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### **Feature Analysis of ToxCast™ Compounds**

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ToxCast™ was initiated by the US Environmental Protection Agency (EPA) to prioritize environmental chemicals for toxicity testing. Phase I generated data for 309 unique chemicals, mostly pesticide actives, that span diverse chemical feature/property space, as determined by quantum mechanical, feature-based, ADME-based, and QSAR-based descriptors. Results in over 450 high-throughput screening (HTS) assays were generated for the chemicals. Deriving associations across such a structurally diverse and information-rich dataset is challenging. Approaches to determine relationships between the bioassay data and chemistry and biology-informed structural features, and methods to meaningfully represent this knowledge are being developed. We initially focus on the Phase I data set, but successful approaches will be applied to the much larger chemical libraries in ToxCast Phase II and Tox21 projects (the latter to screen approximately 10,000 chemicals). These approaches will be used to develop data mining approaches to inform toxicity testing and risk assessment modelling. *This abstract does not reflect EPA or FDA policy.*