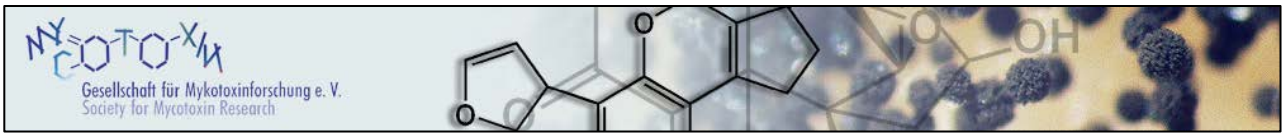


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# Project Aflatox® III - How to use the database to study mycotoxigenic fungi metabolism: a glimpse to the interconnections between molecular structure modifications and biological activity

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The Aflatox® Project (www.aflatox.it), funded by the Cariplo Foundation, is aimed at the development of a biotechnological polyphasic approach to identify and design new bioinorganic compounds possessing biological activities against phytopathogenic fungi contaminating cereals and food/feed derivatives, with a particular focus on aflatoxigenic species. Controlling fungal contamination on crops is considered a priority by sanitary authorities of an increasing number of Countries, due also to the fact that the geographic areas interested in mycotoxin outbreaks are widening. Among the different pre- and post-harvest strategies that may be applied to prevent fungal and/or mycotoxin contamination, fungicides still play a prominent role.
The previous Aflatox® I and II abstracts illustrate, respectively, the experimental flow-chart and the database produced from the evaluation of compounds under analysis.
The present contribution shows some examples of how the search in such a database could be conducted for specific research topics in the study of mycotoxigenic fungi. What we report is how, starting from the collected data, we selected groups of molecules, modified in both structure and chemical-physical characteristics, to analyze different aspects of fungal development and secondary metabolism in *Aspergillus*, *Fusarium* and *Penicillium* species; in particular:

1) the species-specific fungistatic effect of cuminaldehyde-derived molecules on *Penicillium nordicum*, *P. commune*, *Fusarium proliferatum*, *F. verticilloides*, *F. graminearum*, *Aspergillus parasiticus* and *A. carbonarius*;
2) the relationship between predicted antioxidant scavenging ability of jasmone-derived molecules and their effect on sclerotia biogenesis in *A. flavus* aflatoxigenic strains;
3) the differential proteome-changes induced by cinnamaldehyde-derived ligand and relative zinc complex;
4) the importance of lipophilicity in determining thiosemicarbazones anti-aflatoxigenic activity;
5) the molecular docking to predict the interaction between selected molecules and aflatoxins biosynthetic pathway enzymes.

**Acknowledgements**

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