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## Digital Tools for Biodegradation

The application of digital tools to the area of biodegradation has traditionally been relatively minimal, due to the dearth of data and inherent complexity of biological systems. In recent years however, the rapid advancement of machine learning and especially its subsequent application to the areas of chemistry and biology is now showing real outcomes in aiding our understanding of biodegradation.

Starting with traditional statistical techniques, more complex algorithms (such as neural networks) now allow machine learning models to be able to predict biodegradation with high accuracy. These models are already commonly used in the community, mostly for identifying endpoint or half-life biodegradation of small molecules under various conditions relevant for certification: e.g. biodegradation in wastewater after 28 days, or $DT_{50}$ in soil.

Most recently, a number of advancements are offering a more detailed understanding of the biodegradation process. The first real steps are now being taken in prediction of more complex structures such as polymers[1]. Transformer architecture modelling also allows prediction of biodegradation pathways[2], potentially aiding in the identification of persistent metabolites. Additionally, models which predict biodegradation (both endpoints and pathways) are increasingly now becoming of interest to regulators.

This presentation will give an outline of the current advancements in prediction and modelling of biodegradation, as well as an overview of the available tools. We will then offer an insight into the main hurdles identified for future development and how we can best overcome them.

[1] *Environ. Sci. Technol*. 2025, 59, 2, 1253–1263
[2] *J Cheminform*. 2025 Feb 17;17(1):21