**Non-extractable residue formation from pollutants in soil – including biogenic residue in risk assessment**

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Bioremediation of soils contaminated with organic compounds is receiving increasing attention. During biodegradation, generally non-extractable residues (NER) are formed. This process, however, is only little understood, which hampers proper environmental risk assessment. Usually, radiocarbon mass balances are used to quantify NER formation. The possibilities for elucidation of the chemical identity of the NER detected by this method are, however, very limited. Usually it is assumed that most of the NER are either the parent compound or direct metabolites, which are either sorbed or sequestered to soil solids. However, if we assume productive biodegradation of the pollutants, the degrading microbes use the pollutant-derived carbon to build their biomass, which later can be stabilized in soil organic matter. Thus, biogenic NER (bioNER) are formed, and the label can be found in biomolecules such as fatty acids or amino acids. Quantification of NER by radiocarbon analysis therefore may overestimate the environmental risk associated with a compound unless a suitable method for quantification of bioNER based on 14C-labelling has been developed.. BioNER thus need to be quantified for proper risk assessment. A convenient option to quantify the label in specific molecules is stable isotope (13C, 15N) labelling combined with compound specific isotope analysis. This approach thus allows to chemically characterize NER in soil and to quantify the formation of bioNER. For example, it could be found that in the case of 2,4-D and ibuprofen, basically all the carbon remaining in soil after biodegradation could be assigned to bioNER (Nowak et al. 2011; 2013). We follow different approaches to increase information about the quantity of bioNER formation in soil. First of all, further experiments with a range of pesticides are conducted where carbon and nitrogen mass balances are analyzed and bioNER are quantified, thus extending the available data base. In a second approach, compound degradation and NER formation are modelled by a model describing the processes in soil. This allows estimation of NER and bioNER formation without expensive and time-consuming experiments. Finally, we are currently relating literature data on mineralization and NER formation to information on the chemical structure of each compound. The aim is to use QSAR models to predict bioNER formation and thus to create structural alerts for high or low NER or bioNER formation. In summary, our approaches contribute significantly to quantification of bioNER, which are expected to contribute significantly to NER formation in soil from many chemicals, namely always when the chemicals are used as a carbon source by the degrading microorganisms. This will allow more realistic environmental risk assessment of chemicals.

*Bibliography:*

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