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Clustering pesticides according to their molecular properties and their impacts by considering additional ecotoxicological parameters in the TyPol method

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The understanding of the fate of pesticides and their environmental impacts largely relies on their molecular properties. We recently developed 'TyPol' (Typology of Pollutants), a clustering method based on statistical analyses combining several environmental endpoints (i.e. environmental parameters such as sorption coefficient, degradation half-life) and one ecotoxicological one (bioconcentration factor), and structural molecular descriptors (number of atoms in the molecule, molecular surface, dipole moment, energy of orbitals...). TyPol has been conceived on the available knowledge on QSAR of a wide diversity of organic compounds (Mamy et al., 2015). This approach also allows to focus on transformation products present in different clusters and to infer possible changes in environmental fate consecutively to different degradation processes (Servien et al., 2014; Benoit et al., 2016).
The initial version of TyPol did not include any ecotoxicological parameters except the bioconcentration factor (BCF), which informs more on the transfer along the trophic chain rather than on the effects on non-target organisms. The objective was to implement the TyPol database with a data set of ecotoxicological data concerning pesticides and several aquatic and terrestrial organisms, in order to test the possibility to extend TyPol to ecotoxicological effects on various organisms. The data analysis (available literature and databases) revealed that relevant ecotoxicological endpoints for terrestrial organisms such as soil microorganisms and macroinvertebrates are lacking compared to aquatic organisms. We have added seven parameters for acute (EC50, LC50) and chronic (NOEC) toxicological effects for the following organisms: Daphnia, Algae, Lemna and Earthworm.
In this new configuration, TyPol was used to classify about 45 pesticides in different behavioural and ecotoxicity clusters. The clustering results were analyzed to reveals relationships between molecular descriptors, environmental parameters and the added toxicological parameters. Some trends between soil adsorption or Kow coefficient and the acute toxicity towards earthworms or algae were highlighted, and discussed on the basis of the concept of contaminant bioavailability. This proof-of-concept study also showed that the in silico clustering method TyPol can successfully address new questions and can be expanded with other parameters of interest.

Keywords: pesticides, toxicity, QSAR, clustering, PLS

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