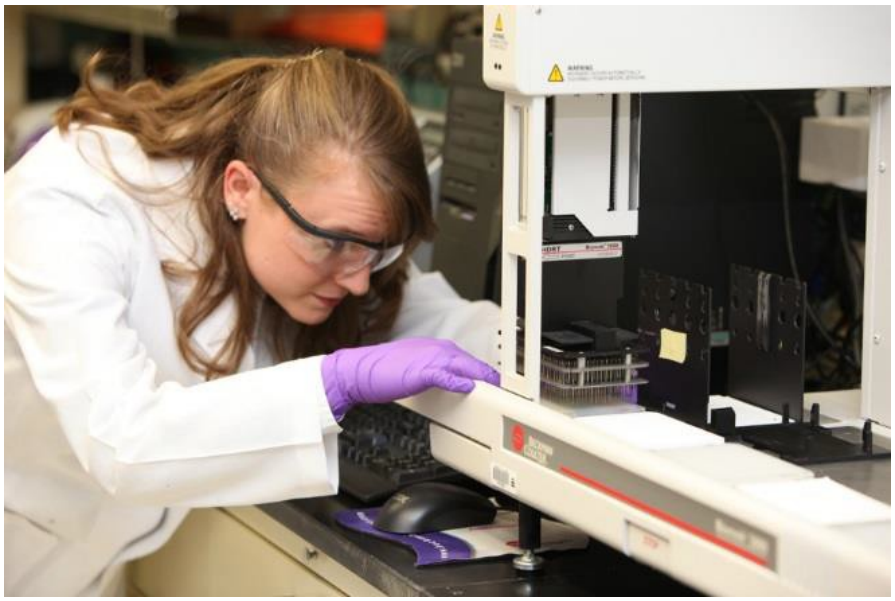
EPA SAFER CHEMICALS RESEARCH
DOWNLOADABLE COMPUTATIONAL TOXICOLOGY DATA

EPA's computational toxicology researchers develop and use new rapid and efficient approaches to evaluate chemicals for potential toxicity and to estimate chemical exposure/dose. These methods quickly evaluate thousands of chemicals, allowing a more efficient approach for prioritizing the chemicals most likely to affect human health.

These new methods produce extremely large data sets that scientists analyze to reveal how chemicals interact with biological processes. As part of EPA's commitment to share scientific data, all computational toxicology data is available for the public to analyze and use. The public can download the full data sets for analysis and access the data through interactive online tools called "Dashboards".



Online Data and Dashboards

ToxCast: High-Throughput Screening

ToxCast uses automated chemical screening technologies, called "high-throughput screening assays", to expose living cells or isolated proteins to chemicals. The cells or proteins are then screened for changes in biological activity that suggest potential health effects. ToxCast has generated data on over 8,000 chemicals evaluated in over 700 high-throughput assay endpoints. ToxCast data is being used to rank and prioritize chemicals in the Endocrine Disruption Screening Program. ToxCast results are contributed to the Toxicology in the 21st Century (Tox21) federal agency collaboration.

Download ToxCast Data:
https://www.epa.gov/chemical-research/toxicity-forecaster-toxcasttm-data

ToxCast dashboard:
https://www.epa.gov/chemical-research/toxcast-dashboard

EDSP21 Dashboard:
https://www.epa.gov/chemical-research/endocrine-disruption-screening-program-21st-century-edsp21

Chemistry Data

The foundation of chemical safety testing relies on chemistry information such as high-quality chemical structures and Physicochemical properties. This information is used by scientists to predict the potential health risks of chemicals. The EPA provides access to chemical structures, as well as experimental and predicted physicochemical and toxicity data, for hundreds of thousands of chemicals. The curated physicochemical property data associated with chemical substances is also mapped to corresponding chemical structures. These data are valuable information for analytical scientists involved in structure identification and can support targeted and non-

targeted screening identification of environmental chemicals.

Download Chemistry Data:
https://www.epa.gov/chemical-research/downloadable-computational-toxicology-data

Chemistry Dashboard:
https://www.epa.gov/chemical-research/chemistry-dashboard

Virtual Tissues: Tipping Point Data

EPA researchers develop mathematical models to predict perturbation of biological systems and determine when cellular systems are no longer able to recover. EPA researchers use these models to determine the "Tipping Point", the point when biological systems are unable to recover from or adapt to chemical exposure. When cellular systems are unable to recover, chemical exposures could lead to adverse outcomes such as cancer.

Download Tipping Point Data:
https://www.epa.gov/chemical-research/downloadable-computational-toxicology-data

Rapid Exposure & Dose Data

EPA researchers develop and use rapid exposure estimates to predict potential exposure for thousands of chemicals. It is important to link the external dose of a chemical to an internal blood or tissue concentration, a process called toxicokinetics. EPA researchers measure the critical factors that determine the distribution and metabolic clearance for hundreds of chemicals and incorporate these data into computer models. The high-throughput toxicokinetic data can be paired with the high-throughput screening data to estimate real-world exposures.

Download High-throughput toxicokinetics data:
https://www.epa.gov/chemical-research/downloadable-computational-toxicology-data

Chemical and Product Categories Database

The Chemical and Product Categories database (CPCat) catalogs the use of over 40,000 chemicals and their presence in different consumer products. The chemical use information is compiled from multiple sources while product information is gathered from publicly available Material Safety Data Sheets (MSDS). EPA continually updates this database as more information is gathered from various data sources.

CPCat Database:
https://www.epa.gov/chemical-research/chemical-and-product-categories-cpcat

For more information:
www.epa.gov/comptox

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