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Evaluation of microbial transformations of dissolved organic matter – what information can be extracted from high-field FTICR-MS elemental formula data sets?

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Transformation of DOC and DOM was and is widespread investigated (1-3). Due to the complex composition of DOC increased attention was payed to DOM quality change during degradation processes. In order to get a better insight in DOM transformation processes both resolution as a function of time and on a molecular level are promising. The observation of DOM quality changes requires sophisticated evaluation techniques. A new evaluation strategy of FTICR-MS elemental formula data sets is introduced. An experiment with seven flumes and leaf leachate was performed. All flumes were sampled on five dates (within 7 days) and the SPEDOM was characterized using high-field FTICR-MS analysis, resulting in together 35 elemental formula data sets. The time dependent change of components abundance was fitted by a simple linear regression model after normalization of mass peak intensities. All components were categorized by calculation of the slope (change of percent intensity per day) in all seven flumes. A positive slope means product formation, a negative slope means degradation of components. Specific data filtration was developed to find out components with relevant change of relative intensity. About 7000 different components were present in at least one of the 35 samples. Of those about 1800 components were present in all of the 35 samples. About 300 components with significant increase of intensity were identified. They were mainly unsaturated and oxygen-rich components (lignin-like or tannin-like) and had molecular masses less than 450 Dalton. A group of about 70 components was partially degraded (significant negative slope, present in all samples). These components were more saturated and less oxygen-rich compared to the product group and had molecular masses > 450 Dalton. A third group of about 150 components was identified with a tendency to total degradation (significant negative slope, not present in all samples, reduced or no abundance at the end of the experiment). They were highly saturated and oxygen-poor (lipid-like).
As a conclusion components of biogeochemical groups (specified by their H/C and O/C coordinates in Van Krevelen diagrams) can be allocated to DOM transformation processes by their tendency of intensity change.
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