

# Computing@PNNL

## SEMINAR

### *Predictive Assessment of the Human and Environmental Toxicity of Chemical Substances*

**Prof. Dr. Gerrit Schüürmann**

Head, Department of Chemical Ecotoxicology,  
UFZ Centre for Environmental Research, and  
Professor, Technical University of Freiberg (Germany)



**August 25 | Noon | CSF Darwin (1007)**

Through the European Directive, REACH, implemented in 2007, alternative methods have increased in importance as non-animal tools for toxicological assessment of chemical compounds. In this context, the “3R” principle of reducing, refining, and replacing animal testing has resulted in a paradigm shift. While the original idea was to replace a given animal test by a single *in vitro* alternative (1:1 replacement), the integrated testing strategy (ITS) aims to exploit the combined information generated from several (n) non-animal methods to partly or fully replace the respective animal experiment (1:n replacement).

In his talk, Prof. Dr. Schüürmann will present the ITS concept and respective non-test (*in silico*) and test (*in chemico*; *in vitro*) methods, including the roles of chemoavailability and the exposome platform for a molecular-level understanding of chemical toxicity. To illustrate ways of application, models for predicting human and environmental toxicity will be shared, focusing on read-across, structural alerts, chemoassays to sense electrophilic reactivity and toxicity, and computational chemistry for predicting reactive toxicity, as well as metabolic toxification and detoxification through P450 and B12 catalysis. Along with industrial chemicals, his discussion will address perfluorinated compounds and pharmaceuticals.

**Host:**

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