

There is a pressing need for accurate in silico methods to predict the toxicity of molecules that are being introduced into the environment or are being developed into new pharmaceuticals. Predictive toxicology is in the realm of structure activity relationships (SAR), and many approaches have been used to derive such SAR. Previous work has shown that inductive logic programming (ILP) is a powerful approach that circumvents several major difficulties, such as molecular superposition, faced by some other SAR methods.