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MASTER THESIS PROJECT

CHARACTERIZING THE ENVIRONMENTAL FATE AND ECOTOXICOLOGICAL EFFECTS OF PESTICIDE TRANSFORMATION PRODUCTS IN AQUATIC ECOSYSTEMS USING THE TYPOL TOOL

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ABSTRACT

After their application for crop protection, pesticides can be degraded into significant number of transformation products (TPs) through biotic and/or abiotic processes, which initiate from the treated soil and crops and can then subsequently contaminate the aquatic ecosystems. However, their fate and ecotoxicity is still poorly understood due to the data lacking though TPs may have different behavior and effects than the active parent compounds. For some years, the TyPol tool (Typology of Pollutants) has been developed to classify organic compounds based on their molecular properties and parameters describing their fate in the environment and their effects. Therefore, the objective of this work was to characterize the fate and ecotoxicological effects of pesticide TPs in aquatic environments using the TyPol tool. Three parent pesticides, namely tebuconazole (fungicide), terbuthylazine (herbicide) and fenoxycarb (insecticide), were selected according to their molecular properties, environmental behavior, and ecotoxicological effects in the aquatic environment, and 214 of their TPs were considered. The values of molecular properties and parameters were obtained thanks to *in silico* approaches using multiple software programs. A total of 40 structural molecular descriptors (constitutional, e.g. number of atoms, geometric e.g. molecular surface area, topological e.g. connectivity indices, and quantum-chemical e.g. ionisation potential), seven environmental parameters (water solubility, partition coefficients (Kow and Koc), Henry's law constants (K_H), vapor pressure (Pvap), bioconcentration factor (BCF), degradation half-life (DT_{50})), and six ecotoxicological parameters, covering both acute (LC_{50}/ EC_{50}) and chronic effects (NOEC) on different trophic levels (fish, daphnia, and green algae), have been taken into account. TyPol allowed to classify the pesticides and their TPs in different clusters characterized by distinct properties showing that some TPs can be assumed to have the same behavior as their parent compounds while others would be more persistent or toxic or, on the contrary, less persistent and toxic. Statistical relationships have been used to identify the molecular properties driving the fate and effects of TPs. The following steps will be to compare this categorization to experimental data obtained on some TPs. The final output will be to use TyPoll to make a priori risk assessment of the fate and effects of pesticide TPs and to select the priority TPs to be monitored in the aquatic environments.

Keywords: pesticide transformation products, TyPol, molecular descriptors, environmental parameter, fate, ecotoxicity