

COMPARISON OF THE STRUCTURE-ACTIVITY RELATIONSHIP OF PURIFIED PEPTAIBOLS EXTRACTED FROM TWO *TRICHODERMA ROSSICUM* STRAINS

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A significant percentage of the 415 filamentous fungal species identified so far from the genus *Trichoderma* plays an important role in agriculture and biotechnology, due to their potential application in biocontrol of phytopathogenic microorganisms and their plant growth-promoting effects. Numerous *Trichoderma* species produce enzymes, as well as secondary metabolites with favourable properties, to which the largest group of peptaibiotics, the peptaibols also belong. Peptaibols are produced by non-ribosomal peptide synthetases (NRPSs) with modular structure. Due to the way of synthesis and the incorporation of non-proteinogenic amino acids to the sequences, the peptaibols are characterized by a high degree of amino acid variability in their sequences. In our study, purified peptaibol extracts from two strains of *Trichoderma rossicum* (TUCIM 3235 and TUCIM 889) were investigated for structure-activity relationships (SAR-s). The two strains produce sequences with similar amino acid composition but different lengths. Their minimal inhibitory concentration values (MIC, mg ml⁻¹) were determined against commonly known eleven Gram-negative and Gram-positive bacterial strains. Through modern molecular modeling techniques such as accelerated molecular dynamics (aMD) we can gain a deeper insight to the structural properties of peptaibol sequences and can improve the knowledge of correlational relationships between conformation and bioactivity. The MIC values and the results of aMD simulations were compared to correlate folded peptaibol dynamics affected by their amino acid content and sequence length to their expressed bioactivity. Results obtained during SAR-s can lead to an efficient selection of peptaibiotic compounds for the practical application in agriculture and plant treatment.