

# Machine Learning for Predicting Microplastics Hazard

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Microplastics toxicity assessment remains fundamentally limited by data scarcity and reliance on monomer-proxy hazard classifications that ignore polymer-specific properties and environmental transformation. We present a computational framework combining transfer learning and polymer informatics to predict microplastics toxicity directly from chemical structure. Our ML pipeline, built on transformer-based polymer representations, was first trained on Tox21 molecular toxicity data. We then transferred this foundation to the polymer domain through fine-tuning on a separate polymer toxicity dataset. This strategy demonstrates that molecular toxicity knowledge can be successfully transferred to polymer hazard prediction, overcoming severe data limitations in polymer toxicology. Building on this validated strategy, we outline two integrated research directions: (i) coupling toxicity forecasts with environmental degradation pathways - photodegradation, hydrolysis, enzymatic transformation - to model how particle structure and hazard evolve across environmental compartments and timescales. (ii) characterizing additive leaching kinetics to quantify how intentionally added substances (plasticizers, flame retardants, stabilizers) are liberated during weathering and contribute to net microplastics toxicity. The integrated framework will transform microplastics risk assessment from static polymer classification into predictive modeling of coupled chemical transformation and ecotoxicological impact, enabling evidence-based polymer design and environmental policy support.

## Bibliography:

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