



IV ASBioSim – Advanced School on Biomolecular Simulation: Protein Engineering with Rosetta, from fundamental principles to tutorials

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***In silico* prospection of plant antimicrobial peptides in transcriptomic data**

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Abstract: Plant antimicrobial peptides (AMPs) are small molecules, generally rich in cysteine, capable of preventing the establishment of invading pathogens. Some of these peptides are shared with other eukaryotes such as defensins and cyclotides, or, still, restricted to the plant kingdom (as snakins). Other AMP classes are specific to some plant taxonomic groups (such as heveins). In order to identify these peptides, bioinformatic approaches may be applied using sequence patterns, usually three techniques are used: BLAST (alignment), HMM (Hidden Markov Models) and/or REGEX (Regular Expressions). HMM and REGEX are more successful to retrieve small sequences (40 amino acids or less) in the databases, since one can search for specific patterns, another point to consider is the structure of these peptides, since they are very conserved into the families, but there are few experimental models solved, thus *ab initio* molecular modeling approaches are needed to understand this characteristic. In this study we are going to use HMM and REGEX patterns to identify sequences of plant antimicrobial peptides in plants and molecular modeling *ab initio* techniques to solve their structure.