Biodegradation of Water-Soluble Polymers – Reviewing In-Silico Methods (Interim state)

D. Skodras¹, M. Hüben¹, J. Klein¹
¹ Fraunhofer Institute for Molecular Biology and Applied Ecology IME, Schmallenberg, Germany

Motivation:
- Water soluble polymers are exempt from REACH.
- If they become subject, assessing biodegradability is obliged.
- In-silico are cost-effective methods used for risk assessment.
- Hence, the current landscape of models is examined.

Pathway Prediction System:
- Predict pathways based on rules mapping functional groups onto products.
- Assign likelihood to rules based on expert knowledge or probability calculations.
- Discriminate reactions and apply recursively to final degradation products.
- Examples: CATABOL³, enviPath⁴, BESS⁵

Connection, Complexity:
- While the degradation process may be modelled at this level, a derivation of biodegradability is not established.
- Modelling specific polymers in itself is a non-trivial task. Including their stochastic nature increases the complexity considerably.

Molecular Modelling:
- Model substances explicitly on the atomic/molecular level.
- Compute energy minima, normal modes, binding-sites for enzymes, interaction strength.
- Examples: GROMACS⁶, AUTODOCK⁷, CHARMM⁸

Outlook:
- Adaptations of the approaches are needed to predict biodegradability of polymers.
- PPS might be most promising.
- Establish degradation rules and assign interdependent likelihoods.
- Determine set of descriptors suited for polymer characterization.

Pathways, Rules:
- To establish pathways, rules for polymer degradation need to be identified and probabilities assigned.
- Due to their variability and macroscopic properties, rules need to include patterns beyond functional groups.

Data, Descriptors:
- Crucial for reliable predictions but sufficiently large and consistent set of water soluble polymer degradation data is lacking.
- Polymers need to be characterized and discriminatory descriptors identified also encompassing macroscopic properties.

Predicting Biodegradability of Polymers

Data, Descriptors:
- Derive substance properties based on regression or similarity.
- Use descriptors/similarity indices to characterize substances.
- Fit models (MLR, RF, SVM, kNN, ANN) to consistent datasets.
- Examples: BIOWIN¹, VEGA²

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