In silico Prediction of the Formation of Non-Extractable Residues (NER) in Soil and relation to their Environmental Hazard

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Organo-clay complexes are the major sink for xenobiotics in soils and sediments. Pollutants can be degraded and transformed by biotic and abiotic mechanisms. Additionally, the parent xenobiotics and their transformation products are immobilized as non-extractable residues (NER). All chemicals are assumed to form NER to different extends, but the actual amount of NER formation depends not only on the chemical structure but also on the environmental conditions.

Three types of NER have recently been classified: Type I are xenobiotics sorbed or entrapped, type II are xenobiotics covalently bound, and type III are biogenic residues. The possible remobilisation of incorporated xenobiotics is of environmental concern and refers particularly to type I NER. Type II or type III NER formation is considered to not cause harm.

The aim of the current project is to predict the potential for both xenobiotic and biogenic NER formation. To this end, structural alerts will be developed and complemented by additional approaches. The models will be implemented and publically made available through the software system ChemProp (UFZ Department of Ecological Chemistry 2014. ChemProp 6.2. http://www.ufz.de/index.php?en=6738).

The paper provides an overview of the approach and reports first modelling results.

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