

EPA Computational Toxicology Data, Tools, Code, and Software

The tables below provide links to the locations where EPA's computational toxicology and exposure data, tools, code, software and other online resources are made available for public access. The locations for the resources below include EPA locations and sites external to EPA. To help users navigate this document, the resources are organized by type. Click on a resource type to jump to that section on the document:

- [Online Applications](#)
- [Data, Databases, APIs, and Software](#)
- [Reports](#)

All resources below have been reviewed and cleared for public release.

Online Applications

Online Application	EPA URL	Software/Code
ChemExpo	https://comptox.epa.gov/chemexpo	
Cheminformatics Modules	https://www.epa.gov/comptox-tools/cheminformatics	
CompTox Chemicals Dashboard	https://comptox.epa.gov/dashboard/	The code for the CCD online application is available on GitHub at the following links: • Dashboard: https://github.com/USEPA/ccd-dashboard-current-public • User Interface (UI) Rebuild: https://github.com/USEPA/ccd-ui-rebuild-public • Application Programming Interface (API) ccdapp1: https://github.com/USEPA/ccdapp1-public • API ccdapp2: https://github.com/USEPA/ccdapp2-public • Batch Search: https://github.com/USEPA/ccdbatchsearch-public • Chemical Files: https://github.com/USEPA/ccdchemicalfiles-public • Similar Compound: https://github.com/USEPA/ccdsimilarcompound-public
EcoTox	https://cfpub.epa.gov/ecotox/	
GenRa	https://comptox.epa.gov/genra/	
SeqAPASS	https://seqapass.epa.gov/seqapass/	

RapidTox	https://comptox.epa.gov/rapidtox/auth/login (Beta version)	
-----------------	---	--

Data, Databases, APIs, and Software

Data Source	Type	EPA Location	Additional/Mirrored Location
CPCat	Database	https://epa.figshare.com/articles/dataset/Chemical_and_Product_Categories_CPCat_database/7871537?file=14656880	
CPDAT	Database	https://epa.figshare.com/articles/dataset/The_Chemical_and_Products_Database_CPDat_MySQL_Data_File/5352997?file=25946270	https://zenodo.org/records/15170627
CvTdb	Database	https://github.com/USEPA/CompTox-PK-CvTdb	https://archive.softwareheritage.org/(search EPA CvTdb)
DSSTox	Database	https://epa.figshare.com/articles/dataset/Chemistry_Dashboard_Data_DSSTox_Identifier_Mapped_to_CAS_Numbers_and_Names/5588566?file=45581535	https://zenodo.org/records/15066221
MMDB	Database	https://epa.figshare.com/articles/dataset/Multimedia_Monitoring_Database_MMDB_/17065024/1?file=3155578	https://zenodo.org/records/15178511
ToxCast (invitroDB)	Database	https://doi.org/10.23645/epacomptox.6062623.v13	https://zenodo.org/records/15191261
ToxRef	Database	https://github.com/USEPA/CompTox-ToxRefDB	https://zenodo.org/records/15041481
ToxVal	Database	https://doi.org/10.23645/epacomptox.20394501.v9	https://zenodo.org/records/15169253
CtX APIs	APIs	https://www.epa.gov/comptox-tools/computational-toxicology-and-exposure-apis	https://cran.r-project.org/web/packages/ctxR/index.html
CtX R	APIs	https://github.com/USEPA/ctxr	https://cran.r-project.org/web/packages/ctxR/index.html
HTTK	Software Package	https://cran.r-project.org/web/packages/httk/index.html	https://zenodo.org/records/15084943

Data Source	Type	EPA Location	Additional/Mirrored Location
HTTr Pipeline Package	Software Package	https://clowder.edap-cluster.com/datasets/61147fefe4b0856fdc65639b#folderId=6616ade1e4b063812d70f779&page=0	https://zenodo.org/records/15085866
invivoPKfit	Software Package	https://github.com/USEPA/CompTox-ExpoCast-invivoPKfit	https://CRAN.R-project.org/package=invivoPKfit
SEEM3	Software Package	https://github.com/HumanExposure/SEEM3RPackage	https://archive.softwareheritage.org/
SHEDs-HT	Software Package	https://github.com/HumanExposure/SHEDSHTRPackage	https://zenodo.org/records/15116145
TEST	Software Package	https://doi.org/10.23645/epacomptox.21379365.v3	
ToxCast-tcpl	Software Package	https://github.com/USEPA/CompTox-ToxCast-tcpl	https://cran.r-project.org/web/packages/tcpl/vignettes/Introduction Appendices.html
ToxCast-tcplfit2	Software Package	https://github.com/USEPA/CompTox-ToxCast-tcplFit2	https://cran.r-project.org/web/packages/tcplfit2/index.html
A combination of high-throughput in vitro and in silico new approach methods for ecotoxicology hazard assessment for fish	Data	https://doi.org/10.23645/epacomptox.26799382.v1	https://zenodo.org/records/15085302
A Comparison of In Vitro Points of Departure with Human Blood Levels for Per- and Polyfluoroalkyl Substances (PFAS)	Data	https://doi.org/10.23645/epacomptox.24645711.v1	https://zenodo.org/records/15085446
ACTOR	Data	https://epa.figshare.com/articles/dataset/AcToR_MySQL_Dump_File/21611286?file=38306889	
Application of Cell Painting for chemical hazard evaluation in support of screening-level chemical assessments	Data	https://doi.org/10.23645/epacomptox.21183481.v1	https://zenodo.org/records/15085483
Bioactivity of the tire preservative 6PPD and degradant, 6PPD-quinone in fish and mammalian-based assays	Data	https://clowder.edap-cluster.com/datasets/677ab279e4b0a7c65d3994d3	https://zenodo.org/records/15098585

Data Source	Type	EPA Location	Additional/Mirrored Location
Bioactivity screening of environmental chemicals using imaging-based high-throughput phenotypic profiling	Data	https://doi.org/10.23645/epacomptox.12132621.v2	https://zenodo.org/records/15085515
Combining phenotypic profiling and targeted RNA-Seq reveals linkages between transcriptional perturbations and chemical effects on cell morphology: Retinoic acid as an example	Data	https://doi.org/10.1016/j.taap.2022.116032	https://zenodo.org/records/15084845
Comparison of Approaches for Determining Bioactivity Hits from High-Dimensional Profiling Data	Data	https://doi.org/10.23645/epacomptox.12589256.v1	https://zenodo.org/records/15061525
EPA Transcriptomics Assessment Product (ETAP): BM2 Data for EPA Perfluoro-3-Methoxypropanoic Acid (MOPA)	Data	https://epa.figshare.com/articles/dataset/BM2_Data_for_EPA_Perfluoro-3-Methoxypropanoic_Acid_MOPA_Transcriptomic_Assessment_Product_ETAP_/25335844?file=44861818	https://zenodo.org/records/15061550
EPA Transcriptomics Assessment Product (ETAP): ETAP Scientific Support Analysis BMDExpress2 Files	Data	https://clowder.edap-cluster.com/datasets/660ad607e4b063812d700fe6?space=65d8b923e4b063812d6a9bfa#	https://zenodo.org/records/15061583
Exploring the effects of experimental parameters and data modeling approaches on in vitro transcriptomic point-of-departure estimates	Data	https://doi.org/10.23645/epacomptox.23736972.v3	https://zenodo.org/records/15083430
High-Throughput Transcriptomics of Water Extracts Detects Reductions in Biological Activity with Water Treatment Processes	Data	https://clowder.edap-cluster.com/datasets/61147fefe4b0856fdc65639b?space=6112f2bee4b01a90a3fa7689#folderId=65c5075ae4b063812d6939f9&page=0	https://www.epa.gov/comptox-tools/computational-toxicology-and-exposure-apis
High-Throughput Transcriptomics Platform for Screening Environmental Chemicals	Data	https://doi.org/10.23645/epacomptox.13368914.v1	https://zenodo.org/records/15085866
High-Throughput Transcriptomics Screen of ToxCast Chemicals in U-2 OS Cells	Data	https://doi.org/10.23645/epacomptox.24938571.v1	https://zenodo.org/records/15084943

Data Source	Type	EPA Location	Additional/Mirrored Location
Optimization of Human Neural Progenitor Cells for an Imaging-Based High-Throughput Phenotypic Profiling Assay for Developmental Neurotoxicity Screening	Data	https://doi.org/10.23645/epacomptox.16695265.v2	https://zenodo.org/records/15085535
Signature analysis of high-throughput transcriptomics screening data for mechanistic inference and chemical grouping	Data	https://doi.org/10.23645/epacomptox.24061563.v1	https://zenodo.org/records/15085230
TempO-seq and RNA-seq Gene Expression Levels are Highly Correlated for Most Genes: A Comparison Using 39 Human Cell Lines	Data	https://doi.org/10.23645/epacomptox.27341970.v1	https://zenodo.org/records/15116172
DCAP Calibration and Example	Data	https://epa.figshare.com/articles/dataset/DCAP_Calibration_and_Example_Chemical_Dataset/28021040?file=51256235	
HTTP	Data	https://epa.figshare.com/articles/dataset/High_Throughput_Phenotypic_Profiling_HTPP_/21502782?file=38102346	https://zenodo.org/records/15061525
HTTr	Data	https://doi.org/10.23645/epacomptox.21502758.v4	https://zenodo.org/records/15083354

Reports

Reports	DOI
US Environmental Protection Agency Center for Computational Toxicology and Exposure's Reports	https://www.ncbi.nlm.nih.gov/books/NBK605696/
US Environmental Protection Agency Center for Computational Toxicology and Exposure's Assessments	https://www.ncbi.nlm.nih.gov/books/NBK605697/
EPA Transcriptomics Assessment Product (ETAP): Perfluoro-3-Methoxypropanoic Acid ("MOPA")	https://doi.org/10.23645/epacomptox.25352962