Computational Toxicology and Exposure Communities of Practice

Sharing research and promoting collaboration

Thursday, January 23, 11 AM-12 PM ET

Agenda:

- **Introduction: Sammy Hanf**
  Communications Specialist, ORD Center for Computational Toxicology and Exposure
- **Presenter: Nisha Sipes and Chelsea Weitekamp**
  Assistant Center Directors, ORD Center for Computational Toxicology and Exposure (CCTE)
- **Q&A**
- **Closing remarks: Sammy Hanf**

CompTox Chemicals Dashboard Version 2.5 & 2.5.1 and updated ToxValDB Data

EPA developed the CompTox Chemicals Dashboard to provide public access to chemistry, toxicity, and exposure data. This information includes chemical structures, experimental and predicted physicochemical and toxicity data, hazard and bioassay data, and additional links to relevant websites and applications. Version 2.5 offers several notable data and feature updates and minor version 2.5.1 resolves issues from Version 2.5. The updated hazard data, ToxValDB v9.5, presents major restructuring of the data, including a modified focus to human health-relevant toxicity information, revised classifications, and improvements to source document accessibility.

EPA United States Environmental Protection Agency

Updates to the CompTox Chemicals Dashboard v2.5 v2.5.1

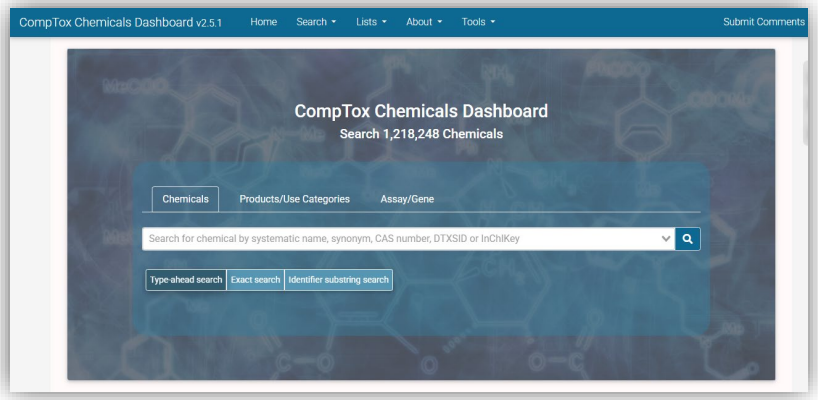
Nisha S. Sipes
US EPA Office of Research and Development

January 23, 2025

The views expressed in this presentation are those of the authors and do not necessarily reflect the views or policies of the US EPA.

CompTox Chemicals Dashboard

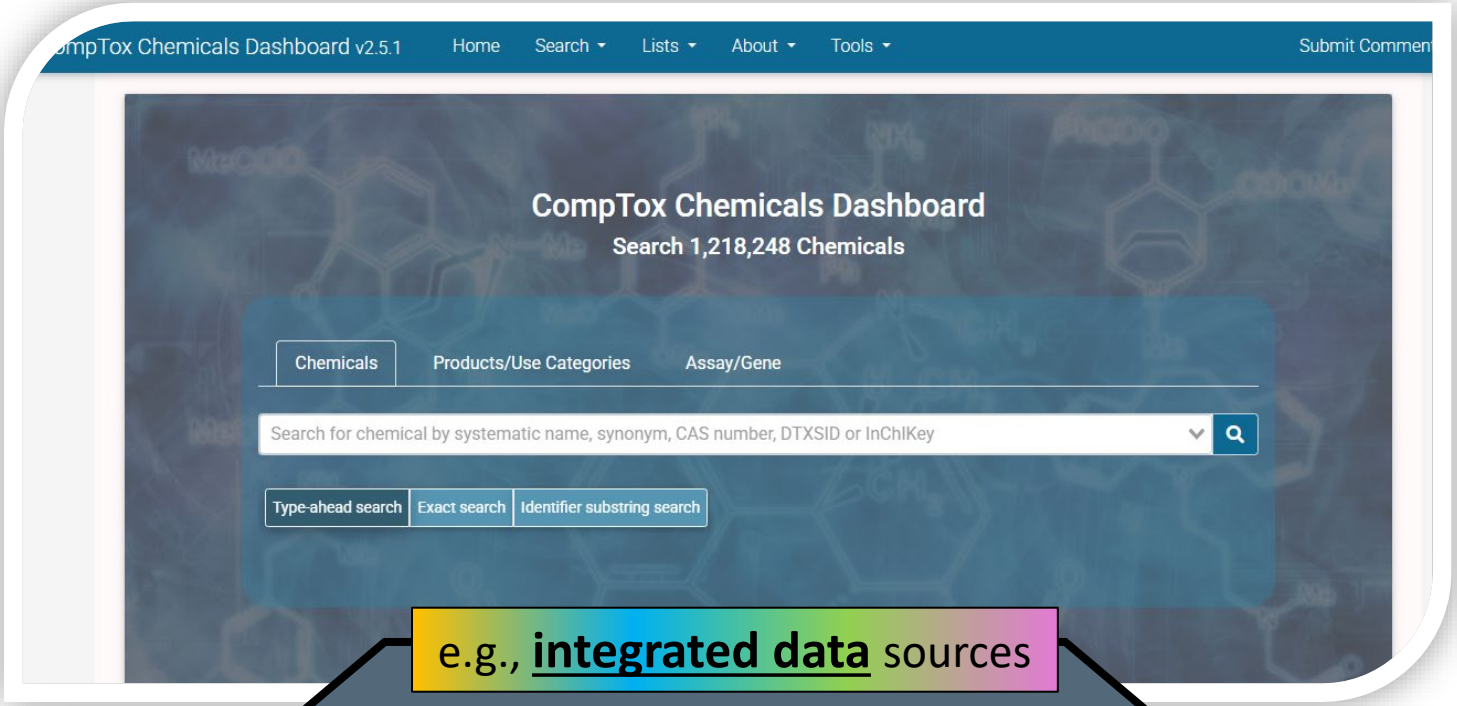
- **Centralized location** for publicly available chemical toxicity data
- Combination of existing legacy, and high throughput and predictive model data
- Publicly accessible, curated, and periodically updated
- Supports EPA and partner decision making
  - e.g., Well-studied chemicals: data can be found in most areas
  - e.g., Data-poor substances: limited data, but may find in vitro and/or modeled data, similar compounds, and literature search information



https://comptox.epa.gov/dashboard/

currently >1.2 million chemicals

*Updated January 13, 2025



e.g., **integrated data** sources

Chemistry

Exposure

Hazard

Bioactivity

DSSTox

Toxicity Estimation Software Tool (TEST)

EPISuite

ECOTOX Knowledgebase

ToxValDB

30+ worldwide sources: e.g., ATSDR, IRIS, HESS, ECHA, EFSA, DOD, Health Canada

OPERA

Percepta/ACD Labs

ToxRefDB

Factotum

NHANES

invitroDB

SeqAPASS

Chemical and Products Database (CPDat)

Chemical and Products Categories (CPCat)

Chemical Data Reporting (CDR)

High Throughput Toxicokinetics (HTTK)

ToxCast

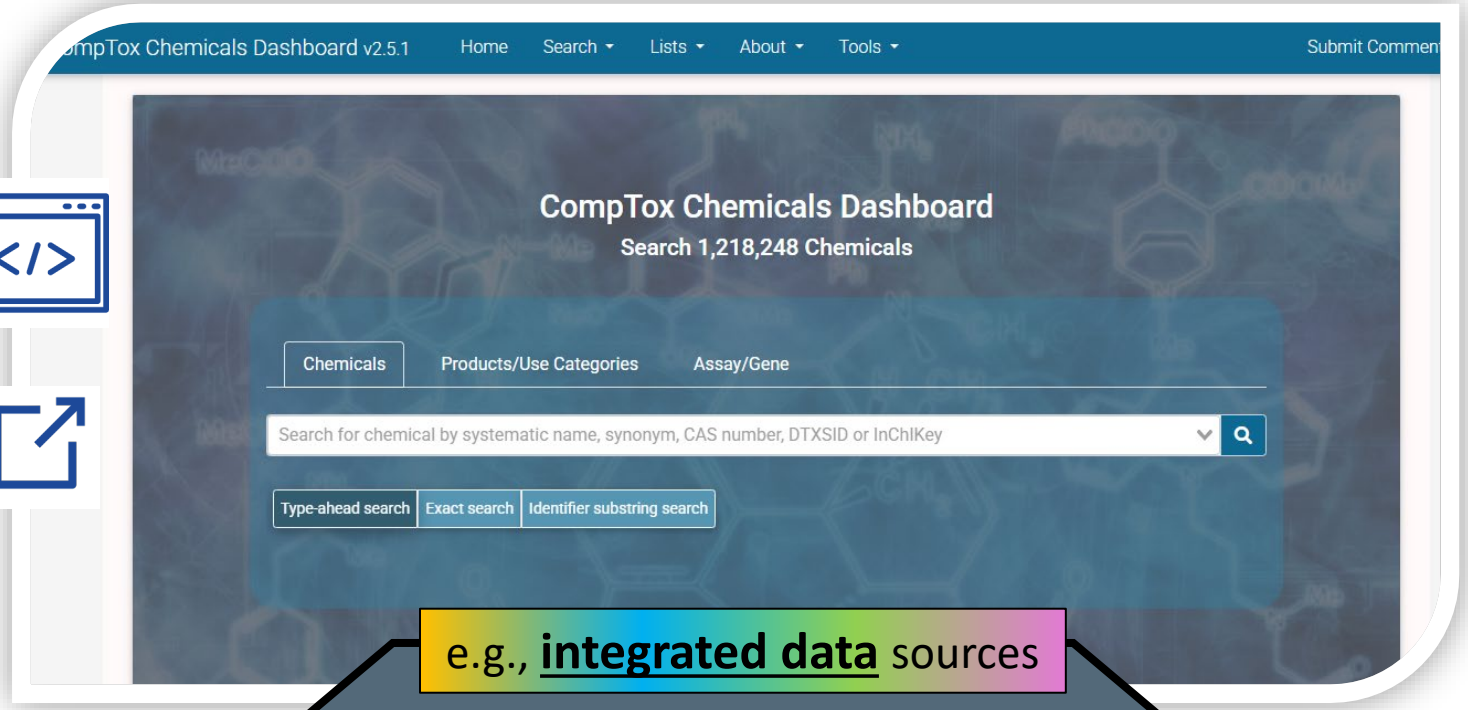
AOP wiki

High Throughput Transcriptomics (HTTr)

High Throughput Phenotypic Profiling (HTPP)

Embedded websites using iframes

Links to websites



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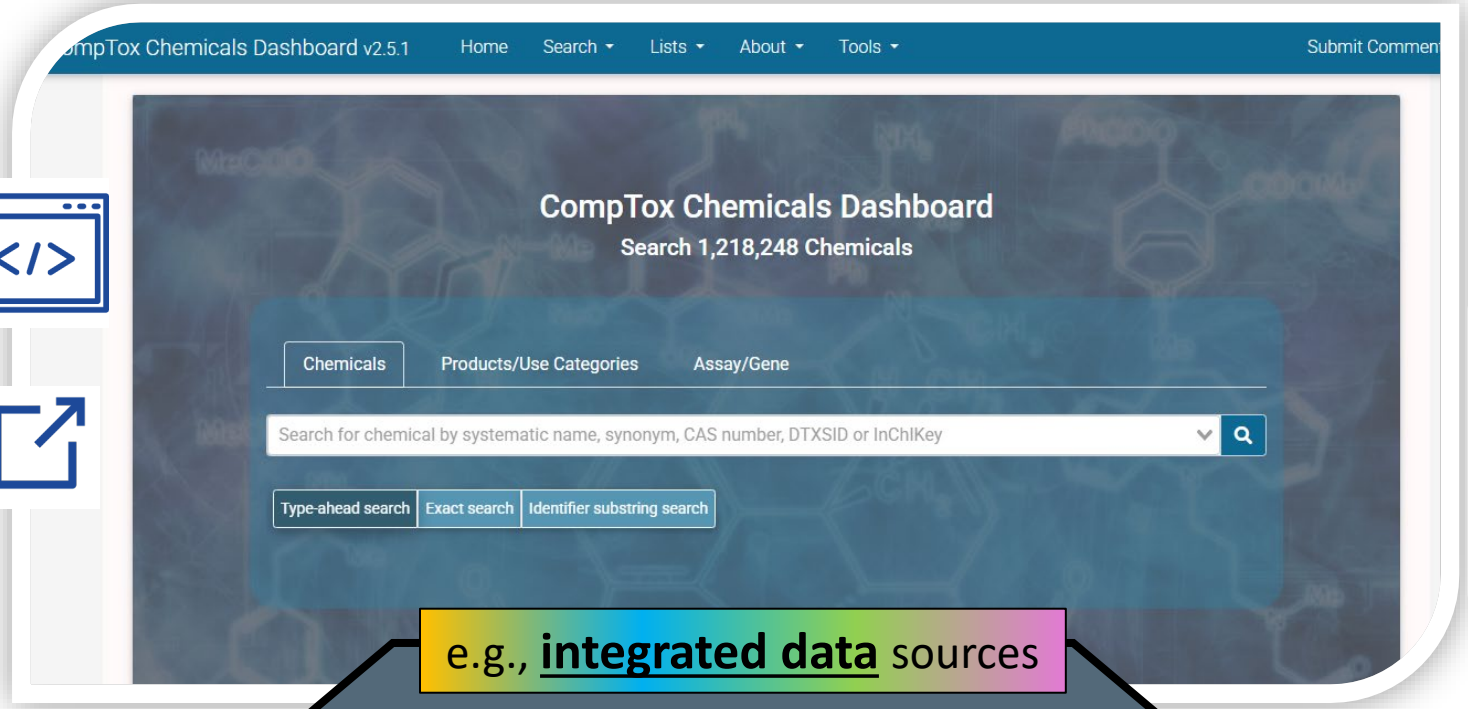

Links to EPA webtools

- **webTEST**
  - hazard and physchem QSAR predictions
- **GenRA**
  - generalized read-across
- **Abstract Sifter**
  - guided literature search

e.g., **integrated data** sources

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Releases & Public Outreach

Online since April 2016 w/numerous updates & presentations

New architecture release

- **Fall 2021 *v2.0***
  - Summer 2022 *v2.0.1, v2.0.2*
- **Fall 2022 *v2.1***
  - Winter 2022 *v2.1.1*
- **Spring 2023 *v2.2***
  - Summer 2023 *v2.2.1*
- **Winter 2023 *v2.3***
- **Spring 2024 *v2.4***
- **Fall 2024 *v2.5***, *v2.5.1*

Jan 13

Presentations / Outreach

- Communities of Practice
- EPA's NAM Training Program
- Presentations and live demos during society meetings (e.g., SETAC, SOT)

SOT Satellite Meeting
Thursday, March 20, 2025
12:00–4:30 PM

U.S. Environmental Protection Agency's CompTox Chemicals Dashboard and Associated Biological Activity and Hazard Data

Training

https://www.epa.gov/chemical-research/new-approach-methods-nams-training

New Approach Methods (NAMs) Training

Resource table

Showing 51 resources (filtered from 151 total entries)

Search: dashboard

Year	Topic	Subtopic	Type	Title	Description
2024	CompTox Chemicals Dashboard	Bioactivity	Slide Deck	CompTox Chemicals Dashboard & Bioactivity Data (pdf) (4.98 MB, April 2024)	Part of the April 2024 NAMs Tools Training Workshop. This presentation covers High Throughput Transcriptomics, High Throughput Phenotypic Profiling, and ToxCast. Presenters: Logan Everett and Madison Feshuk *Related: Database, HTPP*
2024	CompTox Chemicals Dashboard	Toxicity Estimation Software Tool (TEST)	Slide Deck	Toxicity Estimation Software Tool (TEST) - NAMs Workshop (pdf) (2.48 MB, April 2024)	Part of the April 2024 NAMs Tools Training Workshop. TEST software can predict measures of toxicity from physical characteristics of the structure of the chemical, as it contains a compilation of QSAR models. Presenters: Todd Martin
2024	CompTox Chemicals Dashboard	Hazard	Slide Deck	CompTox Chemicals Dashboard & Hazard Data (pdf) (2.3 MB, April 2024)	Part of the April 2024 NAMs Tools Training Workshop. Presenters: Nisha Sipes, Risa Sayre, and Madison Feshuk *Related: ToxRefDB, ToxValDB, Database*
					Part of the April 2024 NAMs Tools Training Workshop.

NAMs Training Resources

- **New to NAMs?** Read background information on NAMs training resources.
- **Have questions?** Contact us.
- Join EPA NAMs email list for training updates.

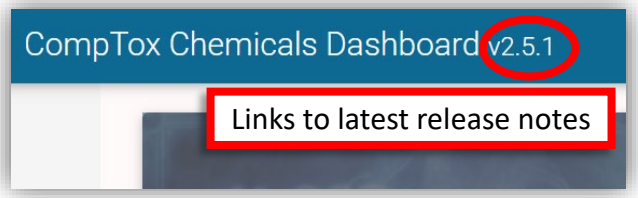
Upcoming Training Events

- CompTox and Exposure Communities of Practice
- EPA Office of Research and Development Events

Related Resources

- EPA New Approach Methods
- EPA Chemical Research
- EPA Computational Toxicology and Exposure Online Resources

New Features for CCDv2.5 *(& fixes for v2.5.1)*



Data Refresh

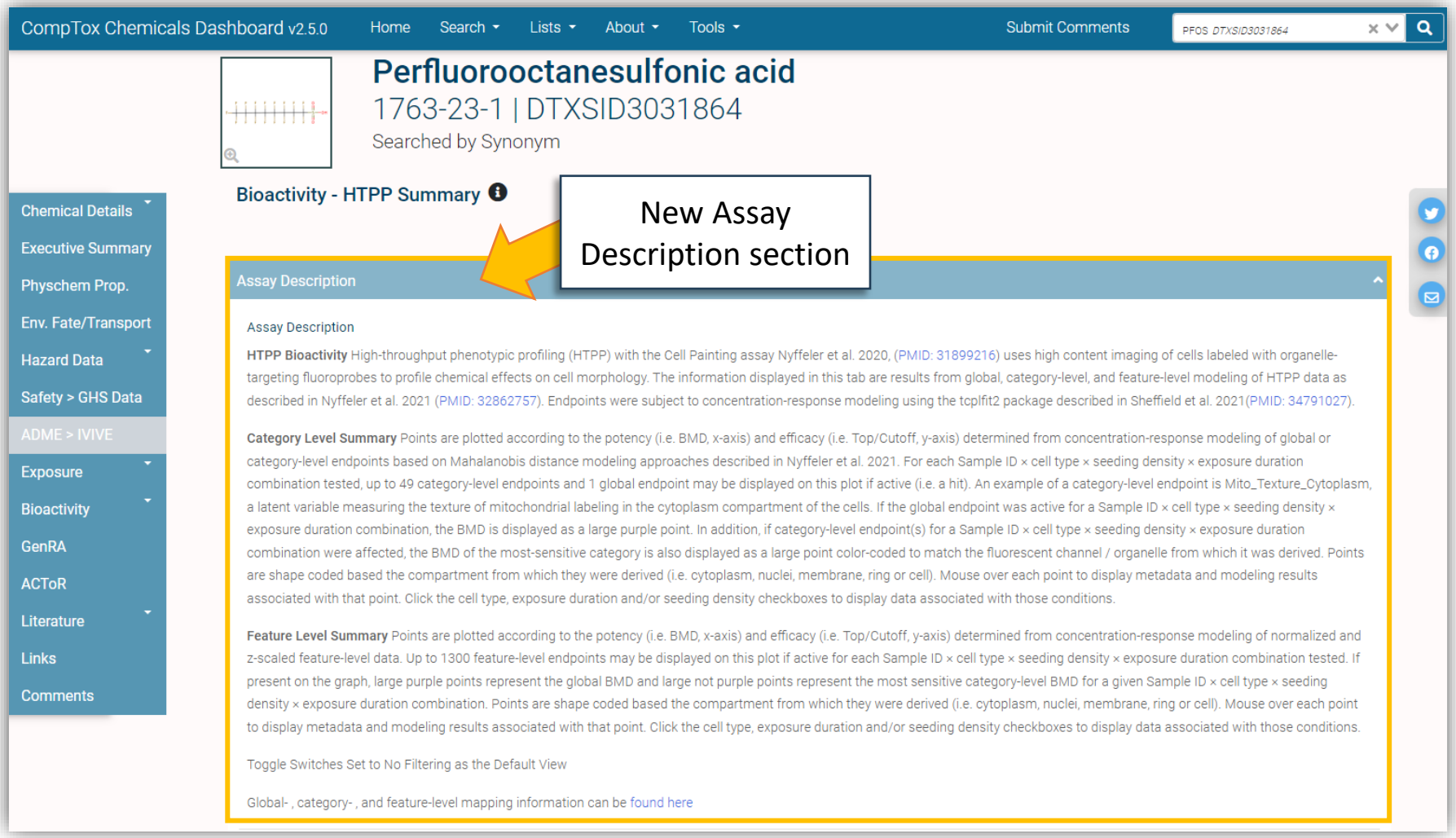
- High Throughput Phenotypic Profiling (HTPP)
- Factotum/CPDat/ChemExpoDB
- SeqAPASS
- ToxValDBv9.5

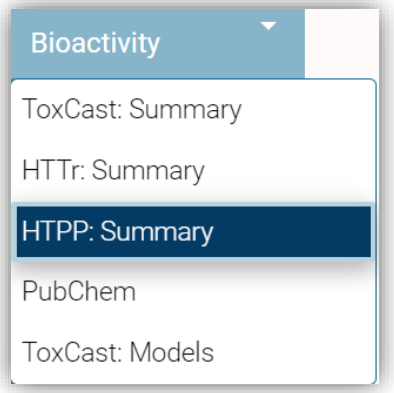
Page Updates

- Bioactivity > HTPP: Summary , ToxCast: Summary
- Exposure > Product & Use Categories, Chemical Weight Fraction, Chemical Functional Use
- Batch Search
- Advanced Search > *Molecular Formula Search new option, Formula Contains (default)*
- Hazard data > Hazard, Genotoxicity, Skin/Eye subtabs
- Executive Summary

High Throughput Phenotypic Profiling (HTPP)

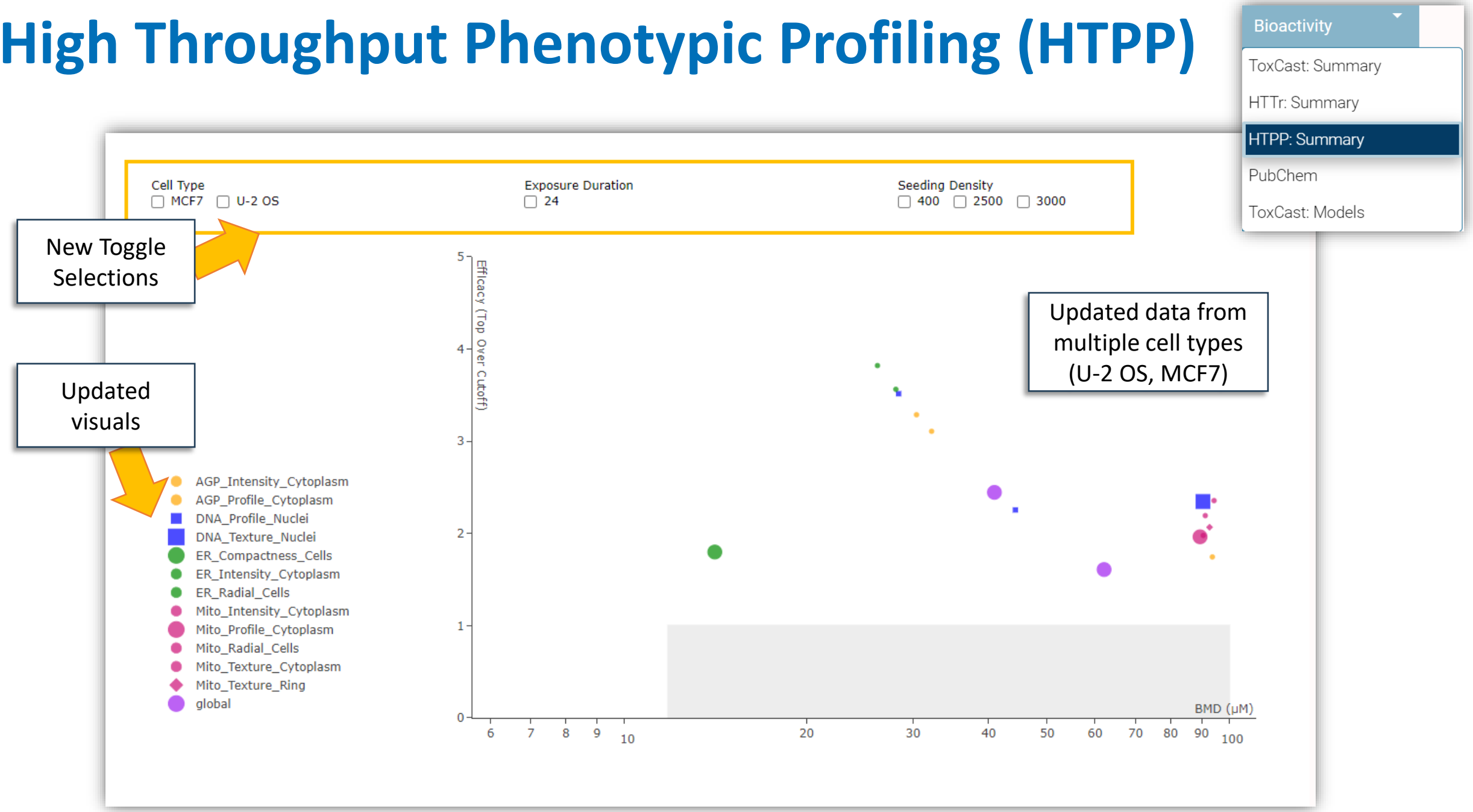
Image-based phenotypic profiling measures a large variety of morphological features of individual cells in *in vitro* cultures.
For more information: https://www.epa.gov/chemical-research/high-throughput-profiling-using-transcriptomics-and-high-content-imaging





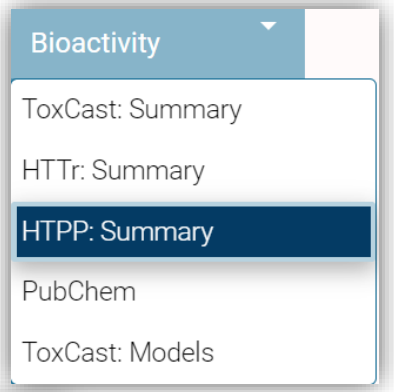
Example https://comptox.epa.gov/dashboard/chemical/htpp-summary/DTXSID3031864

High Throughput Phenotypic Profiling (HTPP)



Example https://comptox.epa.gov/dashboard/chemical/htpp-summary/DTXSID3031864

High Throughput Phenotypic Profiling (HTPP)



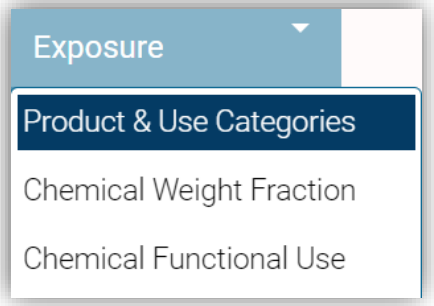
New columns

Sample ID	Cell Type	Seeding Density	Exposure Duration (hrs)	Endpoint	Endpoint Description	BMD	Hit Call
EPAPLT0180F03	U-2 OS	400	24	f 524	Cells Non-Border - DNA_Nuclei_Morph_STAR Symmetry 13 SER-Spot	-	0.06
EPAPLT0180F03	MCF7	2500	24	f 525	Cells Non-Border - DNA_Nuclei_Morph_STAR Symmetry 13 SER-Valley	-	0.02
EPAPLT0180F03	U-2 OS	400	24	f 525	Cells Non-Border - DNA_Nuclei_Morph_STAR Symmetry 13 SER-Valley	-	0.03
EPAPLT0180F03	U-2 OS	400	24	f 526	Cells Non-Border - DNA_Nuclei_Morph_STAR Symmetry 13 SP-Filter	-	0.00
EPAPLT0180F03	MCF7	2500	24	f 526	Cells Non-Border - DNA_Nuclei_Morph_STAR Symmetry 13 SP-Filter	-	0.01
EPAPLT0180F03	U-2 OS	400	24	f 527	Cells Non-Border - DNA_Nuclei_Morph_STAR Symmetry 14	61.2	0.99
EPAPLT0180F03	MCF7	2500	24	f 527	Cells Non-Border - DNA_Nuclei_Morph_STAR Symmetry 14	-	0.84
EPAPLT0180F03	MCF7	2500	24	f 528	Cells Non-Border - DNA_Nuclei_Morph_STAR Symmetry 14 SER-Bright	-	0.00
EPAPLT0180F03	U-2 OS	400	24	f 528	Cells Non-Border - DNA_Nuclei_Morph_STAR Symmetry 14 SER-Bright	-	0.00
EPAPLT0180F03	MCF7	2500	24	f 529	Cells Non-Border - DNA_Nuclei_Morph_STAR Symmetry 14 SER-Dark	-	0.00

Example https://comptox.epa.gov/dashboard/chemical/htpp-summary/DTXSID3031864

Factotum/CPDat/ChemExpoDB

CPDat 4.0.0-alpha.3 (March 2024)



New data

Product and Use Categories (PUCs)

Search PUC

EXPORT

Product Use Categories (PUCs)

Product Use Category	Categorization Subtype	Number of Products
Arts and crafts/office supplies:body paint:tattoo ink	Formulation	2
Cleaning and safety:cleaning products:industrial hand cleaner	Occupation	2
Cleaning products and household care:dishwasher and dishes:c	Formulation	
Cleaning products and household care:shoes	Formulation	
Medical/dental	Occupation	
Not yet Categorized		
Personal care:body hygiene:bar soap	Formulation	
Personal care:body hygiene:body wash	Formulation	
Personal care:body hygiene:hand soap	Formulation	
Personal care:deodorant	Formulation	

General Use Keywords

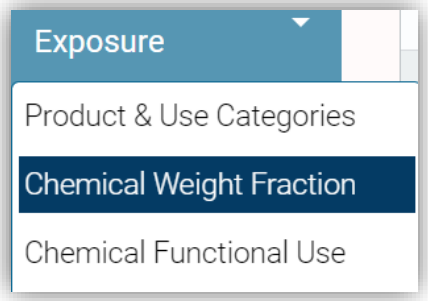
General Use Keywords	Number of Sources
active_ingredient, Europe, Pesticides	1
active_ingredient, Pesticides	5
Canada, pharmaceutical	2
children, Europe	1
Cleaning products and household care - shoes, Europe	2
detected, drinking_water, MN Chemical Screening	5
detected, Europe, Other direct contact consumer goods	1
detected, MN Chemical Screening, surface_water	6
detected, MN Chemical Screening, wastewater	1
detected, wastewater	1
Europe	2
Europe, Food contact items	1
Europe, Furniture and Furnishings, nondetect	1
Europe, Personal care	1
Europe, Personal care - body hygiene - hand soap	1

Data collected by EPA about how chemicals are used in commerce and how they occur in consumer and industrial products. For more detailed information: https://comptox.epa.gov/chemexpo

Example https://comptox.epa.gov/dashboard/chemical/product-use-categories/DTXSID5032498

Factotum/CPDat/ChemExpoDB

CPDat 4.0.0-alpha.3 (March 2024)



New data

Chemical Weight Fractions (CWF)

Search Chemical Weight Fractions

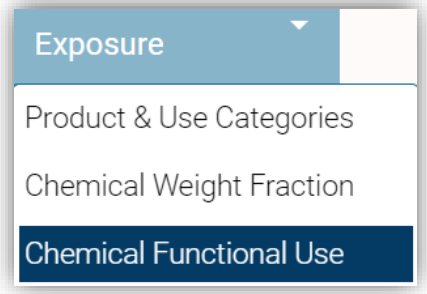
EXPORT

Product Name	Product Use Category	Categorization Subtype	Minimum Weight Fraction	Maximum Weight Fraction	Data Type	Source	Product Count
7188 purell antibacterial lotion so...	Personal care:body hygiene:h	Formulation	0.00	1.00e-2	reported	SIRI	1
9212-12 dermapro antimicrobial l...	Cleaning and safety:cleaning	Occupation	0.00	1.00e-2	reported	SIRI	1
9751 purell antibacterial lotion so...	Personal care:body hygiene:h	Formulation	0.00	1.00e-2	reported	SIRI	1
9752 purell antibacterial lotion so...	Personal care:body hygiene:h	Formulation	0.00	1.00e-2	reported	SIRI	1
AHAVA Dermud Intensive Foot Cr...	Personal care:foot care	Formulation	-	-	reported	Environme...	2
Ahava Dermud Intensive Foot Cr...	Personal care:foot care	Formulation	-	-	reported	Environme...	2
Ahava Dermud Intensive Hand Cr...	Personal care:general moistur	Formulation	-	-	reported	Environme...	1
AHAVA Dermud Nourishing Body...	Personal care:general moistur	Formulation	-	-	reported	Environme...	1
AHAVA Purifying Mud Mask (old f...	Personal care:facial cleansing	Formulation	-	-	reported	Environme...	1
amber antibacterial hand soap	Personal care:body hygiene:h	Formulation	-	-	reported	Vi-Jon	1
AMOREPACIFIC Treatment Cleans...	Personal care:facial cleansing	Formulation	-	-	reported	Environme...	2

Example https://comptox.epa.gov/dashboard/chemical/chemical-weight-fraction/DTXSID5032498

Factotum/CPDat/ChemExpoDB

CPDat 4.0.0-alpha.3 (March 2024)



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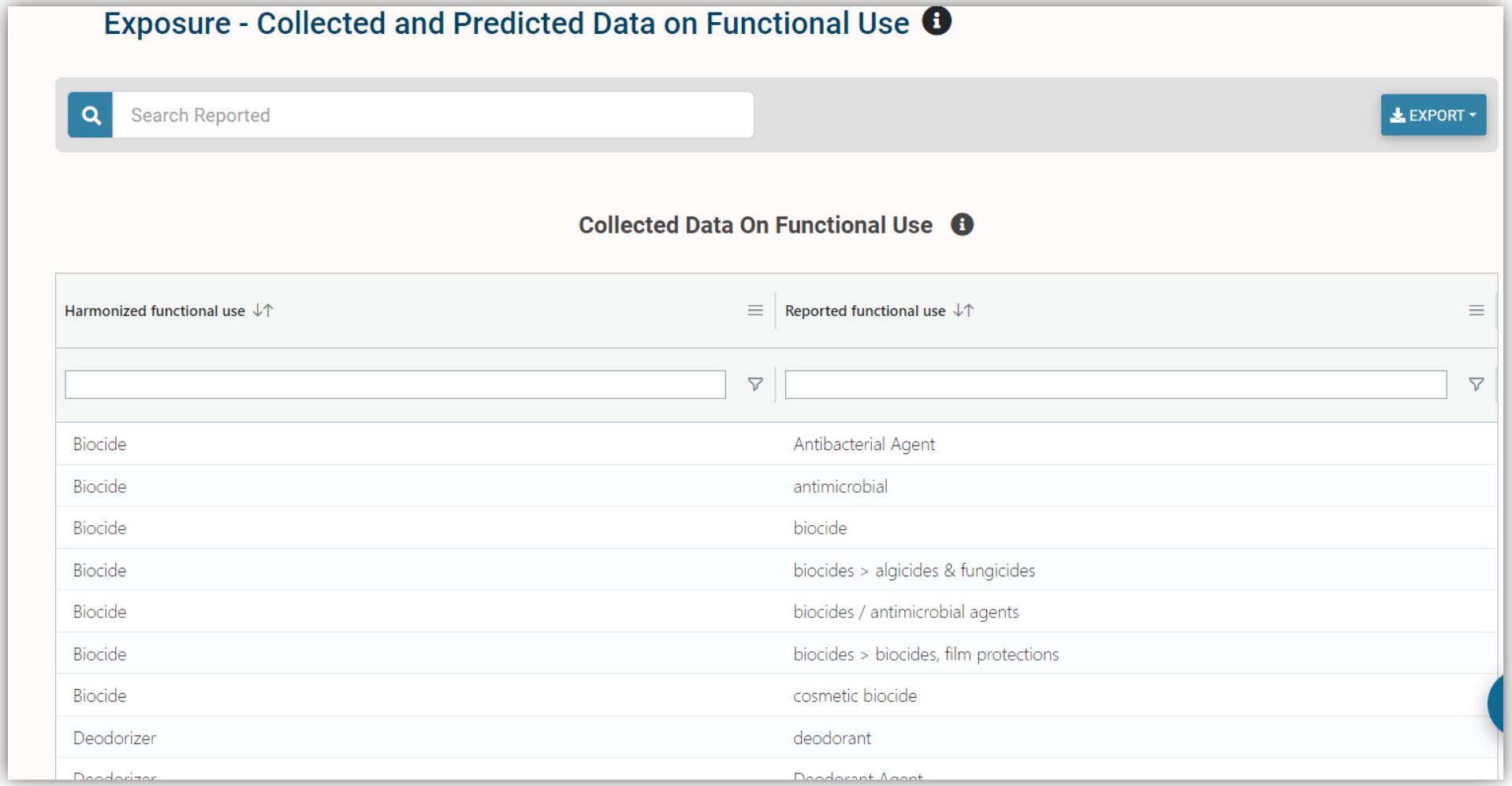
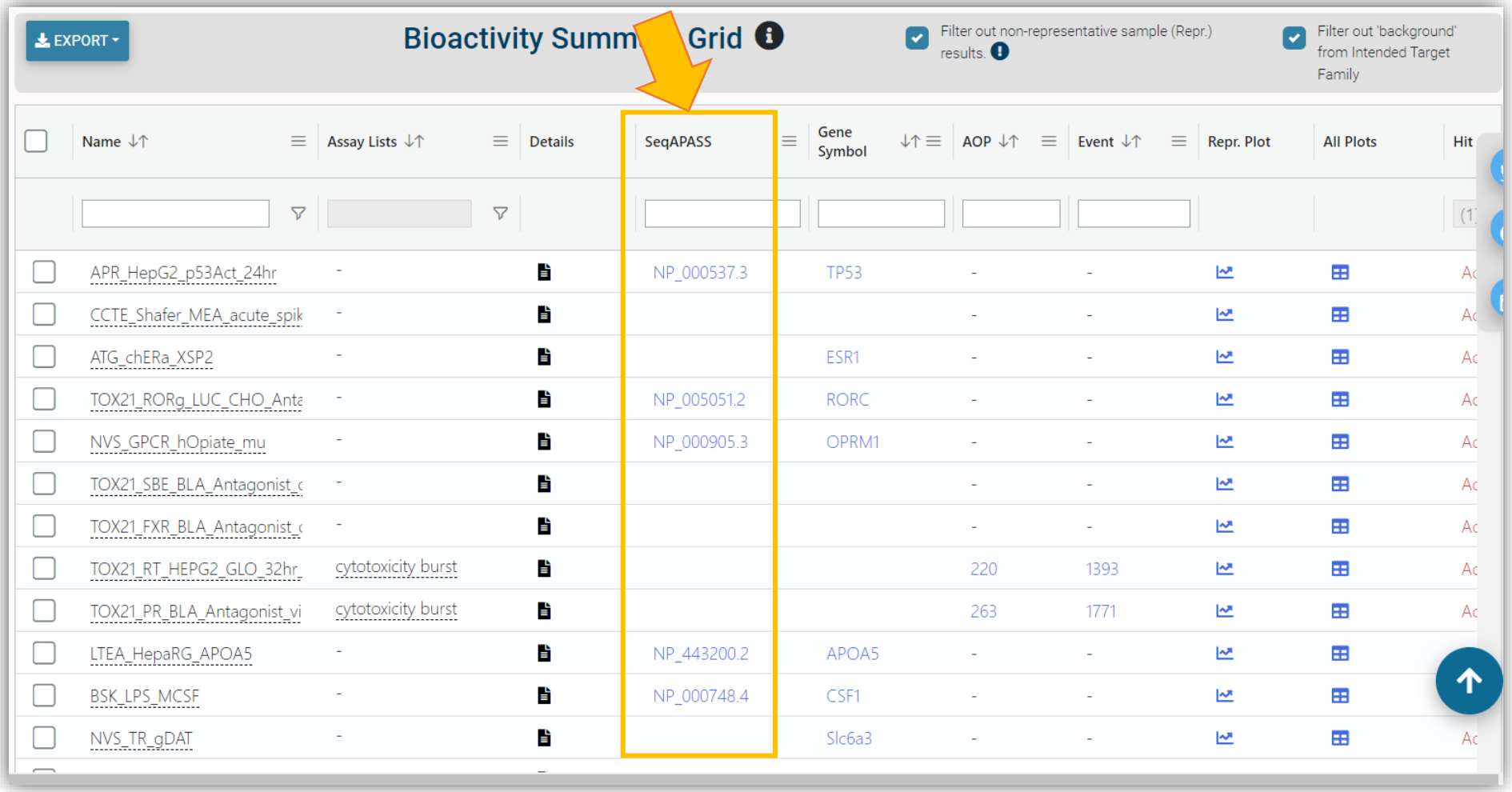


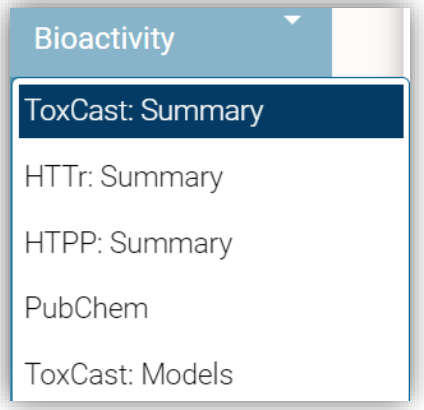
Example https://comptox.epa.gov/dashboard/chemical/chemical-functional-use/DTXSID5032498

SeqAPASS Sequence Alignment to Predict Across Species Susceptibility

SeqAPASS data version 8

Allows one to extrapolate toxicity information across species. For more information on SeqAPASS: https://www.epa.gov/comptox-tools/sequence-alignment-predict-across-species-susceptibility-seqapass-resource-hub



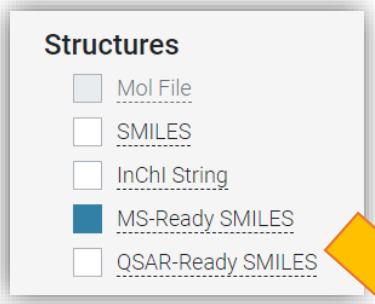


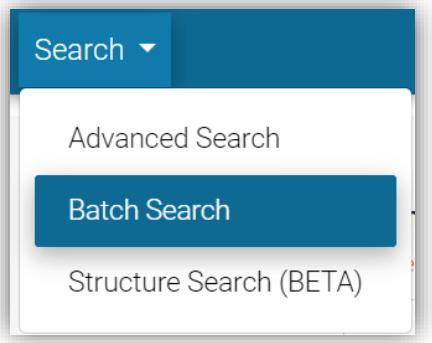
New data

Example https://comptox.epa.gov/dashboard/chemical/invitrodb/DTXSID5032498

Batch Search

- MS-Ready SMILES selection - MS-Ready mass and MS-Ready formulae are now included in the download

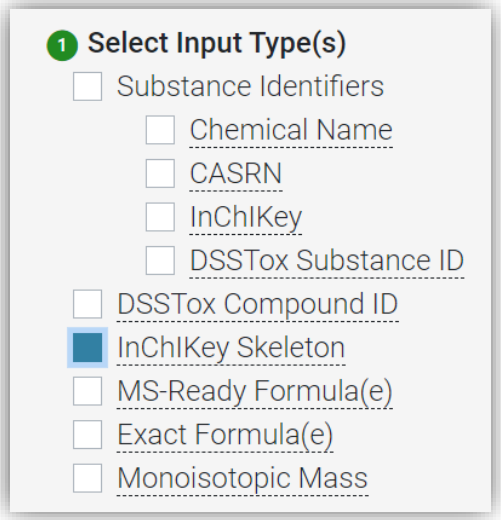


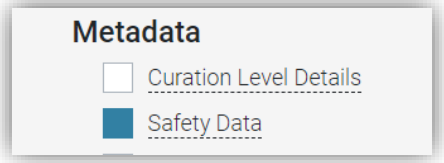


	A	B	C	D	E	F
1	INPUT	FOUND_BY	PREFERRED_NAME	MS_READY_SMILES	MS_READY_MASS	MS_READY_FORMULAE
2	bpa	Synonym	Bisphenol A	CC(C)(C1=CC=C(O)C=C1)C1=CC=C(O)C=C1	228.291	C15H16O2
3	atrazine	Approved Name	Atrazine	CCNC1=NC(NC(C)C)=NC(Cl)=N1	215.69	C8H14ClN5
4	triclosan	Approved Name	Triclosan	OC1=C(OC2=CC=C(Cl)C=C2Cl)C=CC(Cl)=C1	289.54	C12H7Cl3O2

- Enhanced accessibility with informational text added to the Batch Search Workflow

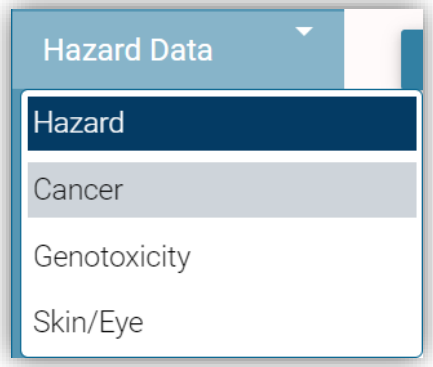
- Several bug fixes including,
  - InChIKey Seleton search
  - Safety Data selection

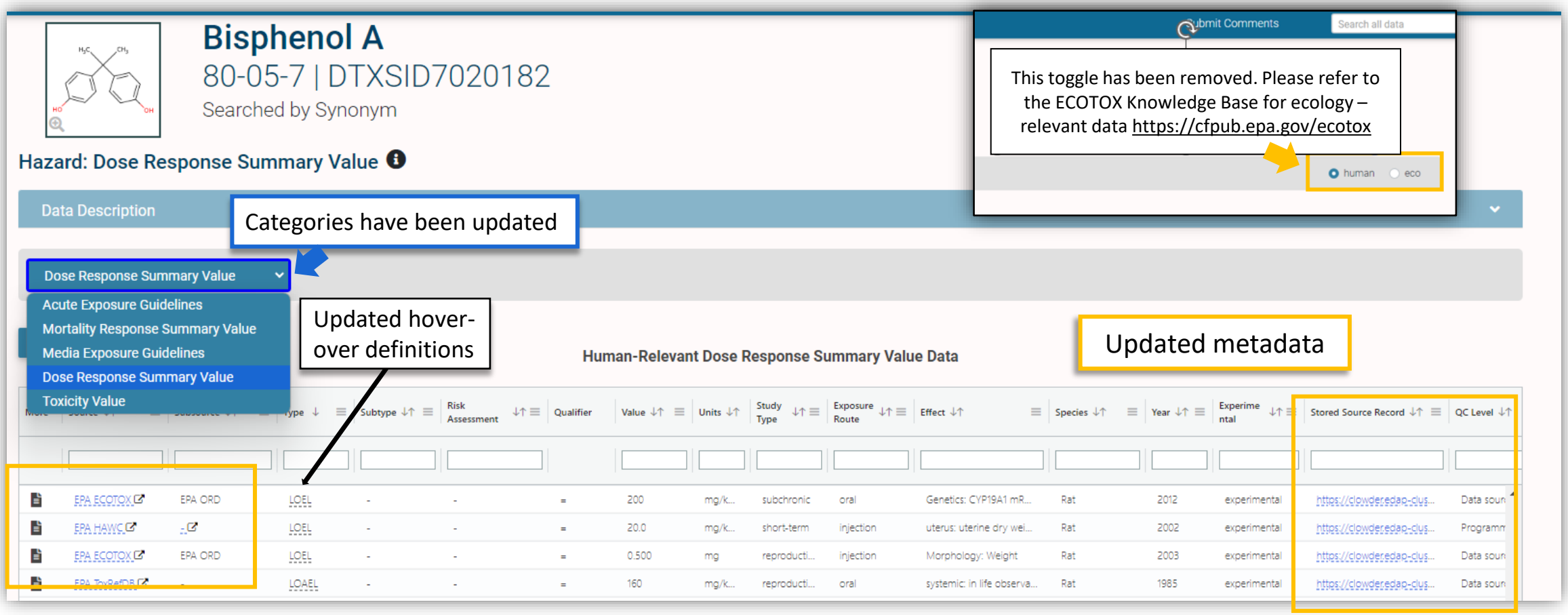




ToxValDBv9.5 (Hazard data)

- Major restructuring of the data
- Modified focus to human health-relevant toxicity information
- Revised classification categories
- Improvements to source document accessibility





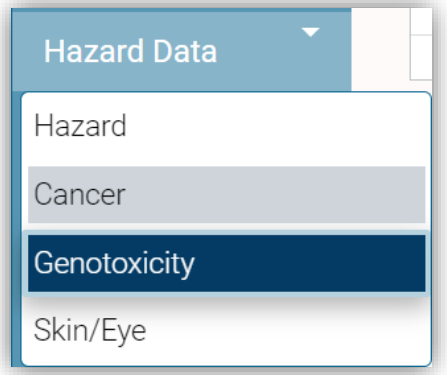
ToxValDBv9.5 (Executive Summary)

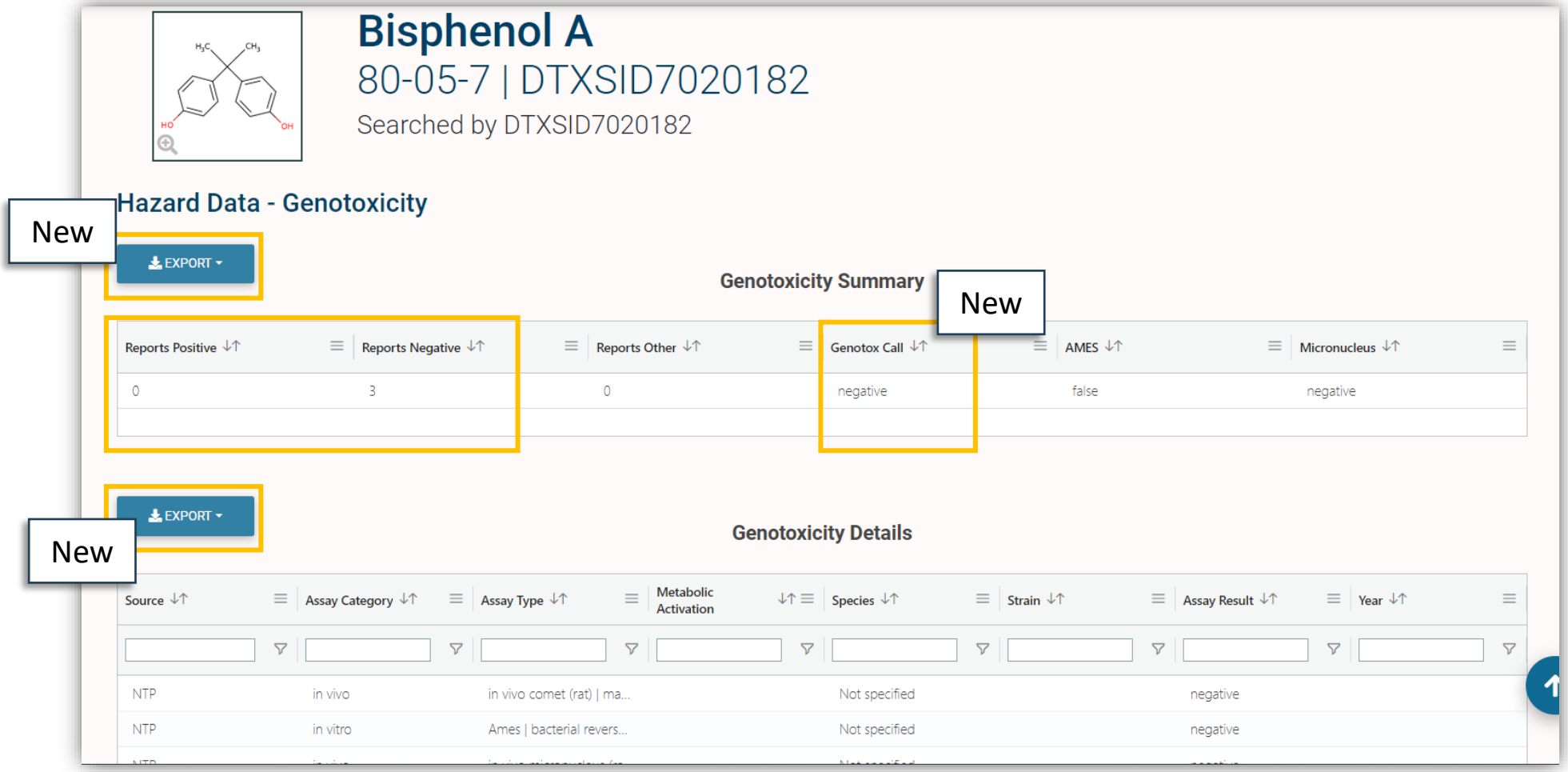
Updated based on ToxValDB categories

- Reproductive & Developmental toxicology endpoints are now displayed together
- Removed subacute, endocrine system, IVIVE POD, occupational exposure

ToxValDBv9.5 (Genotoxicity data)

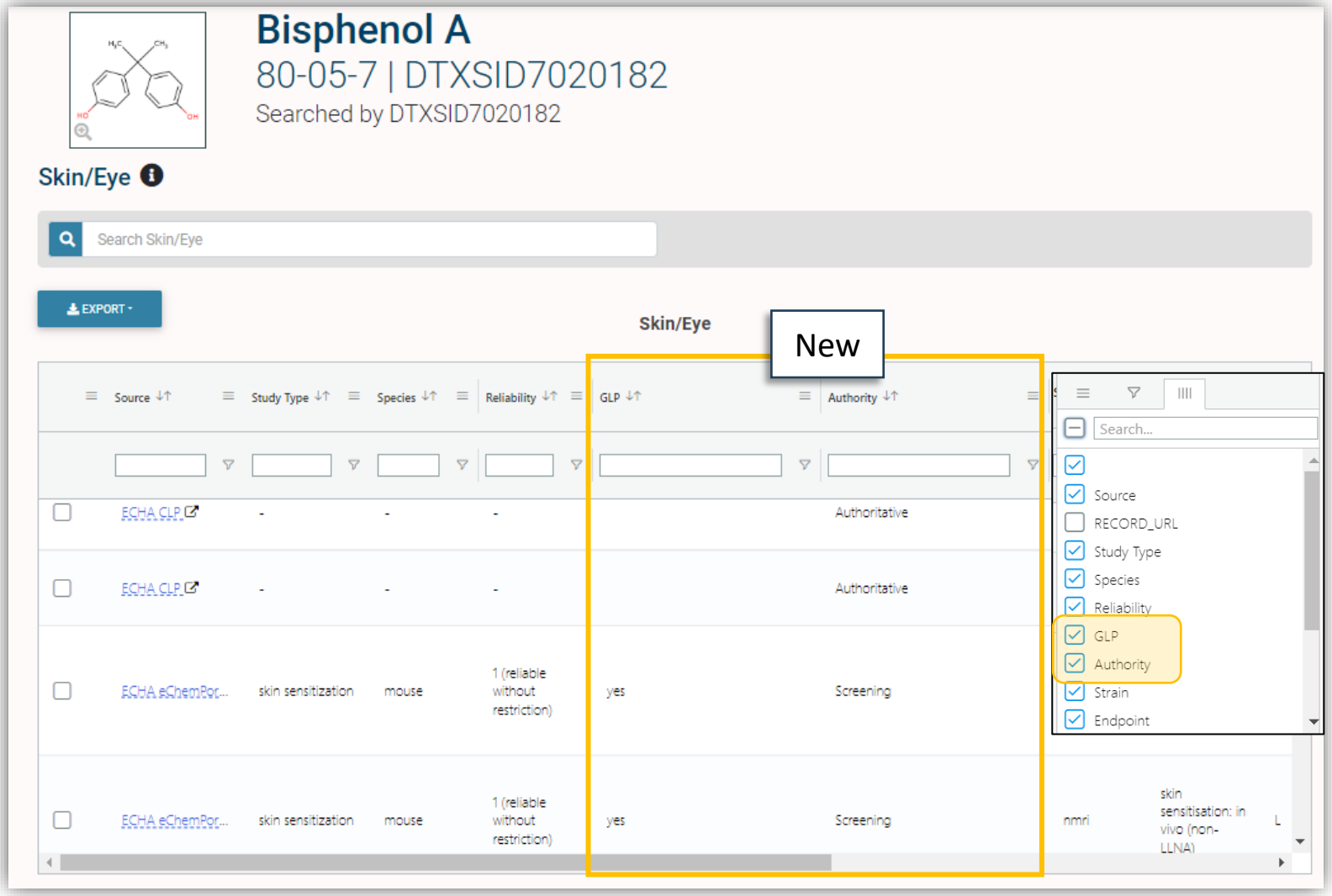
- Genotoxicity aggregation for number of reports positive and negative are correct
- Genotoxicity subtab Export option is now available
- Genotox Call column has been added to the Summary table

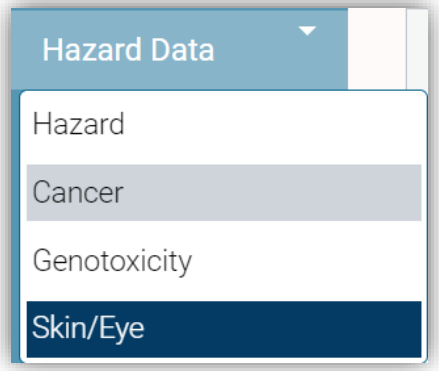




ToxValDBv9.5 (Skin/Eye data)

- New GLP and Authority columns
- Updated source link





GLP and Authority columns can be made visible by selection any column heading & making them visible.

*note: all columns are downloaded in the export

Team Approach

EPA/ORD/Center for Computational Toxicology and Exposure

Efforts include many more than who are shown here

Many external collaborators provided data & links

EPA United States Environmental Protection Agency

We value your feedback!

Nisha S. Sipes, PhD

Assistant Center Director

US EPA ORD Center for Computational Toxicology and Exposure

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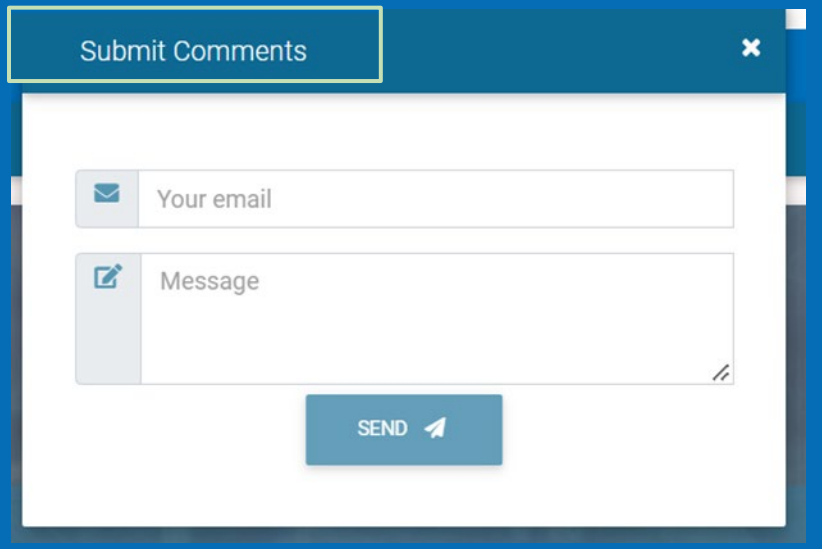

https://comptox.epa.gov/dashboard/

Updates to the Toxicity Values Database, ToxValDB

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Computational Toxicology and Exposure Communities of Practice

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ToxValDB Overview

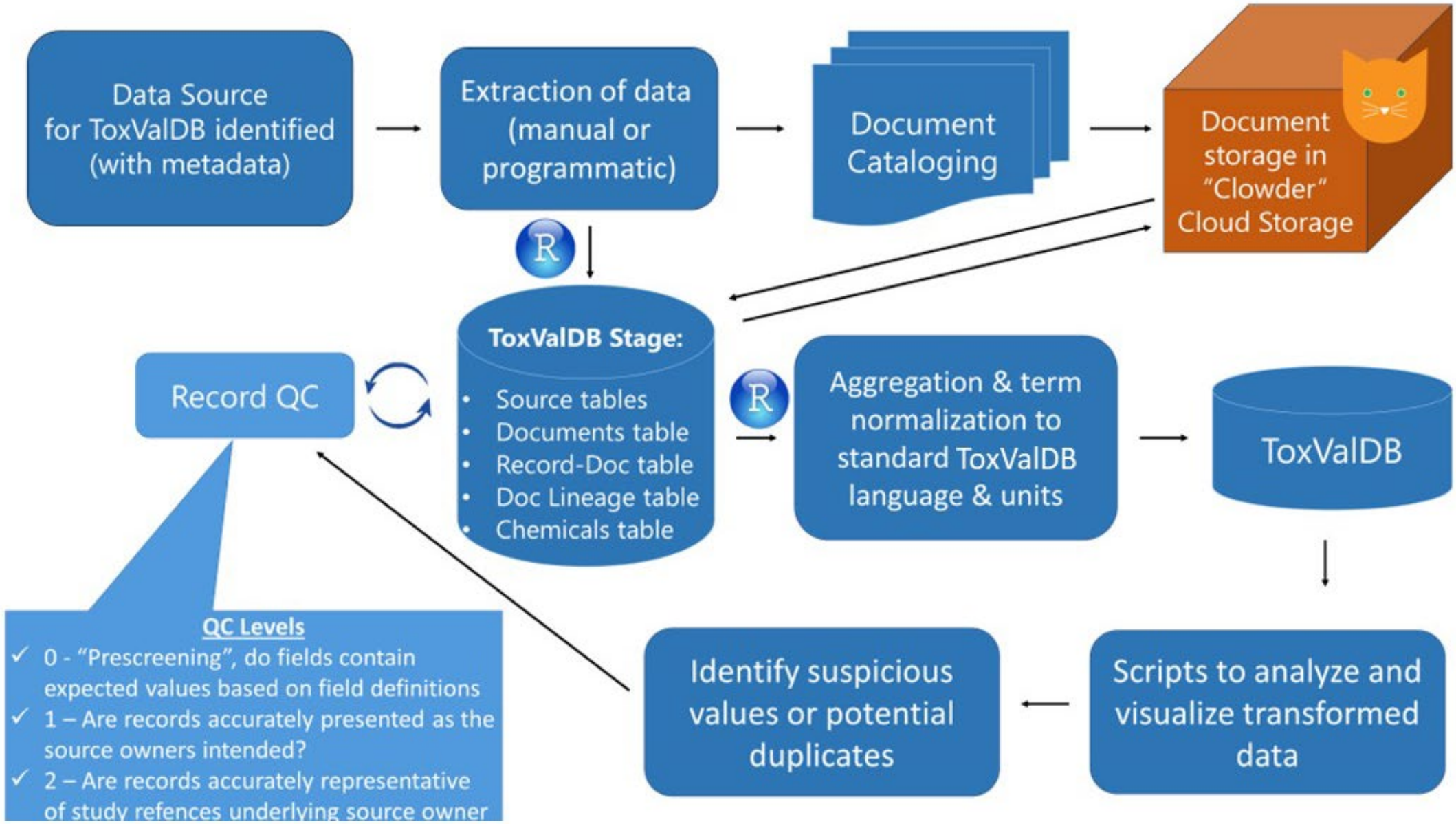
- The Toxicity Values Database (ToxValDB) is a large compilation of human health-relevant toxicology data, including
  - Experimental *in vivo* toxicity data
  - Derived toxicity values
  - Exposure guideline values
- First publicly released in 2016 (v3)
- Applications in NAM development, evaluation, and/or validation
- CompTox Chemicals Dashboard v2.5.1 surfaces ToxValDB v9.5

Major Updates in Version 9.5+

- Narrowed scope to human health relevance
  - Represents removal of ecotoxicity data
    - Most ecotoxicity data can be accessed directly via the ECOTOX Knowledgebase
- Improved curation and quality control
- Revised record categorization scheme
- Summary of version 9.5:
  - 231,485 records
  - 39,434 unique chemicals
  - 43 sources

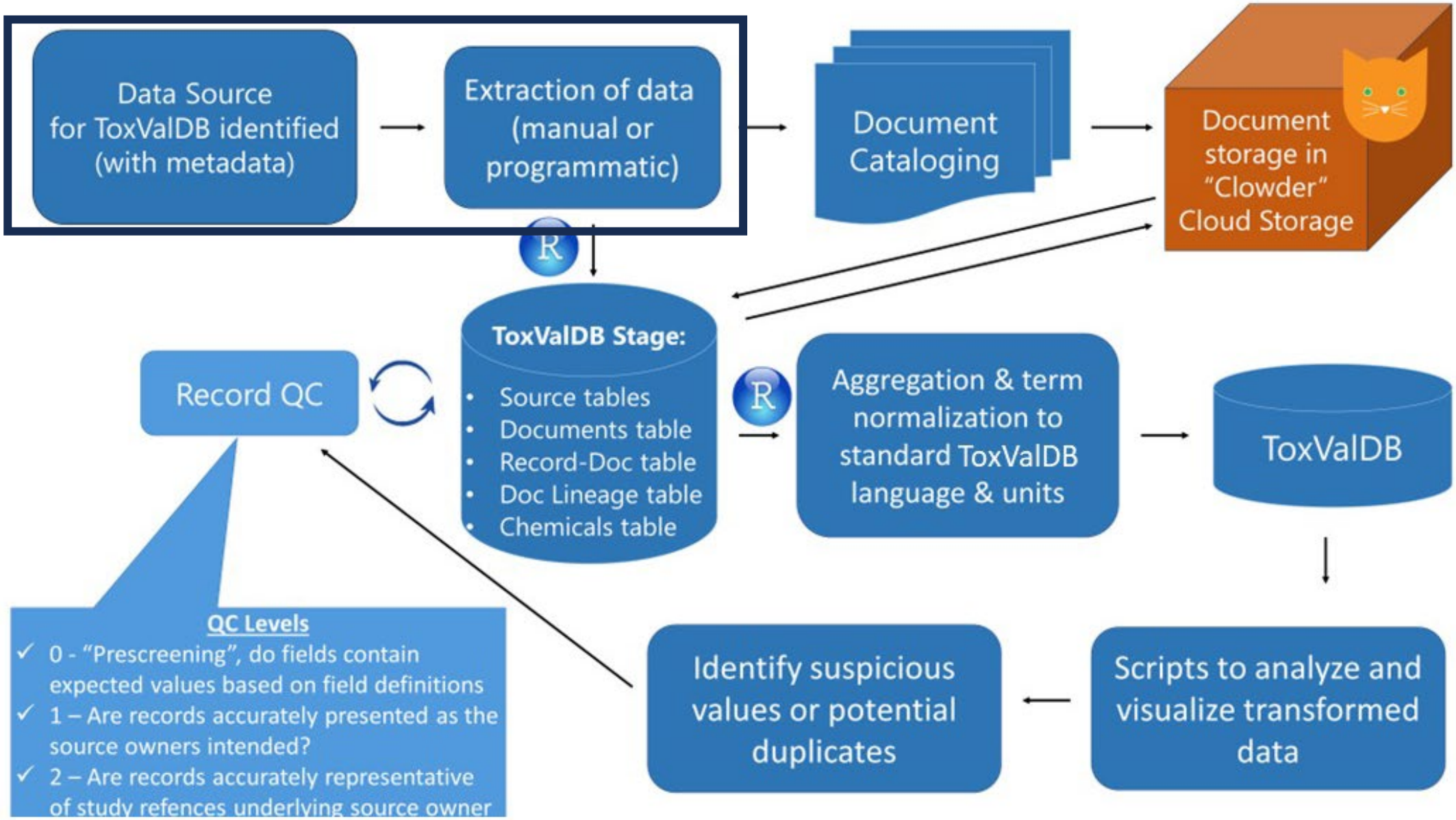
Database Development

- MySQL platform – open-source relational database management system
- Important steps in ToxValDB development:
  - Curation
  - Storage
  - Quality control
  - Standardization



Wall et al., *in prep*

Curation



Wall et al., *in prep*

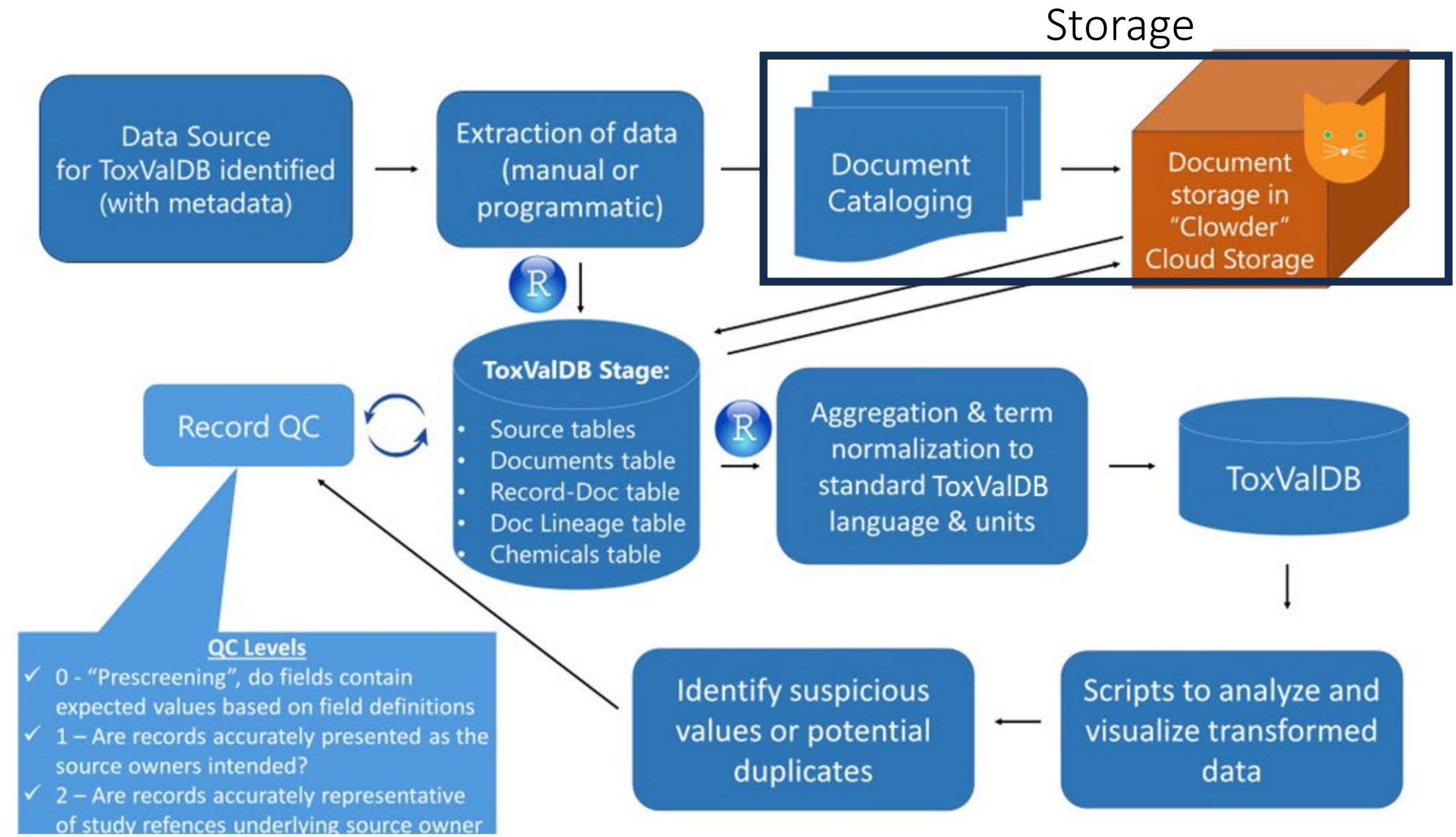
Data Curation – Source Identification

- Focus is on data published by authoritative sources
  - Data are not pulled from the open literature
- Three categories of relevant information:
  - Results from *in vivo* toxicity experiments (e.g., NOAEL, BMDL)
  - Risk assessment values (e.g., RfD, MRL)
  - Media exposure guidelines (e.g., MCL, AEGL)
- Included species are limited to those commonly used in human health assessment

NOAEL = No Observed Adverse Effect Level; BMDL = Benchmark Dose Level; RfD = Reference Dose; MRL = Minimal Risk Level; MCL = Maximum Contaminant Level; AEGL = Acute Exposure Guideline Level

Data Curation – Extraction of Data

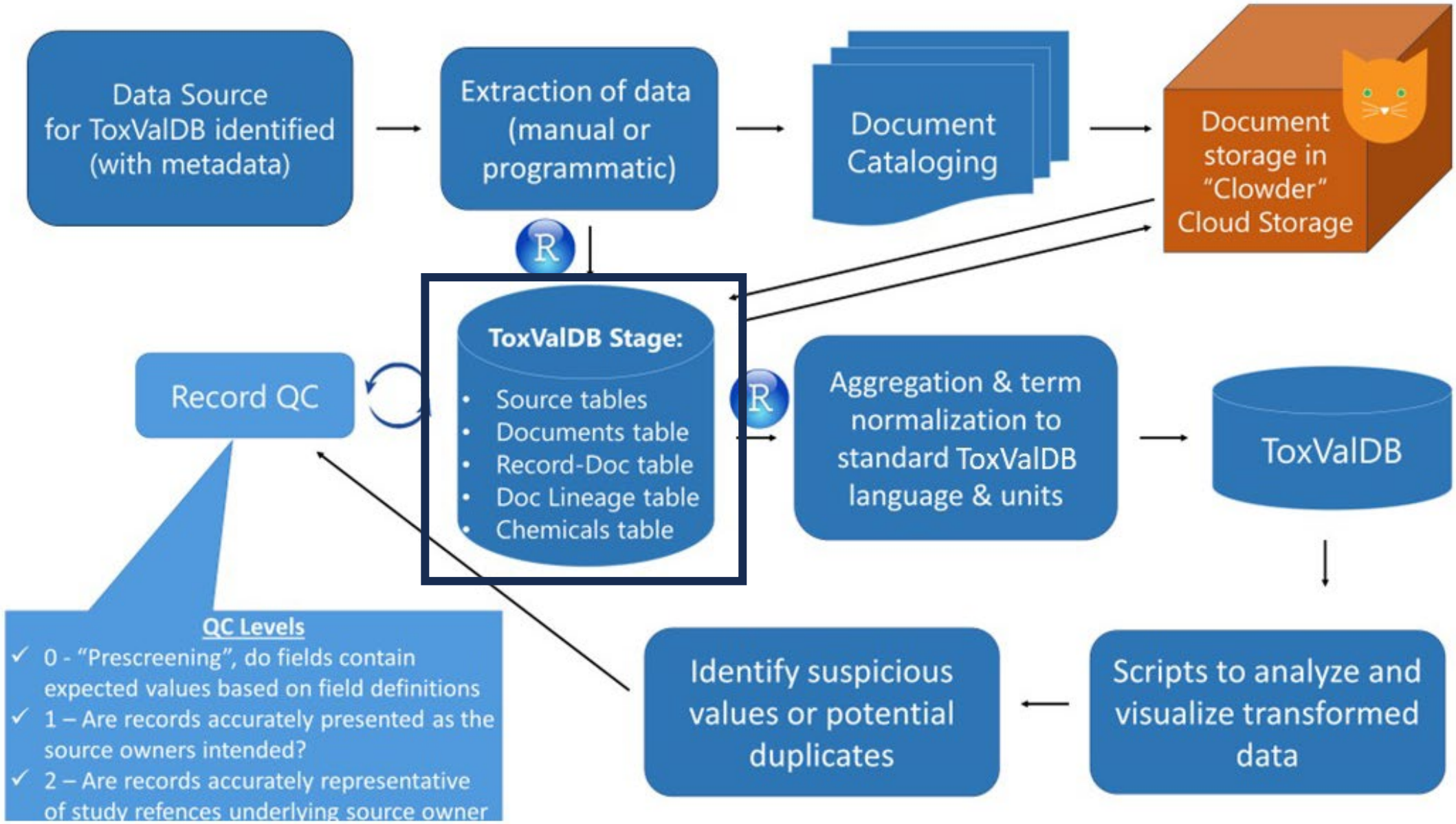
- Programmatically curated
  - Structured, machine-readable source data
  - Custom script is developed for each source that follows a standard template and uses common, generic functions when possible
- Manually curated
  - Complex, text-based, unstructured data
  - Expert and trained curators manually extract information into standardized Excel template



Wall et al., *in prep*

Document Cataloging and Storage

- Documents are retrieved and stored in a file management system (Clowder)
- Documents include:
  - Flat file or report from which data were extracted
  - Original (underlying) source documents (when available)
  - Screenshots of webpages
- Documents are associated to individual records and accessible via hyperlink



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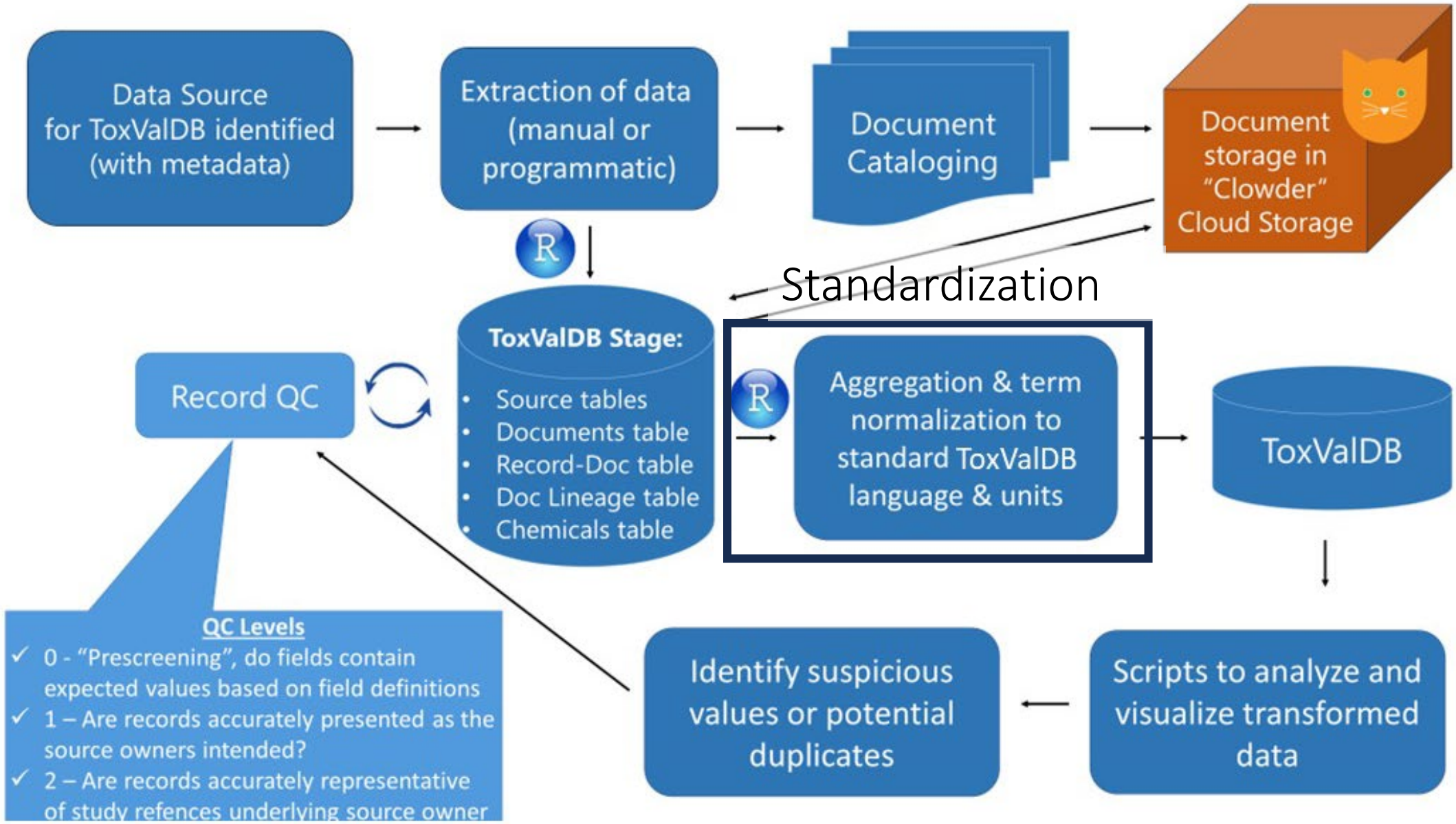

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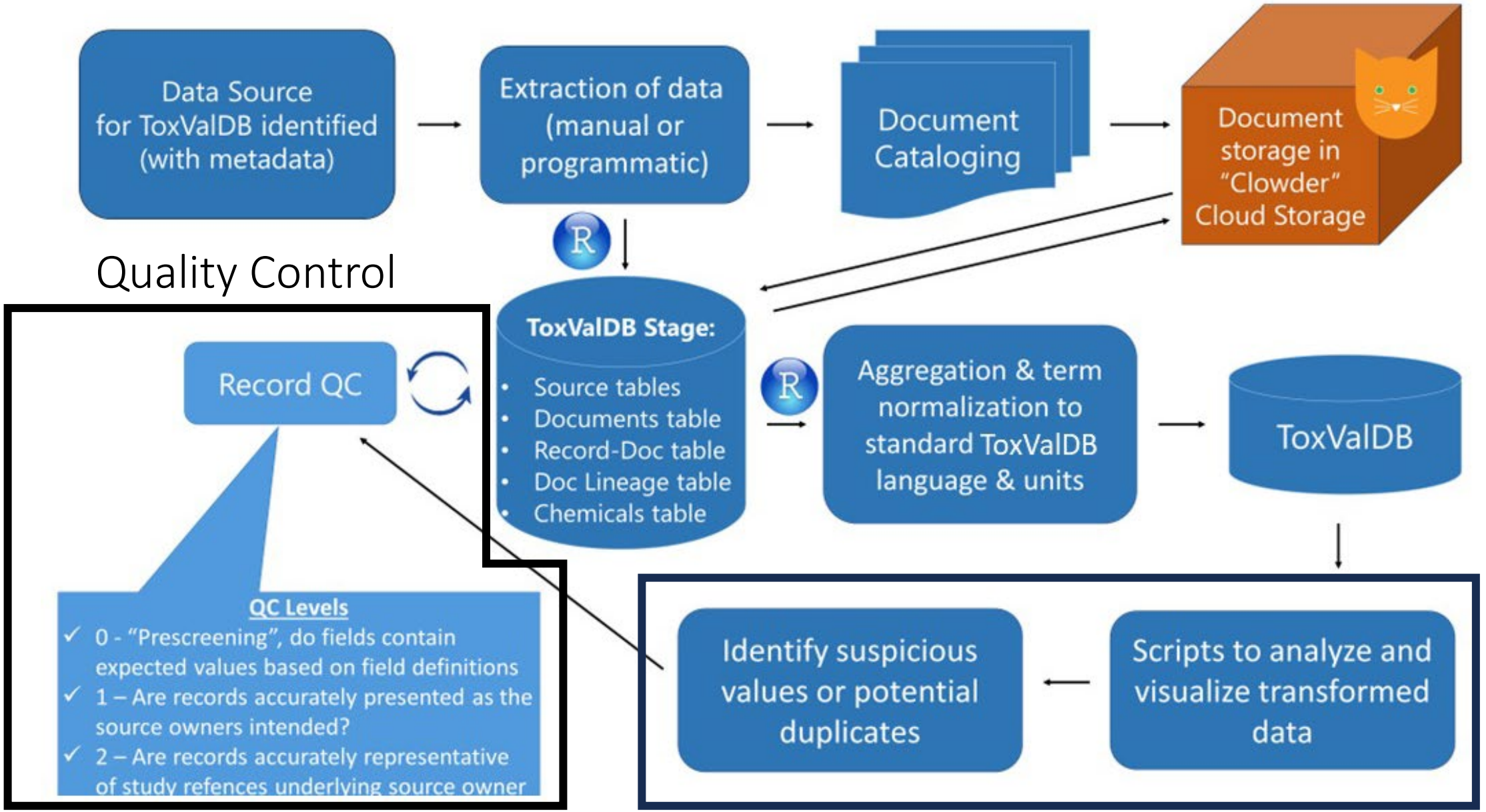
Standardization Steps

- Because ToxValDB extracts data from diverse sources, there is heterogeneity for many terms
- A large part of the value of ToxValDB is in the standardization that facilitates comparisons across the database
- Terms are standardized using a common controlled vocabulary per field
- Where possible, units are converted and standardized to mg/kg-d for oral exposures and mg/m^3 for inhalation exposures

Record Categorization

Effect Type Example	Effect Type Supercategory	Study Type	Risk Assessment Class	Experimental Record
BMDL, NOAEL	Dose Response Summary Value	Acute, Short-term, Subchronic, Chronic, Developmental, Reproduction Developmental, Clinical, Epidemiologic, Occupational	N/A	Experimental Not Experimental Undetermined
LD50, LC10	Mortality Response Summary Value	Acute	N/A	Experimental Not Experimental Undetermined
RfD, MRL	Toxicity Value	N/A	Cancer, Non-cancer	Not experimental
MCL, MEG	Media Exposure Guidelines	N/A	Water, Air, Soil	Not experimental
AEGL, PAC	Acute Exposure Guidelines	N/A	Water, Air, Soil	Not experimental

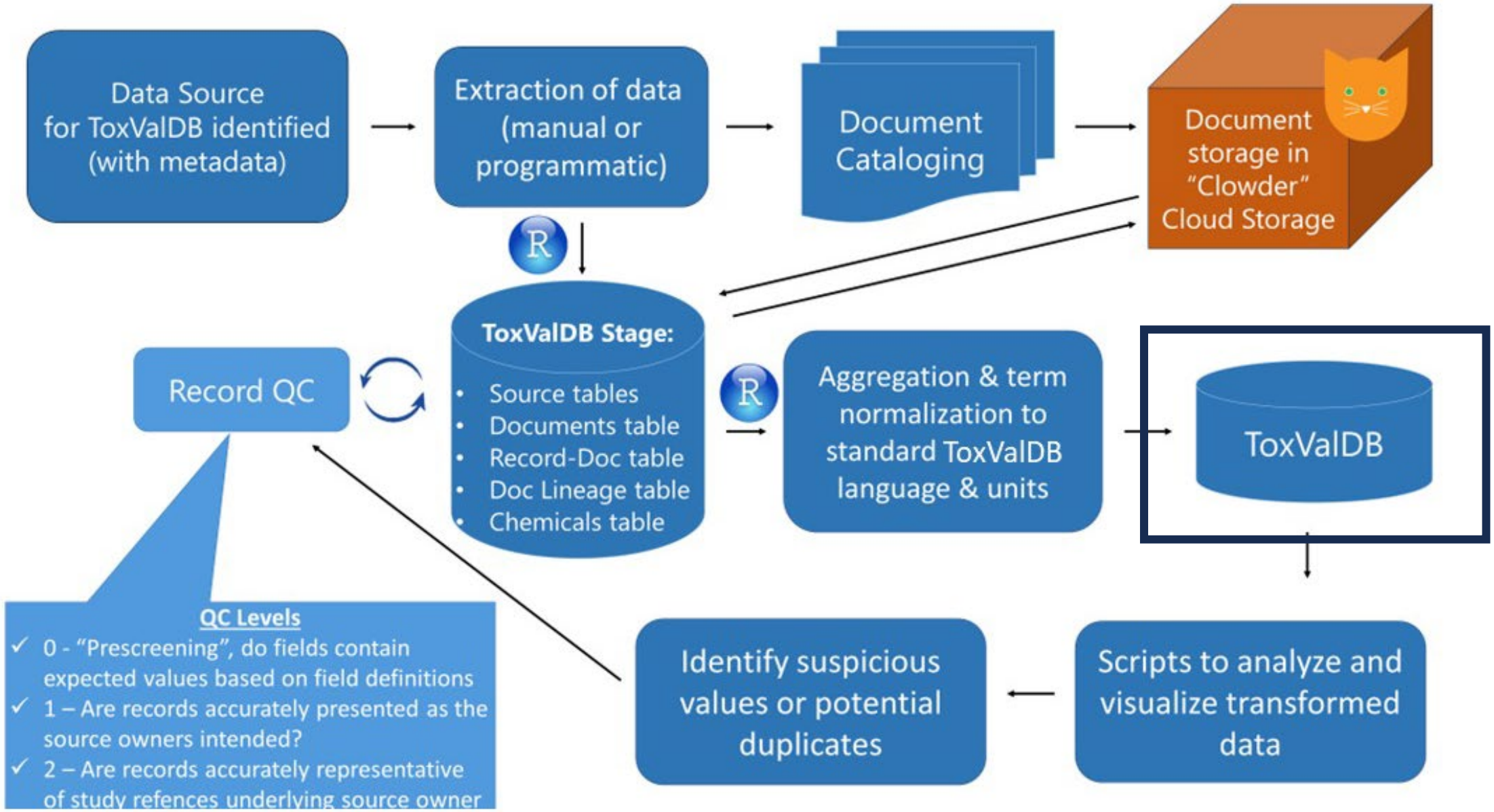
BMDL = Benchmark Dose Level; NOAEL = No Observed Adverse Effect Level; LD = Lethal Dose; RfD = Reference Dose; MRL = Minimal Risk Level; MCL = Maximum Contaminant Level; MEG = Military Exposure Guideline; AEGL = Acute Exposure Guideline Level; PAC = Protective Action Criteria



Wall et al., *in prep*

Quality Control

- Quality control is a multi-level and iterative process
- Three tiers of quality control on non-standardized data
  - Level 0 QC
    - To check for systematic errors in the data importation step
    - 100% of sources
  - Level 1 QC
    - To evaluate extraction accuracy by comparing ToxValDB records to source documents
    - Programmatically extracted sources: ≥10% of records
    - Manually extracted sources: ≥20% of records
  - Level 2 QC
    - To check record against cited reference documents
- Quality control on standardized data
  - Data profiling reports to flag records or fields for review that could be potentially erroneous.



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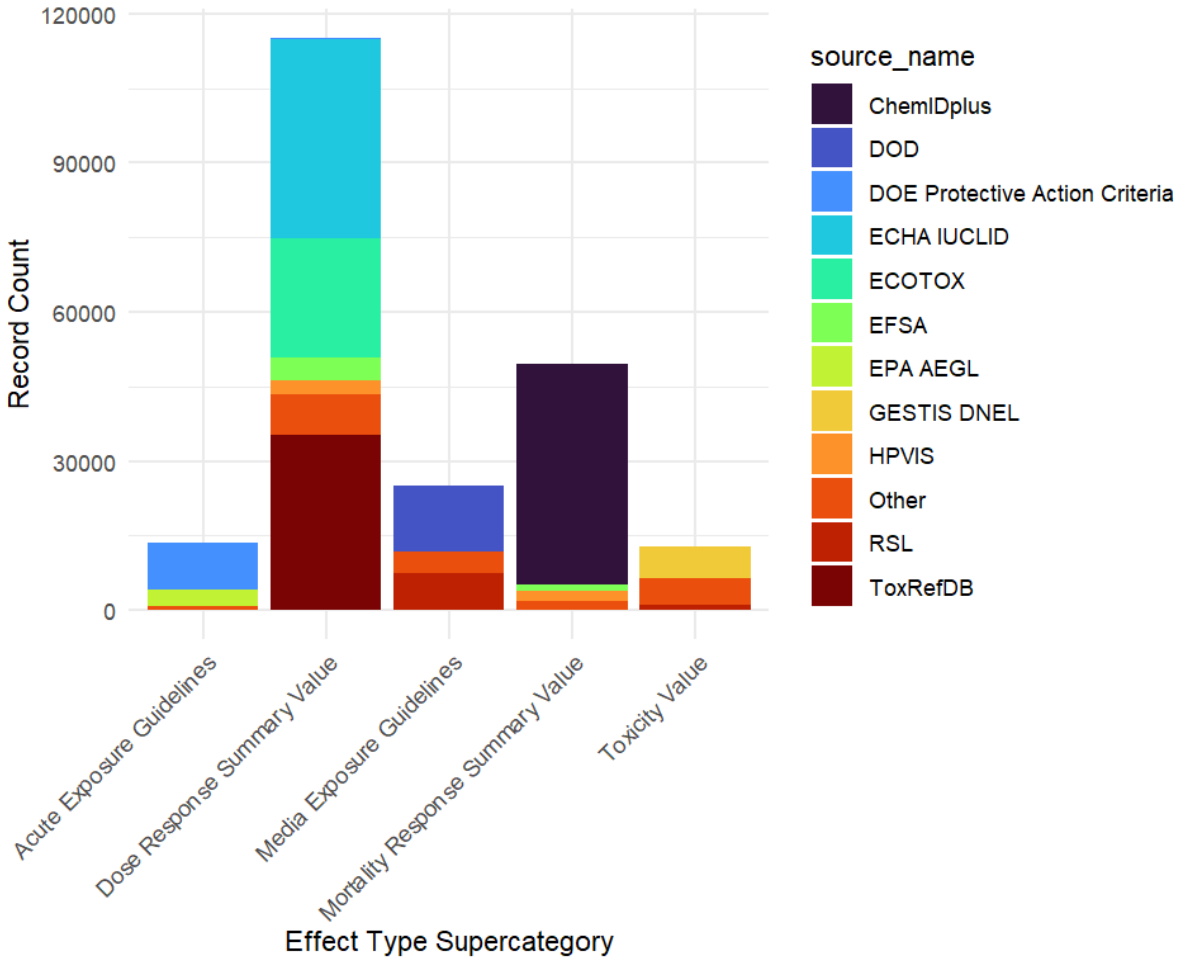
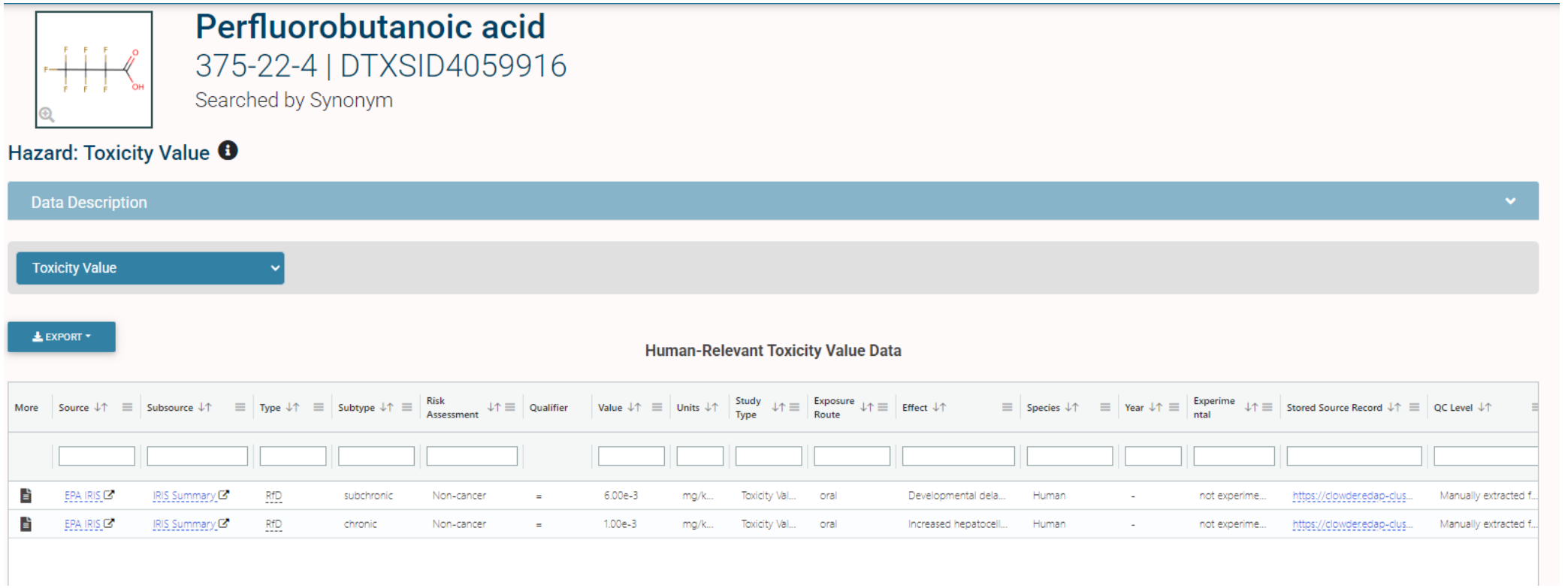
Sources in ToxValDB



- Version 9.5 includes 43 data sources
- Most records are dose response summary values
- Largest sources by record count:
  - ChemIDplus
  - ECHA IUCLID
  - ToxRefDB
  - ECOTOX Knowledgebase

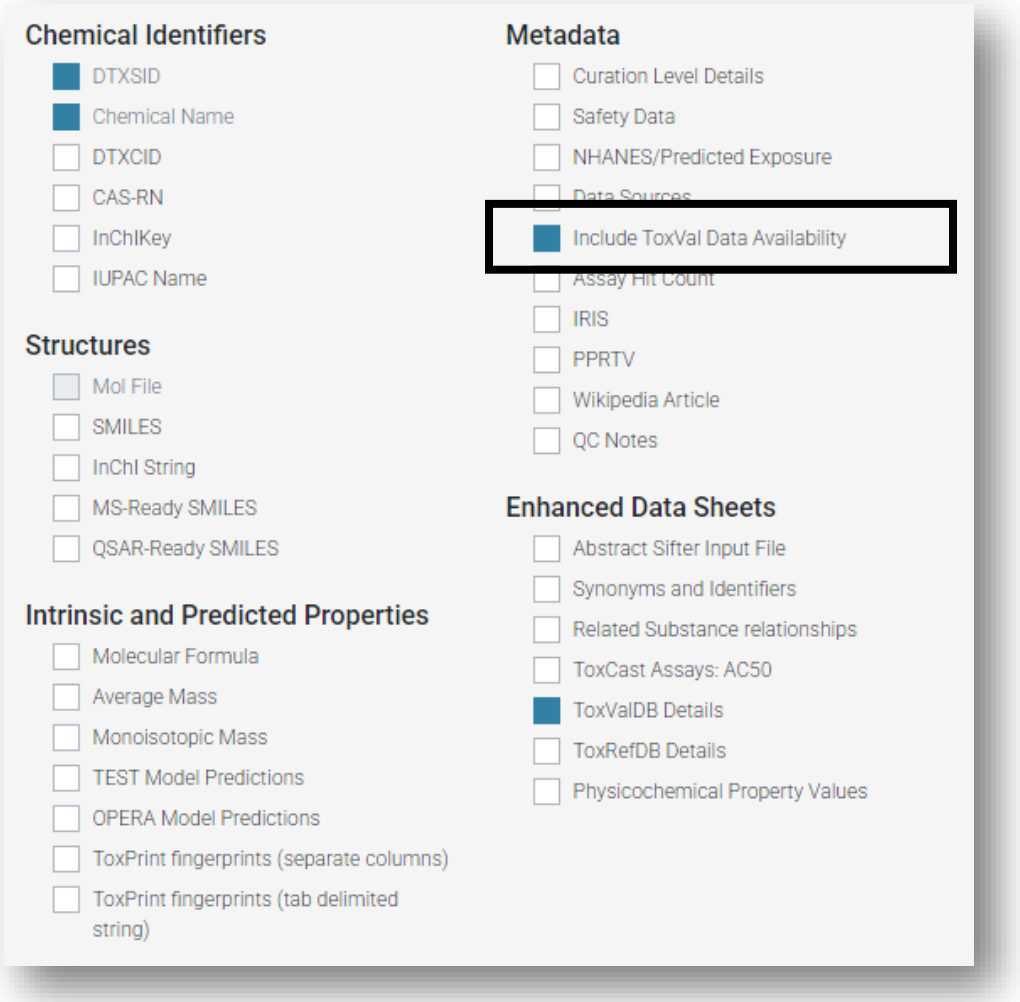
Database Access – CompTox Chemicals Dashboard Hazard Tab

- Live demo of hazard tab



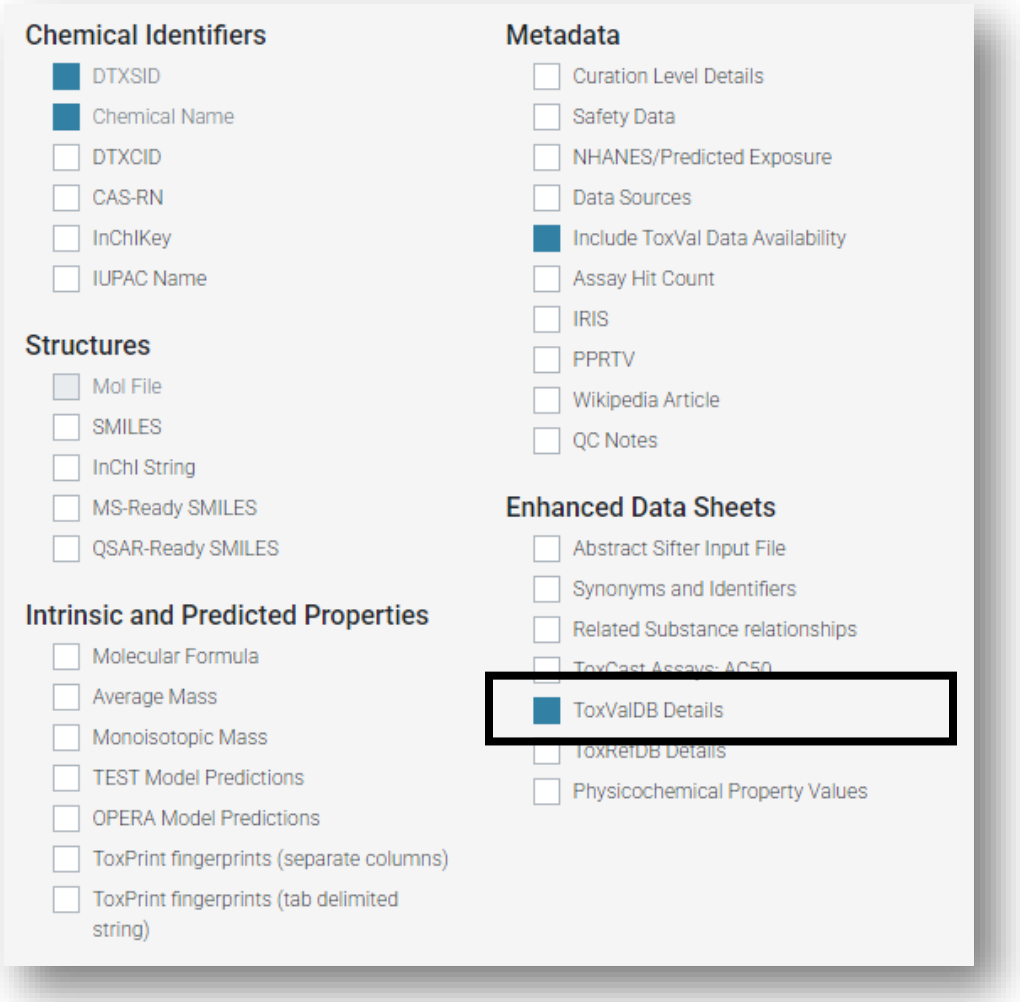
Database Access – CompTox Chemicals Dashboard Batch Search

- Metadata: Include ToxVal Data Availability
  - Provides binary Y/blank if hazard data are in the current Dashboard version of ToxValDB
  - Y is hyperlinked to Dashboard chemical page

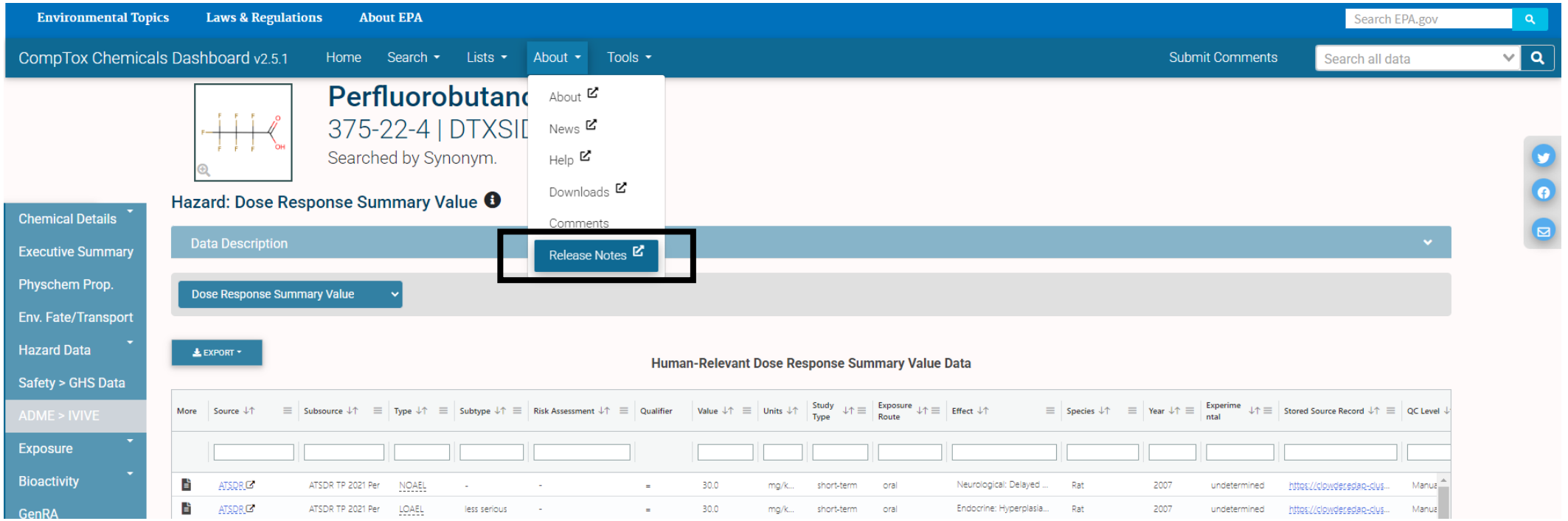


Database Access – CompTox Chemicals Dashboard Batch Search

- ToxValDB Details: Access to all ToxValDB data fields
  - Includes both standardized and original fields



Database Access – CompTox Chemicals Dashboard Version Information



Database Access – Data Downloads

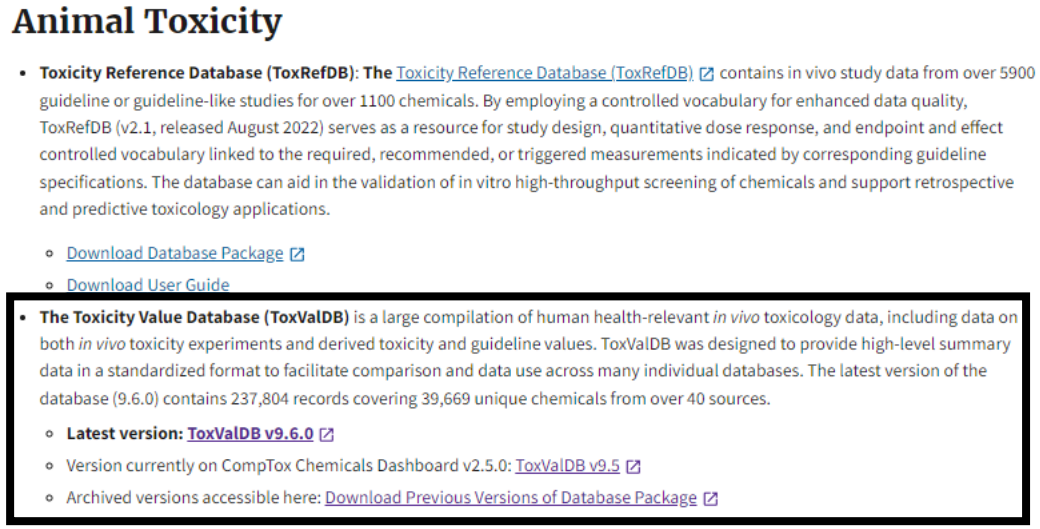
- Latest version of ToxValDB is v9.6.0
  - Includes additional record processing, deduplication, and quality control
- Download from US EPA Clowder Repository as a series of Excel files (one per source) and as a MySQL dump file

Downloadable Computational Toxicology Data

On this page:

High-Throughput Screening | Rapid Exposure and Dose Information | Animal Toxicity | ACToR | Ecotoxicology | Chemicals and Chemistry Data | CompTox Chemicals Dashboard | Virtual Tissues | Literature Mining

www.epa.gov/comptox-tools/downloadable-computational-toxicology-data



Animal Toxicity

- **Toxicity Reference Database (ToxRefDB)**: **The** Toxicity Reference Database (ToxRefDB) contains in vivo study data from over 5900 guideline or guideline-like studies for over 1100 chemicals. By employing a controlled vocabulary for enhanced data quality, ToxRefDB (v2.1, released August 2022) serves as a resource for study design, quantitative dose response, and endpoint and effect controlled vocabulary linked to the required, recommended, or triggered measurements indicated by corresponding guideline specifications. The database can aid in the validation of in vitro high-throughput screening of chemicals and support retrospective and predictive toxicology applications.
  - Download Database Package
  - Download User Guide
- **The Toxicity Value Database (ToxValDB)** is a large compilation of human health-relevant *in vivo* toxicology data, including data on both *in vivo* toxicity experiments and derived toxicity and guideline values. ToxValDB was designed to provide high-level summary data in a standardized format to facilitate comparison and data use across many individual databases. The latest version of the database (9.6.0) contains 237,804 records covering 39,669 unique chemicals from over 40 sources.
  - **Latest version: ToxValDB v9.6.0**
  - Version currently on CompTox Chemicals Dashboard v2.5.0: ToxValDB v9.5
  - Archived versions accessible here: Download Previous Versions of Database Package

Please Share Your Feedback!

Contributors (Version 9.5+):

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Please reach out with questions or comments

- Chelsea Weitekamp – weitekamp.chelsea@epa.gov
- "Submit Comments" button on the CompTox Chemicals Dashboard

Learn More at an SOT Satellite Meeting

- Society of Toxicology annual meeting in Orlando, FL
- *Thursday, March 20, 2025, 12pm–4:30pm*
- U.S. Environmental Protection Agency's CompTox Chemicals Dashboard and Associated Biological Activity and Hazard Data
  - Nisha Sipes (Chair); Scarlett VanDyke (Co-Chair)
- Speakers:
  - CompTox Chemicals Dashboard: Nisha Sipes
  - Toxicity Forecaster: Katie Paul Friedman
  - Toxicity Values Database: Chelsea Weitekamp
  - Toxicity Reference Database: Madison Feshuk

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Creating a Safer and Healthier World by Advancing the Science and Increasing the Impact of Toxicology