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# Structure Elucidation and Characterization of Patulin Synthase, Insights into the Formation of a Fungal Mycotoxin

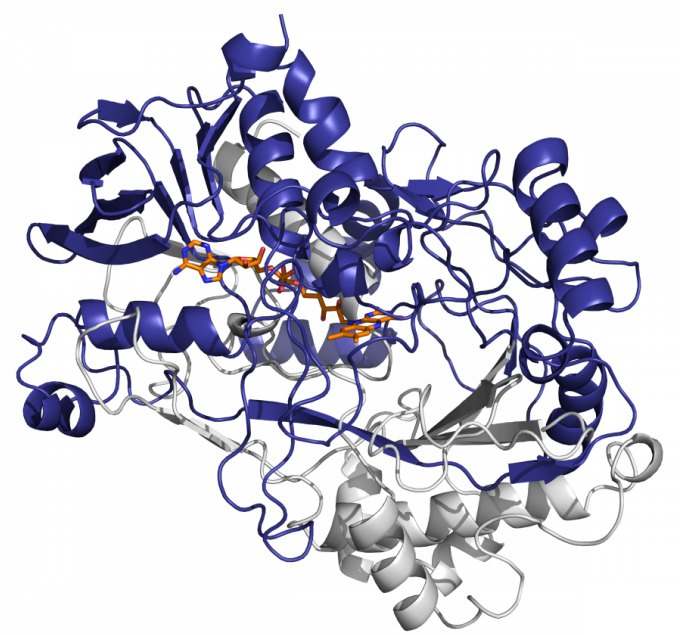
## AUTHORS

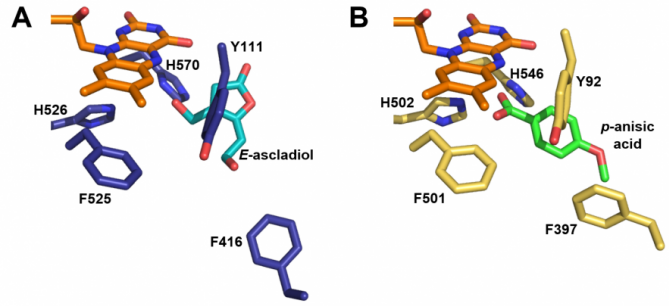
Gwen TJALLINKS / UNIVERSITY OF GRONINGEN, NIJENBORGH 4, GRONINGEN
Alessandro BOVERIO / UNIVERSITY OF GRONINGEN, NIJENBORGH 4, GRONINGEN
Ivana MARIC / UNIVERSITY OF GRONINGEN, NIJENBORGH 4, GRONINGEN
Henriette ROZEBOOM / UNIVERSITY OF GRONINGEN, NIJENBORGH 4, GRONINGEN
Mark ARENTSHORST / LEIDEN UNIVERSITY, SYLVIUSWEG 72, LEIDEN
Jaap VISSER / LEIDEN UNIVERSITY, SYLVIUSWEG 72, LEIDEN
Arthur RAM / LEIDEN UNIVERSITY, SYLVIUSWEG 72, LEIDEN
Andrea MATTEVI / UNIVERSITY OF PAVIA, VIA FERRATA 9, PAVIA
Marco FRAAIJE / UNIVERSITY OF GRONINGEN, NIJENBORGH 4, GRONINGEN

## PURPOSE OF THE ABSTRACT

Elucidating the three-dimensional structure of biological macromolecules yields a wealth of information facilitating developments in biotechnology such as modern drug design.[1] Patulin synthase is an enzyme involved in the biosynthesis of the secondary metabolite patulin, a mycotoxin often present in apples and apple-derived products.[2,3] Penicillium expansum, also termed as apple blue mold, is the major contributor to the presence of patulin on apples and has resulted in significant postharvest losses.[4] Hence, understanding and characterizing the functioning of patulin synthase involved in the key step of patulin production is of utmost importance. In this study, the P. expansum patE gene was expressed in Aspergillus niger, purified via a C-terminally added His-Tag to show that patulin synthase is active exclusively on aromatic alcohols including 5-hydroxymethyl furfural (HMF) and the natural substrate ascladiol. By elucidating its crystal structure (Figure 1), details on its catalytic mechanism were revealed. Several aspects of the active site architecture are reminiscent of that of fungal aryl alcohol oxidases (Figure 2). Overall, this study provides detailed insights into the functioning of patulin synthase and has shown that it can also be used for selective oxidation of a large number of aromatic compounds. This can be of help in strategies to lower the risk on formation of this mycotoxic, for example by developing patulin synthase inhibitors, while it may also develop as a useful biocatalyst for synthetic chemistry, e.g. for conversion of HMF.

## FIGURES






### FIGURE 1

Monomeric structure of patE. In deep blue the flavin-domain, in gray the substrate-domain and in orange the FAD cofactor is represented.

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### FIGURE 2

A: docked binding pose of (E)-ascladiol (blue sticks) in the active site of patE (deep blue). B: binding pose of p-anisyl (green sticks) in the active site of aryl-alcohol oxidase from P. eryngii (yellow, PDB ID: 5OC1) [5].

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## KEYWORDS

Flavoprotein | Patulin | Crystallography | Biocatalysis


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