**NER formation and identification of a model herbicide in soil**

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The fate of pesticides in soil, depending on the substance used, comprises different pathways. The substance may be (i) fixed to the soil particles or (ii) leach and volatilize from the soil and will be (iii) metabolized incl. mineralization. The contributions of the different mechanisms depend on the properties of the compound, e.g., water solubility, log KOW etc., on soil properties and on the microorganism community. The ecotoxicological risk of a compound that is brought to the environment depends on how far and how fast it is detoxified and on its bioavailability. The more similar it becomes during metabolization compared to natural compounds of the soil organic matter the less toxic it can be considered. In current discussion is the bioavailability and potential ecotoxicity of so called bound or non-extractable residues. Based on the original IUPAC definition and according to recent experimental findings Kästner et al. (2014) differentiated NER into Type I, which contains xenobiotic NER derived from parent pesticides and primary metabolites that are sorbed or entrapped within the soil organic matter; type II, describing compounds that are covalently bound to soil organic matter and type III, comprising biogenic residues, resulting from conversion of carbon, nitrogen and other elements from the compounds into microbial biomass.

Up to now, non-extractable residues are counted for as not bioavailable. The main question herein is how probable these compounds may be released into the environment and become bioavailable and how toxic these released residues remain. It is out of question that biogenic residues (Type III NER) pose no risk to the environment but this is not easily decided for type I and type II NER.

In our experiments, we have incubated a standard soil with a 14C-labeled model substance (the herbicide pendimethalin) in order to investigate the formation of xenobiotic NER (type I and II). In a parallel experiment, soil is incubated with the 13C/15N-labeled model substance and the formation of biogenic NER (Type III NER) will be investigated.

First we analyzed the fulvic acid fraction containing radioactive residues (18 and 6 % of applied radioactivity after 120 days of incubation) by high performance size exclusion chromatography (JUNGE et al. 2011). We observed that the major part of residues during the chromatographic separation was still bound to the fulvic acid fraction and only minor amounts of low molecular weight residues represented free parent compound or metabolites. To gain further information the fulvic acids and the extracted soil will be silylated with trimethylchlorosilane in order to disintegrate the humic matter aggregates into smaller fragments, which are naturally held together by hydrogen bonds and other noncovalent interactions. This procedure has proven helpful in identification of non-extractable residues (BERNS et al. 2005; HAIDER et al. 2000).

Barriuso (1997) showed that the addition of compost will enhance the formation of NER of several herbicides in soil. This method is used in an additional experiment to obtain a higher amount of NER to facilitate the analysis of the non-extractable residues.

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