

Reactome-based encoding of microbial communities and their application to contaminant biotransformation prediction

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The growing number of chemicals used in the different sectors of society has led to their inevitable presence in the environment. Development of predictive methods to estimate their potential risk to human and environmental health is therefore of utmost importance.

The biotransformation of contaminants by environmental microbial communities is one of the most efficient mechanisms to avoid long-term exposure of the environment to contaminants (Fenner 2013). Thus the understanding of microbial degradation processes is crucial for an accurate modelling of environmental contaminants fate and plays a key role in the environmental risk assessment of chemicals.

Presently, biotransformation models suffer from several limitations. One of these limitations is the fact that neither functional characteristics of the microbial communities nor any other environment-specific conditions that may influence degradation are considered in the development of the most part of these models.

However, a high variability of biotransformation rate constants can be observed for the same contaminant under different environmental conditions, ultimately due to the different microbial communities present and their specific biochemical machineries. With respect to chemical risk assessment, this leads to the following main question: Would *in silico* methods, i.e., (Quantitative) Structure Biodegradability Relationships, (Q)SBRs, need to also consider information on the microbial community and environmental conditions to yield more accurate predictions of biotransformation rates and pathways of environmental contaminants?

To explore this question, the main objective of this work is to develop a new method to encode the active biochemical machinery of a microbial community relevant for contaminant biotransformation in a numerical fixed length representation (set of descriptors). This set of descriptors should enable the prediction of contaminant biotransformation rate constants in different microbial communities, e.g., different waste water treatment plants (WWTPs). The strategy is to establish a link between the gene expression profile and the catalyzed enzymatic reactions of a microbial community. This descriptor set, a reactome-based description of the microbial community, is then used in combination with molecular descriptors of the contaminant and additional environment-specific information to establish a novel class of quantitative relationships for biotransformation prediction, i.e., (Q)SRBR – Quantitative Structure/Reactome-Biodegradability Relationships. We will present the details of the reactome-based encoding of microbial communities gene expression profiles from 10 activated sludges collected in WWTPs (Helbling 2012) and the preliminary results of their use as descriptors in (Q)SRBR models for the prediction of biotransformation rate constants of contaminants.

References

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