High-Throughput Exposure Potential Prioritization for ToxCast Chemicals

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The U.S. EPA must consider lists of hundreds to thousands of chemicals when prioritizing research resources in order to identify risk to human populations and the environment. High-throughput assays to identify biological activity *in vitro* have allowed the ToxCast™ program to identify potential chemical hazard, but without similar assessment of potential for exposure, high-throughput risk assessment for chemicals with no other available information cannot be completed. Using models (USEtox and RAIDAR) identified by the EPA Exposure-Based Prioritization Challenge nearly 1000 ToxCast chemicals have been prioritized with respect to far-field exposure potential (*e.g.* partitioning into environmental media). The ToxCast (Phase I and II) chemicals include industrial compounds, pesticides, and pharmaceuticals that failed in human trials, all of which have been tested in over 500 dose-response assays for potential bioactivity. For most of these chemicals, the descriptors necessary for fate and transport modeling (*i.e.* model parameters) were not available and had to be predicted based upon structure using Episuite and QikProp (accessed through the Aggregated Computational Toxicology Resource – https://actor.epa.gov). The prioritizations (*i.e.* rank order) of the two models will be compared with each other as well as ground-truthed with respect to exposures inferred from the Centers for Disease Control National Health and Nutrition Examination Survey (NHANES), pesticide residues, and other similar data sources.
[*This abstract does not necessarily reflect U.S. EPA policy*.]