

New Approach to Identify and Categorize Pesticide Metabolites in Soil Combining Suspect Screening Metabolomics with *In Silico* Molecular Typology

Veronika Storck, Fabrice Martin-Laurent

INRA, UMR Agroécologie, Dijon, France; Enoveo, Lyon, France

Federico Ferrari

Aeiforia srl, Spinoff Università Cattolica del Sacro Cuore, Fidenza, Italy

Luigi Lucini, Marco Trevisan

Università Cattolica del Sacro Cuore, Istituto di Chimica Agraria ed Ambientale, Piacenza, Italy

Laure Mamy, Pierre Benoit

INRA, UMR EcoSys, Grignon, France

Evangelia S. Papadopoulou, Panagiotis A. Karas, Dimitrios G. Karpouzas

University of Thessaly, Department of Biochemistry and Biotechnology, Larissa, Greece

Sofia Nikolaki

University of Patras, Department of Environmental and Natural Resources Management, Patras, Greece

Remi Servien

INRA, UMR Toxalim, Toulouse, France

Extended Abstract

Once released into the environment, pesticides are transformed by abiotic and biotic processes into numerous metabolites which might be detrimental to living organisms. However, pre-registration environmental risk assessment considers only potentially relevant metabolites and needs improvement to prevent premature pesticide market introduction. One of the major challenges to predict or interpret pesticide degradation in the environment is the gap of knowledge on produced pesticide metabolites.

In order to fill this gap, we report the development of an innovative approach based on quadrupole time-of-flight mass spectrometry, which allows identifying and clustering of known and unknown metabolites in environmental samples without the need of reference standards. This approach combines (i) creation of an empirical and theoretical pesticide metabolite library, (ii) chemical analysis by non-target MS with suspect screening metabolomics against the library to detect metabolites, and confirmations by target tandem MS and molecular structure correlation and (iii) *in silico* clustering of metabolites by molecular typology ('TyPol' methodology)^a. As a case study, results obtained by applying this new approach to field study where the triazole fungicide tebuconazole was applied at the recommended dose to winter wheat crop, will be presented and discussed.

Overall, 76 metabolites were contained in the library, 34 (22 empirical and 12 unknown metabolites) were detected and clustered into different groups according to a range of molecular descriptors considered by the TyPol. Environmental parameters like the DT₅₀ of suspected tebuconazole metabolites were estimated *in silico* by similarity to other pesticides for which they were available. This approach has the potential to be used in pre-registration environmental risk assessments and to address post monitoring

activities of various pesticides as a basis to rationalize the choice of the metabolites to be intensively studied for environmental risk assessment.

Servien, R., Mamy, L., Li, Z., Rossard, V., Latrille, E., Bessac, F., Patureau, D., & Benoit, P. (2014). Typol - A New Methodology For Organic Compounds Clustering Based On Their Molecular Characteristics And Environmental Behaviour. *Chemosphere*, 111, 613-622.