

Degradation of ochratoxins A and B by lipases: a kinetic study unraveled by molecular modelling.

Santos, J.^{1,2}, Castro, T.^{1,2}, Venâncio, A.^{1,2}, Silva, C.^{1,2}

¹*Centre of Biological Engineering, University of Minho, Campus de Gualtar, 4710-057 Braga, Portugal;* ²*LABBELS - Associate Laboratory, 4710-057 Braga, 4800-058 Guimarães, Portugal*
joanasantos587@hotmail.com

Mycotoxins are toxic substances produced by fungi that are present in a variety of food commodities, being ochratoxin A (OTA) and B (OTB), a non-chlorinated OTA equivalent, examples of fungal toxins. These compounds differ in some chemical groups, promoting different levels of toxicity, being OTA the most common and hazardous for humans and animals.

To reduce OTA exposure, many approaches for its degradation using microorganisms have been proposed in the last 20 years, both bacteria and fungi. However, the application of isolated enzymes seems to be one of the most promising strategies. Although there are some studies of OTA degradation using enzymes, they are few and produce unsatisfactory results, when compared to studies using living organisms. When considering simultaneous degradation studies of OTA and OTB, the available knowledge becomes even more limited.

We investigated the potential of five isolated lipases to hydrolyze OTA and OTB into non-toxic chemicals. Amano lipase from *Aspergillus niger* (ANL) and porcine pancreatic lipase A (PPL) effectively degraded both substrates: OTA was totally degraded by ANL after 3 hours, and OTB by PPL after 9 hours. The impact of the chlorine group on the enzymatic hydrolysis of OTA was assessed using molecular dynamics. The analyses support the experimental findings that OTA has a greater affinity for PPL due to an interaction with chloride ions, impairing hydrolysis. To understand how the halogen affects the catalytic activity, the kinetic parameters were determined. These results demonstrate the applicability of these enzymes to detoxify co-occurring ochratoxins A and B in food matrices.

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