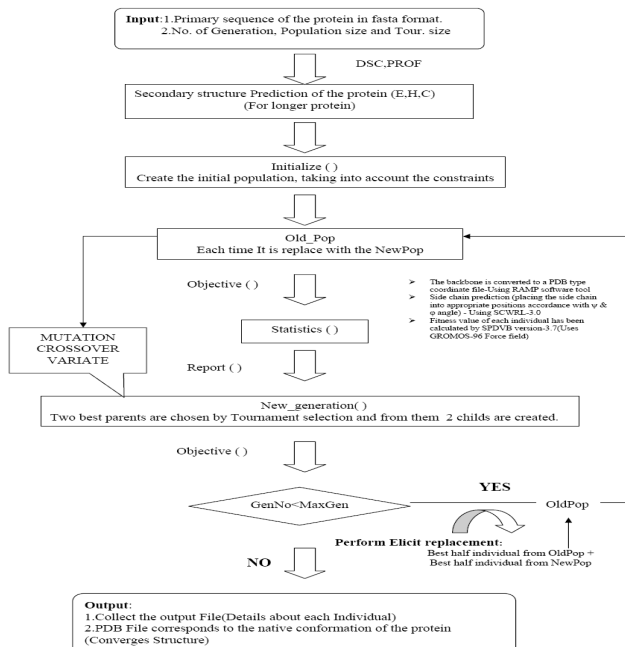


Fig -2 : Distribution of ϕ (left) & ψ (right) along the 36 bins

Flow Chart



Pentapeptide studied : Met-Enkephalin

Tyr-Gly-Gly-Phe-Met (PDB ID:1LPW).

Opioid Peptides produced by brain.

known to play an important role in motivation, emotion, attachment behavior, the response to stress and pain, and the control of food intake.

Results & Discussion

Input parameters:

Input sequence
No of generation:50
Population size:20
Tournament size:2

Output obtained:

converged in 23 cycles
Time taken: 41 Mints (To converge)
No of Mutation: 2813
No of Crossover: 188
No of Variation: 696
RMSD : 5.07 Å°

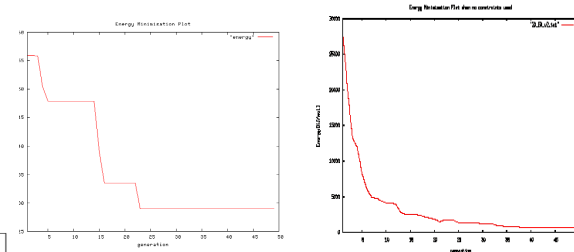


Fig-4: Comparison of results in presence & absence of Filters

Conclusion

➤ The Real Valued Genetic Algorithm proved to be very efficient for the pentapeptide - Met Enkephalin

➤ The Algorithm can be extended to longer polypeptide.

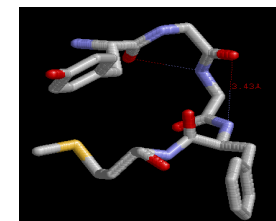


Fig -5: Converged structure