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science BRIEF

INNOVATIVE RESEARCH FOR A SUSTAINABLE FUTURE

EPA SAFER CHEMICALS RESEARCH
DOWNLOADABLE COMPUTATIONAL TOXICOLOGY DATA

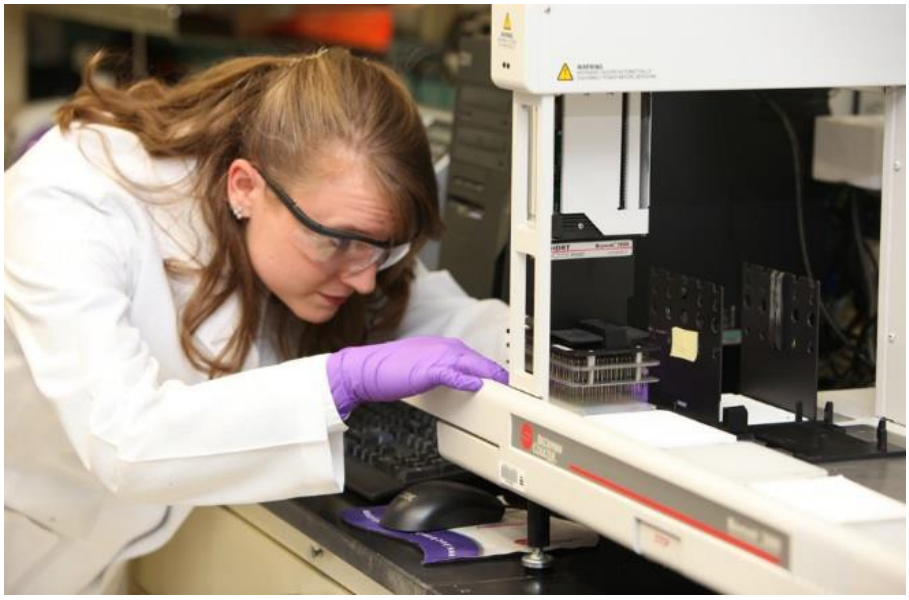
EPA's computational toxicology researchers develop and use new rapid and efficient approaches to evaluate chemicals for potential toxicity and to estimate chemical exposure/dose. The exposure data is used together with toxicity data to help thoroughly evaluate thousands of chemicals for potential health effects.

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 transparency, computational toxicology data, databases and software packages are available for the public to analyze and use. The public can access this information through an interactive online tool called the CompTox Chemicals Dashboard and full data sets, software packages, and databases can also be downloaded for independent analysis.

Online Tools

CompTox Chemicals Dashboard

The CompTox Chemicals Dashboard, formerly the Chemistry Dashboard, provides online access to chemistry, hazard and exposure information for over 760,000 chemicals. The Dashboard helps decision-makers and scientists quickly and efficiently access information to thousands of chemicals.



The Dashboard can be searched by chemical (e.g. Name and CASRN), assays/genes associated with high-throughput screening data, and consumer product use categories. The Dashboard contains chemical lists, assay lists, a literature mining tool and the ability to download all data available within the dashboard.

CompTox Chemicals Dashboard: https://comptox.epa.gov

Downloadable Data, Databases and Software Packages

ToxCast: High-Throughput Screening Information

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 4,500 chemicals evaluated in over 700 high-throughput assay endpoints.

The ToxCast high-throughput screening data is being used for the development, proof of concept and implementation of the Toxic Substance Control Act's Pre-prioritization strategy, TSCA's Alternatives

chemicals strategy and to screen chemicals for potential endocrine disruption.

The ToxCast database, data and software packages are available for download.

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

Rapid Exposure and Dose

Rapid, also called high-throughput, exposure predictions or ExpoCast provide rapid exposure estimates for thousands of chemicals. ExpoCast quickly and efficiently looks at multiple routes of exposure to provide exposure estimates. ExpoCast uses, enhances and evaluates two well-known exposure models to provide exposure predictions.

The high-throughput exposure models are being improved by adding more refined indoor and consumer use information from the EPA Chemical and Products Database (CPDat), a database that maps more than 49,000 chemicals to a set of terms categorizing their use or function in 16,000 consumer products (e.g. shampoo, soap) types based on what chemicals they contain.

The information in the database comes from collating electronic material safety data sheets (MSDS), analyzing consumer product purchasing behavior and data resulting from testing consumer products for the presence of chemicals using a technology called non-targeted analysis. The high-throughput exposure predictions and CPDat is a part of the CompTox Chemicals Dashboard.

EPA researchers are also developing more precise methods for estimating chemical concentrations in humans following exposure. While they are a valuable tool, typical high-throughput assays are hampered by uncertainty in estimating exposure dose. To address this limitation, EPA scientists developed a method to make its high-throughput results more applicable to humans by replacing the traditional constant exposure rate with more realistic human exposure pathways.

EPA researchers developed four toxicokinetic models within a R software package called high-throughput toxicokinetics to estimate chemical concentrations in humans. The package can currently use human high-throughput screening data to make predictions for 391 chemicals in humans, rats, mice, dogs, and rabbits, including 76 pharmaceuticals and 282 ToxCast chemicals. The package can also be used to provide a more rapid and less resource intensive method for understanding population specific differences in exposure and dose. This method allows you to adjust exposure models to account for these population specific susceptibilities

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

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

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