Development of an Antimicrobial Peptide Activity Detector Using Machine Learning for the Discovery of New Drugs

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Antimicrobial peptides have a broad spectrum of antimicrobial activities against bacteria, fungi, and even viruses, and there have been over 5000 AMP's discovered. Individual peptides can be analyzed for hundreds of physicochemical descriptors (charge, polarity, solvent accessibility…), which are quantitative chemical properties. The goal of this study is to develop an antimicrobial activity detector using machine learning methods to create testable candidate peptides against Escherichia coli. The Support Vector Machine and the Random Forest were used to create the first model to detect antimicrobial activity of any kind in a random peptide. Five thousand random peptides were used to generate antimicrobial peptides with an unknown target. Then a second model was created using the same machine learning tools, and it acted as a target classifier to predict peptides candidates that potentially had antibiotic efficacy on E. coli. The output to the antimicrobial activity detector was inputted into the function identifier, and 36 candidate peptides were generated for E. coli. The feature importance was also collected to understand the relationship between chemical properties to efficacy. This systemic approach takes advantage of modern machine learning tools and thousands of antimicrobial peptides to create potentially useful drugs for future development.

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