



Machine learning meets ecotoxicology: A look into the ADORE dataset

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The MLtox project between the Departments of Environmental Toxicology (Utox) and Systems Analysis, Integrated Assessment and Modeling (SIAM) aims to explore the possibilities and limitations of machine learning in ecotoxicology.

An important element for the comparability of studies on in silico methods is the use of common and defined data sets. The recent publication of the ADORE benchmark dataset in the journal Nature ScientificData contributes to this. Christoph Schür, PostDoc in the MLtox project, has written an article on [the Nature Communities Blog](#) about the path to this and the associated added value.

Publication

Schür, Christoph, Lilian Gasser, Fernando Perez-Cruz, Kristin Schirmer, und Marco Baity-Jesi. „A Benchmark Dataset for Machine Learning in Ecotoxicology“. Scientific Data 10, Nr. 1 (18. Oktober 2023): 718.

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