



# ChemTunes Databases

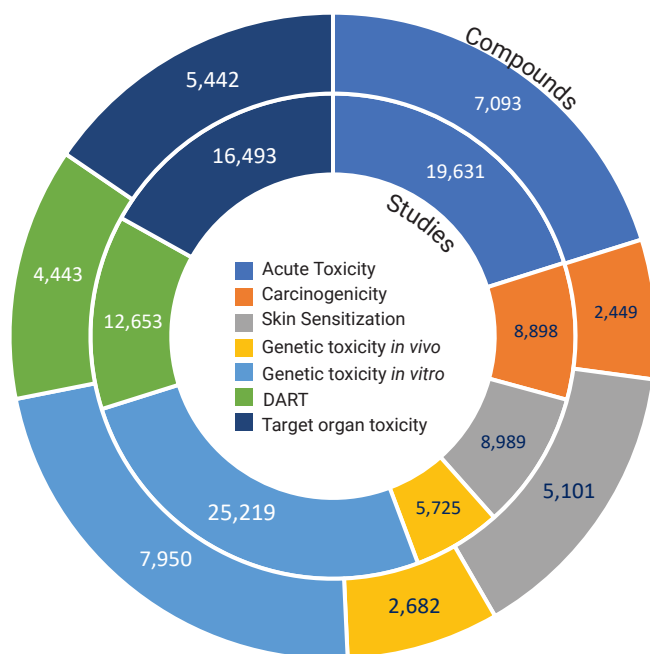
Expert-Reviewed Data for  
Chemical Safety Assessment

**ChemTunes** is a chemoinformatics platform to store, manage, search, and retrieve chemical substances and *in vivo* and *in vitro* toxicity (human-health and environmental studies), bioavailability, physiologically-based kinetics, and metabolism data. It also provides a unique safety evaluation database with Health-Based Guidance/Limit Values (HBGV or HBLV) from a variety of safety/risk assessment programs.

The easy-to-use interface facilitates chemistry, regulatory, and toxicity searches to retrieve relevant information tailored to the needs of toxicologists to support the safety, risk, and PBT assessment processes of chemical substances.

## Database Statistics

### Toxicity Database



### ADME

- **PBK data:** PK/TK/TD data on food, drugs, pesticides
- **Metabolism:** ADMET data for metabolites of drugs and pesticides
- **ADE:** *in vivo* and *in vitro* oral and dermal absorption, permeability
- **Data sources:** ECHA, IUCLID-6, SCCS, open literature, US FDA, EFSA opinions

## Key Facts

- Over 118,000 test substances
- Over 120,000 studies across 128 endpoints
- Diverse chemical space and regulatory use types including food substances, drugs, cosmetics, industrial chemicals, pesticides, and impurities

## Available Databases

### Toxicity and Ecotoxicity

- Comprehensive human health-related and environmental endpoints with dose-level findings
- **Toxicity endpoints:** acute, dermal (irritation and sensitization), genetic, neuro, developmental/reproductive, and carcinogenicity
- **Ecotoxicity studies:** PBT assessment support
- **Data sources:** ECHA, EFSA, SCCS, US CIR, NTP, US EPA (IRIS, ToxRefDB), US FDA (CDER, CFSAN), CPDB, IARC, HESS Japan, IUCLID-6, literature, Fraunhofer ITEM RepDose (optional)

### Safety Evaluation and Risk Assessment Results

- **POD:** NO(A)EL/LO(A)EL, LD50, BMD10/BMDL10, TD50, EC3, hazard, potency category
- **Health-Based Guidance Values:** MOS, MOE, RfD, TDI, ADI determined from critical studies with sites, effects, and other meta information
- **Data sources:** EFSA, SCCS, ECHA, US EPA, US FDA, JECFA/WHO, HESS Japan, IARC, CPDB, etc.