**OPTIMIZING POTENTIAL GREEN REPLACEMENT CHEMICALS – BALANCING FUNCTION AND RISK**

Judson, Richard

NCCT, ORD, US EPA, Research Triangle Park, NC

An important focus of green chemistry is the design of new chemicals that are inherently less toxic than the ones they might replace, but still retain required functional properties. A variety of methods exist to measure or model both functional and toxicity surrogates that could be used in a global green optimization scheme. I present an approach that uses multiple methods including in vitro screening assays, in vitro-based toxicokinetics modeling, QSAR and docking modeling to help rank-order potential replacement chemicals. This ranking needs to account for both differences in inherent toxicity but also differences in properties related to intended use. This approach will be illustrated using data and modeled parameters for a collection of pyrethroid insecticides. These cover a diverse range of chemical structures and differential toxicity (e.g. chemicals in the class hit different ion channel targets and show different rates of detoxifying liver metabolism) and differential pesticidal activity (mainly via different ion channel activities) so provide a good example for testing out “green” optimization approaches.
This abstract does not necessarily reflect U.S. EPA policy.