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Interpretable Machine Learning for Environmental Fate: From Small Molecules to Polymers

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Abstract

Predicting environmental fate is difficult because chemical space is vast and environmental conditions vary widely, limiting the transferability and mechanistic value of many traditional QSARs. This talk presents an end-to-end workflow that integrates rigorous data curation, physics-guided feature engineering, and interpretable machine learning to build system-aware predictive models. Two applications are highlighted. For **small molecule reduction**, we harmonized a comprehensive dataset for Fe(II)-associated reductants by unifying free, complexed, sorbed, and structural Fe(II) into one modeling matrix, achieving high accuracy for organics ($R^2 = 0.83$) and recovering classic Hammett/LFER trends through model interpretation. For **polymer biodegradation**, we addressed sparse, inconsistent macromolecular data by combining literature meta-analysis, targeted experiments, and synthetic "failure-mode" data, yielding $R^2 = 0.66$, capturing non-linear behaviors and identifying thermal decomposition temperature as a key proxy for recalcitrance. Model interpretation analysis confirms mechanistic consistency and enables large-scale virtual screening (e.g., ~38% of DSSTox), supporting safe-by-design chemicals and materials with reduced environmental persistence.