

Cysteine Proteases of Plants That Act on the Coagulation Cascade: Approach from Bioinformatics

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Abstract : The MEROPS system is an information resource for proteases that classifies them into clans according to their catalytic type. Within the Plant kingdom, cysteine proteases are one of the best known, as they are the catalytic type on which the first studies on plant proteases were focused. Plant cysteine proteases have a similar mechanism of action to serine proteases, and some are known to have activity on factors of the blood coagulation cascade, such as a potent antithrombotic effect, and also cause increased fibrinolysis. Of a few plant cysteine proteases, the three-dimensional structure is known, so a method of interest to be able to predict their potential activity on the factors of the coagulation cascade would be to know their structure. Phylogenetics is the study of the evolutionary relationships between biological entities, often species, individuals, or genes (which can be called taxa). It is essential to identify the evolutionary position and the possible distribution of these enzymes in the plant kingdom, particularly those that act on coagulation factors. Bioinformatic tools, such as Clustal Omega / Jalview and Mega6, can be used to create phylogenetic trees. From the results of the alignment, it can be seen that although there is a certain degree of conservation (Conservation) and consensus (Consensus) among the eleven sequences, the functionally important motifs (those corresponding to the active site), the degree of conservation and consensus is very low. We could then infer that although activity on coagulation is reported for these enzymes, linked to their structural and mechanistic similarity with serine proteases, this activity may not have a direct or primary relationship with the proteolytic activity associated with their common, poorly conserved active site in this case. This ultimately could be related to modifications in the reaction mechanism of several of the enzymes studied, which would require more detailed study. Also, below, we will deal with factors that may have a greater influence on this result. The results of this work enrich the understanding of how species (and molecular sequences in general) evolve. Through phylogenetics, we learn not only how sequences came to be the way they are today but also the general principles that allow us to predict how they will change in the future. For pharmaceutical sciences, phylogenetic selection of biologically related species can help identify closely related members of a species with compounds of pharmacological importance, such as plant cysteine proteases, in addition to identifying structural features that may influence their pharmacological activity and which can be valuable for drug design.

Keywords : computational simulation, proteases, coagulation, bioinformatics

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