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IDENTIFICATION AND QUANTIFICATION OF CANDIDATE METABOLITES OF TEBUCONAZOLE

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ABSTRACT

Tebuconazole belongs to the family of triazole fungicides, used for crop protection and human health applications. In the environment, the dissipation of the parent molecule leads to the formation of metabolites that are of unknown identity or toxicity.

In order to identify and determine the putative identity of those metabolites and their potential toxicity, a quadrupole time-of-flight (Q-TOF) approach is often used. Q-SAR approaches help to predict their toxicity by comparing them to a known database of molecules with known properties. All together the information on the candidate by-products may help to select relevant sub-set of metabolites for further quantification by LC or GC coupled with MS. It is thereby possible to select putative toxic compounds for further quantification using chemical analysis.

Previous work allowed the identification of potential metabolites of tebuconazole. Triazole, triazolyl acetic acid and p-chlorophenol were suspected to result from the decomposition of tebuconazole. Tebuconazole degradation kinetics was followed for 125 days by quantifying the dissipation of the parent molecule and the emergence of the three candidate metabolites by LC/MS for tebuconazole, triazol and triazolyl acetate and by GC/MS for p-chlorophenol. Results will be presented and discussed further.