Modeling of Amino Acids' Chemical Reactivity Against Cancer

Vasnetsov, Catherine (School: The TASIS School in Dorado)
Vasnetsov, Victor (School: The TASIS School in Dorado)

The composition and structure of variable side chains in amino acids determine peptides' unique functions in a wide range of applications. The APD database served as the primary data source for theoretical modeling research on various amino groups and their properties in relation to amine composition, size, 3-dimensional structure, positive charge at the amino group, and the type and length of the side organic chain. Our research objective was to identify chemical, physical, and structural properties that define peptides' activity against both types of pathogens: viruses and cancers. There were 1,547 physicochemical features extracted with the propy package in Python, and these features characterize the sequence through the percentage of each amino acid present in the sequence (amino acid composition, 20 features); the percentage of each pair of amino acids in the sequence (total of 400 features). Additional factors include correlations between pairs of amino acids in a specific feature, such as charge, polarizability, free energy, and van der Waals forces. We discovered that specific properties were correlated with all three targeted anti-disease activities: anti-virus, anti-cancer, and dual action. Our analysis revealed that specific pairs of amino acids possess the most important specific properties for anti-cancer and anti-virus activity. A promising framework for accelerated development of drugs with multiple targets is proposed to benefit experimental chemists by pre-selecting specific groups of amino acids based on their targeted reactivity against pathogens. This should lead to faster and more productive laboratory experiments, identifying more viable candidates for clinical trials.

Awards Won:
Fourth Award of $500