Ab-Initio Conformational Epitope Structure Prediction Using Genetic Algorithm and SVM for Vaccine Design

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Highlights

- The paper proposes a new approach using a **G**enetic **A**lgorithm for **P**redicting the **E**pitope **S**tructure (**GAPES**).
- The proposed teriatry structure prediction of epitopes in GAPES is based on ab-initio force field prediction model.
- The prediction accuracy and the Area Under Receiver Operating Characteristic (ROC) Curve (AUC) were calculated as the performance measures.
- GAPES achieved the highest AUC in the Immune Epitope Data Base (IEDB) from El-Manzalawy benchmark and HLA-DRB1*0101 allele of the Wang benchmark dataset.
- An average prediction accuracy of **93.50%** and an average AUC of **0.974** in the similarity-reduced IEDB dataset is achieved.
- A prediction accuracy of **95.125%** and an AUC of **0.987** on the HLA-DRB1*0101 allele of the Wang benchmark dataset is achieved.
- Results showed that GAPES is a promising technique that will help the researchers and scientists in the intelligent design of new epitope-based vaccines and in the protein structure prediction.