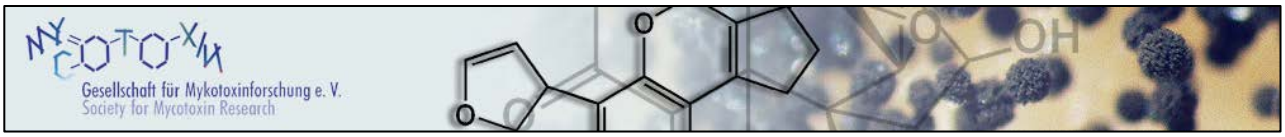

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Project Aflatox® II - A full-experimental database to collect and handle chemical and biological data for the development of new antiaflatoxigenic agents

Marianna Pioli, Francesca Degola, Nicolò Orsoni, Giorgio Spadola, Serena Montalbano, Jennifer Bartoli, Franco Bisceglie, Dominga Rogolino, Annamaria Buschini, Claudia Zani, Donatella Feretti, Mauro Carcelli, Francesco M. Restivo, Giorgio Pelosi.

During the three years of the Aflatox® Project (www.aflatox.it) we worked to synthesize and examine properties of a large number of chemical compounds. Our attention focused on the research of very specific aflatoxin production inhibitors. At the same time, these molecules must be safe for human cells, for the plants on which fungi grow and for the whole ecosystem.
To achieve our goal, the project has been divided into three different sections.The first was the design and synthesis of some parent compounds from natural molecules. The second was the study of their biological effect and cytotoxicity. The third was the chemical modification of the most active compounds in order to study the mechanism of action and to improve the biological activity. In this last stage of the project, the compounds which had shown good results were not only modified in their chemical scaffold, but also used as chelating agents for bio-metal ions like zinc, copper or iron.
What we obtained is a panel of more than 170 compounds fully characterised and tested for antifungal and antiaflatoxigenic properties. Toxicological and genotoxicological evaluations were conducted on three different human cell lines, and on *A. cepa* root apices.
This huge amount of data would be certainly impossible to be analysed as a whole, so we managed to create a database which allows to produce Q-SAR (Quantitative structure-activity relationship) evaluation profiles. To build this database we used the InstanJChem software by ChemAxon which can record and handle large volumes of data coming from different fields. It allows also to run queries and make graphs based on the recorded information. This full-experimental database is a powerful tool to identify important requirements to be taken into account for the development a new generation of pesticides, responding to “greener” and environmentally sustainable agricultural strategies.

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