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Speech Title	Structure-guided machine learning prediction of the relationship between single amino acid variations, cancer, and drug resistance

Abstract(200 words)：

Single amino acid variation (SAV) refers to a substitution of an amino acid in a protein sequence, which can potentially affect the overall structure and function of the protein, as well as its binding affinity. Protein destabilization is linked to various diseases, including several types of cancer, and SAVs may contribute to resistance against anticancer drug therapy. In our study, we transformed all characteristics of SAVs derived from protein sequences, structures, and their microenvironments into feature vectors. These vectors were then processed through an integrated prediction system utilizing a support vector machine and genetic algorithms. We focused on identifying critical features that help estimate the relationship between SAV properties, cancer, and drug resistance. We developed a prediction system capable of distinguishing whether an SAV is associated with cancer, which achieved a five-fold cross-validation accuracy of 89.73%, a Matthews correlation coefficient of 0.74, and an F1 score of 0.81. Additionally, we constructed another machine learning model to predict mutations related to cancer drug resistance, which attained an accuracy of 86%, a Matthews correlation coefficient score of 0.57, and an F1 score of 0.66. Our innovative approach has great potential to serve as a valuable tool in cancer research and precision medicine.