

## INVESTIGATING THE EFFECTS OF PEPTAIBOLS THROUGH STRUCTURE- ACTIVITY RELATIONSHIPS

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In terms of agriculture and biocontrol, the role of filamentous fungi from the genus *Trichoderma* has been increasing in the recent years. Among the secondary metabolic products of *Trichoderma* species, peptaibols are of particular importance, and due to their characteristic properties, peptaibols may potentially be used in agriculture in the future. Peptaibols exert inhibitory effects against various plant pathogenic Gram-positive bacteria as well as fungal plant pathogens. Based on previous experiments, peptaibols may have the potential to support plant growth and provide protection against plant pathogenic microorganisms. In addition to laboratory tests of the purified peptaibol extracts, we can deepen our knowledge about the effects of peptaibols through *in silico* studies, such as accelerated molecular dynamics (aMD) simulations.

In our experiments, the peptaibol production of 8 strains of *Trichoderma* species were determined, and purified peptaibol extracts were examined through laboratory tests and modern molecular modeling tools. The peptaibol extracts were tested against commonly known 11 Gram-positive and Gram-negative bacterial strains, as well as two plant pathogenic fungal species. The minimum inhibitory concentration (MIC, mg ml<sup>-1</sup>) and effective concentration (EC, mg ml<sup>-1</sup>) values of the purified peptaibol extracts were determined and the results were compared with the characteristic properties of the most produced peptaibol sequences simulated by aMD.

Correlations were studied through the investigation of structure-activity relationships (SARs) of peptaibols. By examining peptaibols from different aspects we can gain a wider insight into their bioactivity and promote their possible future application in crop protection and agriculture.