

US EPA ARCHIVE DOCUMENT

SAR Validation Study

Structure Activity Relationships, or SAR, is a technique routinely used by EPA to estimate aquatic toxicity of chemicals reviewed by the EPA in response to premanufacture notices. As part of their Project XL commitment, PPG, working with EPA, conducted a validation study to compare measured aquatic toxicity data with SAR predictions from ECOSAR (Ecological Structure Activity Relationships) a personal computer software program that is used to estimate the toxicity of chemicals used in industry and discharged into water. The program estimates a chemical's acute (short-term) toxicity and, when available, chronic (long-term or delayed) toxicity for the same set of PPG polymers. SAR predictions were generated for 38 polymeric chemicals submitted by PPG to EPA as PMNs. These predictions were compared to measured data on the same set of chemicals. The results indicate 87-90% agreement between the predictions and measured data. Data were considered to be in agreement if SAR predictions were: (1) within the same order of magnitude (less than a ten-fold difference) as measured data; or (2) no effects at saturation (NES) and the measured data showed no effects at the maximum attainable or limit test values. The actual data are TSCA Confidential Business Information and can not be released, however an abstract of the study was presented as a poster at the March 2001 annual meeting of the Society of Toxicology in San Francisco, CA. In addition the study has been submitted for publication. For information contact Jean Chun, PPG, chun@ppg.com or Vince Nabholz, EPA, Nabholz.Joe@epa.gov