A Novel Evolution-Based Technique for Generating Anticancer Peptides (Year 2)

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Cancer threatens millions of individuals every year and remains a central issue in the scientific community. It's important to search for new alternative treatments, and anticancer peptides (ACP's) are a potential key solution. Characterized by peptides between the length of 10-25 amino acids, ACP's can target a variety of cancers while avoiding common side effects caused by conventional drugs. The current in vitro method of discovery of ACP's is both time-consuming and expensive, so computational tools have the potential to expedite the discovery process. The goal of this study is to build a machine learning-based genetic algorithm that can produce new anticancer peptide candidates through generations of training. First, a random forest and a support vector machine model were trained with a 91.2% testing accuracy to determine if a randomly given peptide carries anticancer properties. Then, these classifiers were used to construct a genetic algorithm. A population of 100 random peptides was generated and evaluated using the classifiers trained before, and the top five performing peptides are chosen to repopulate a new generation of 100 peptides with random mutations. After training for 25 generations, the population's average chance of exhibiting anticancer properties grew to 81%, and the top five peptides in the final generation averaged a fitness score of 0.9. These results reflect the potential of evolutionary algorithms in developing new ACP-based treatments for cancer.

Awards Won: