

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.

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

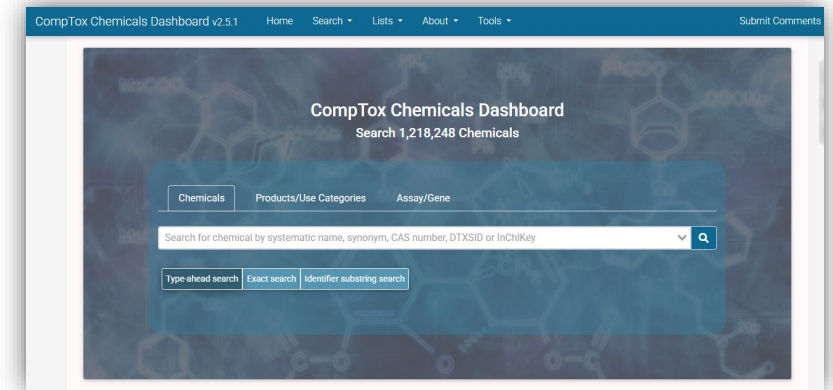
Nisha S. Sipes

US EPA Office of Research and Development

January 23, 2025

CompTox Chemicals Dashboard

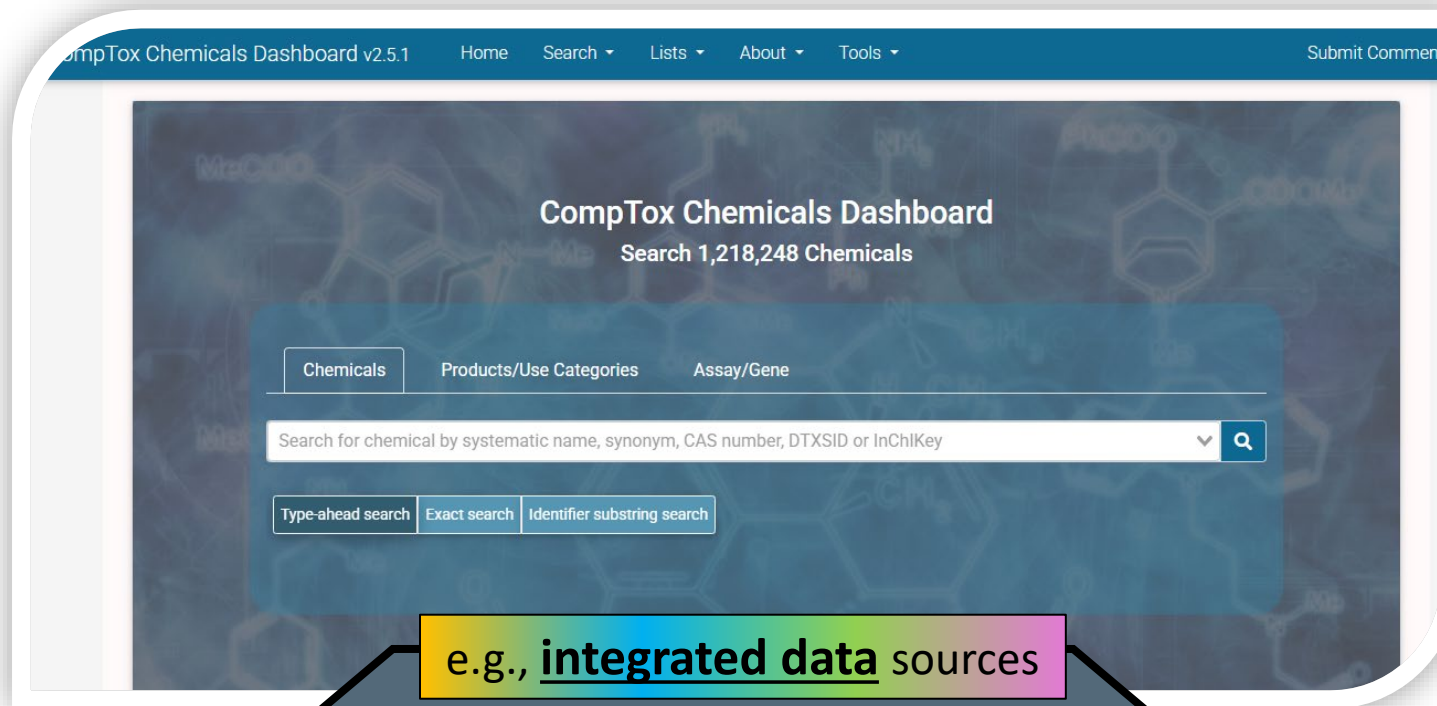
- **Centralized location** for publicly available chemical toxicity data
- Combination of existing legacy, and high throughput and predictive model data
- Publicly accessible, curated, and periodically updated
- Supports EPA and partner decision making
 - e.g., Well-studied chemicals: data can be found 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



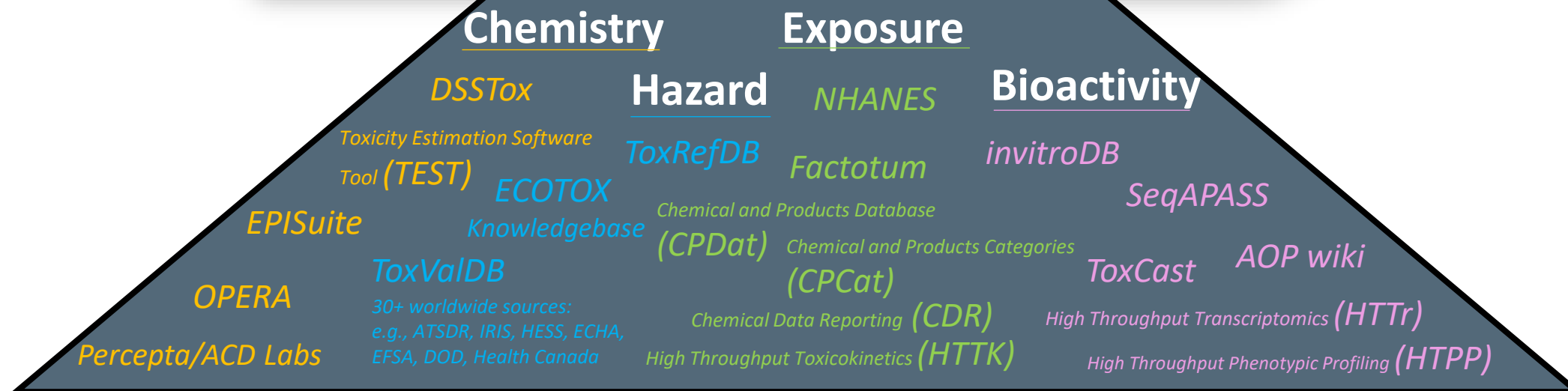
<https://comptox.epa.gov/dashboard/>

currently >1.2 million chemicals

***Updated January 13, 2025**



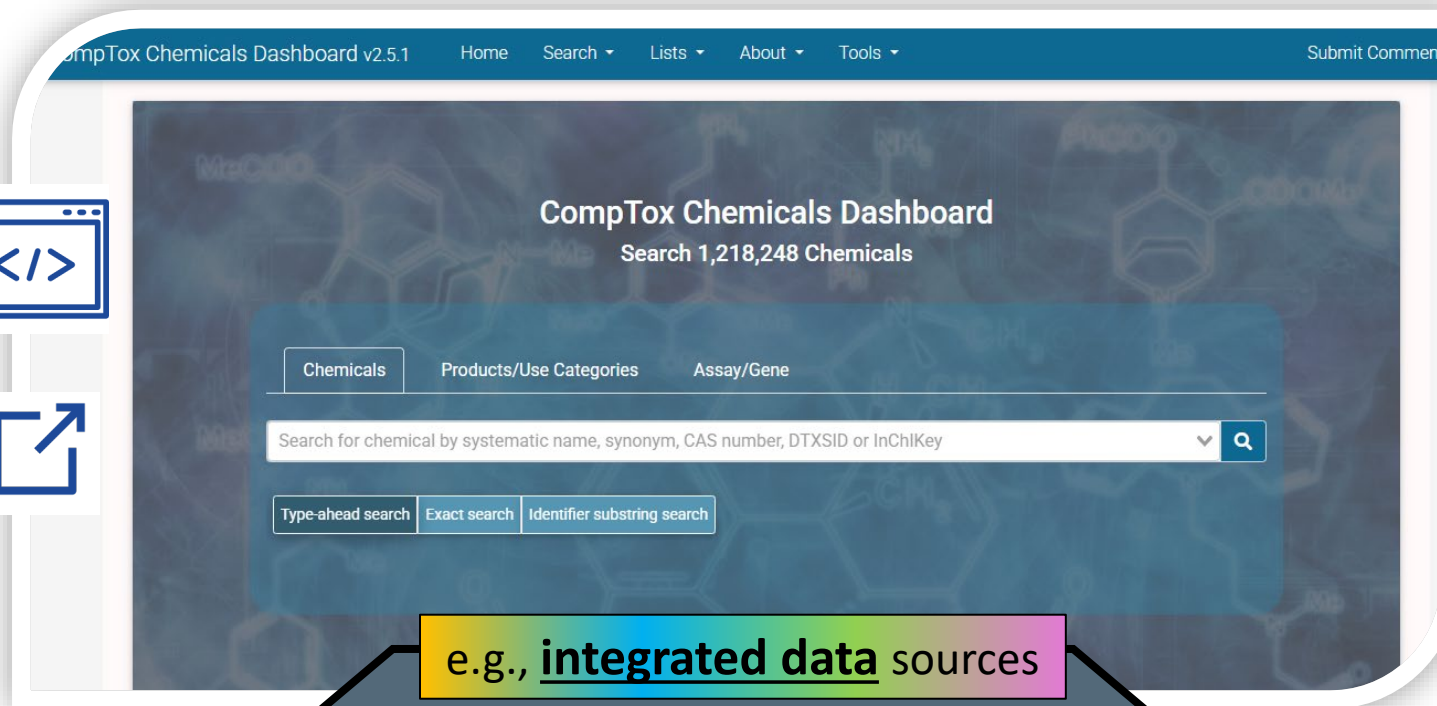
e.g., integrated data sources



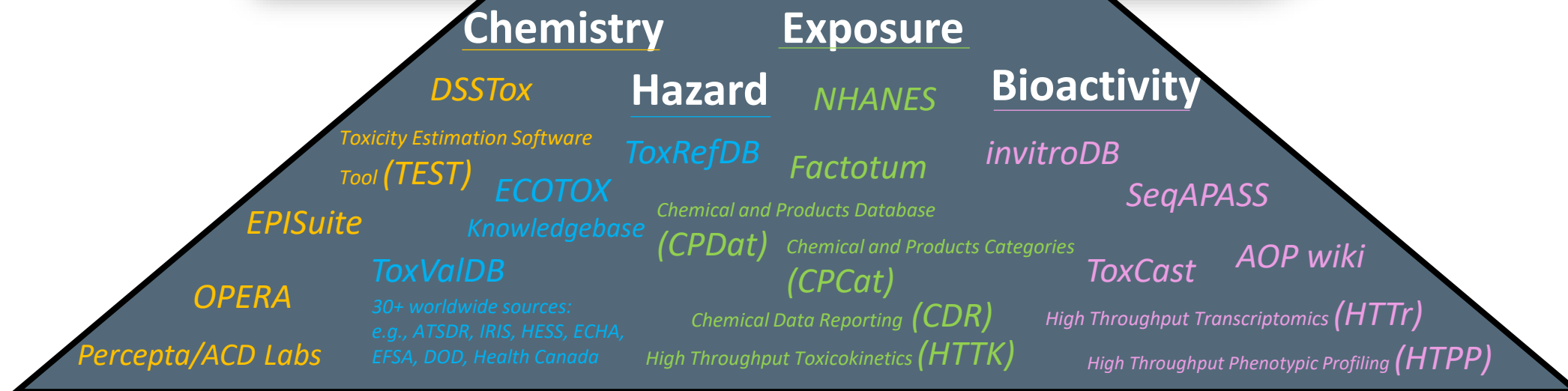
Embedded websites
using iframes



Links to websites



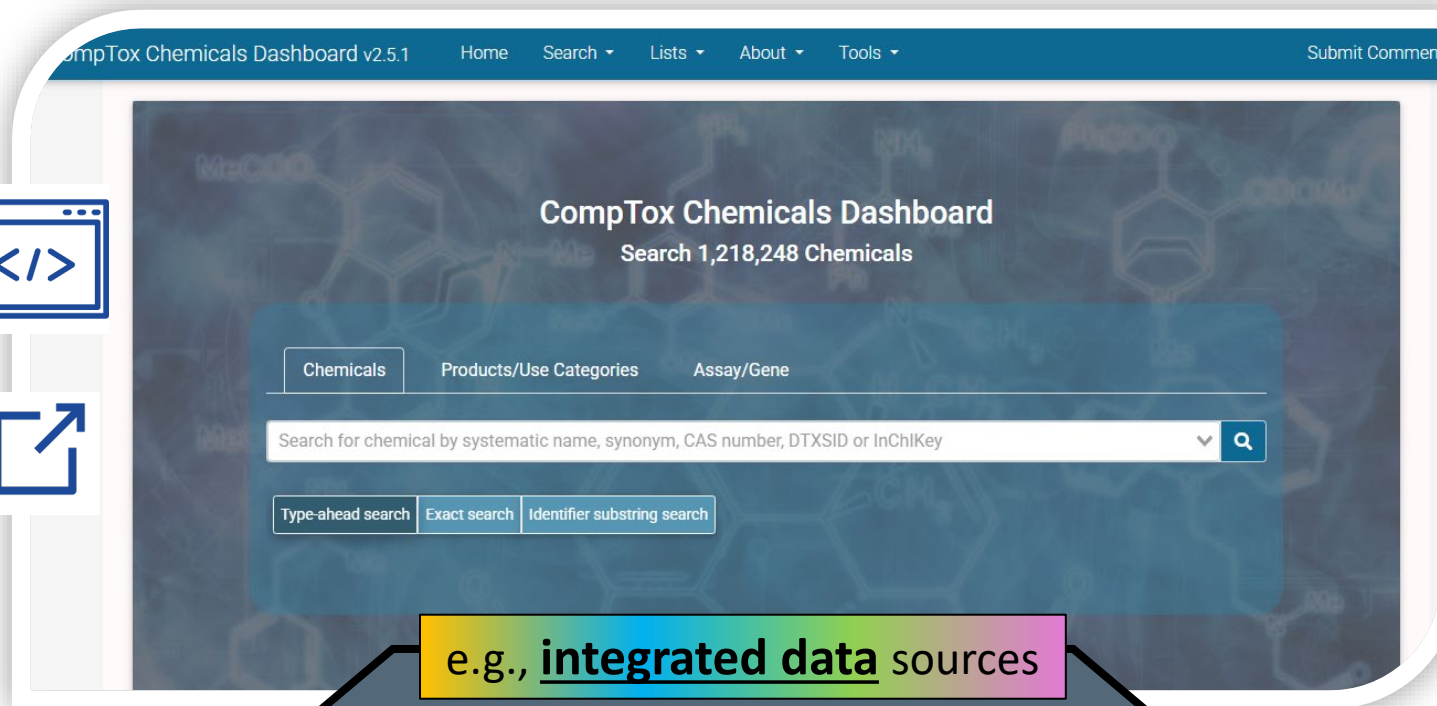
e.g., integrated data sources



Embedded websites
using iframes



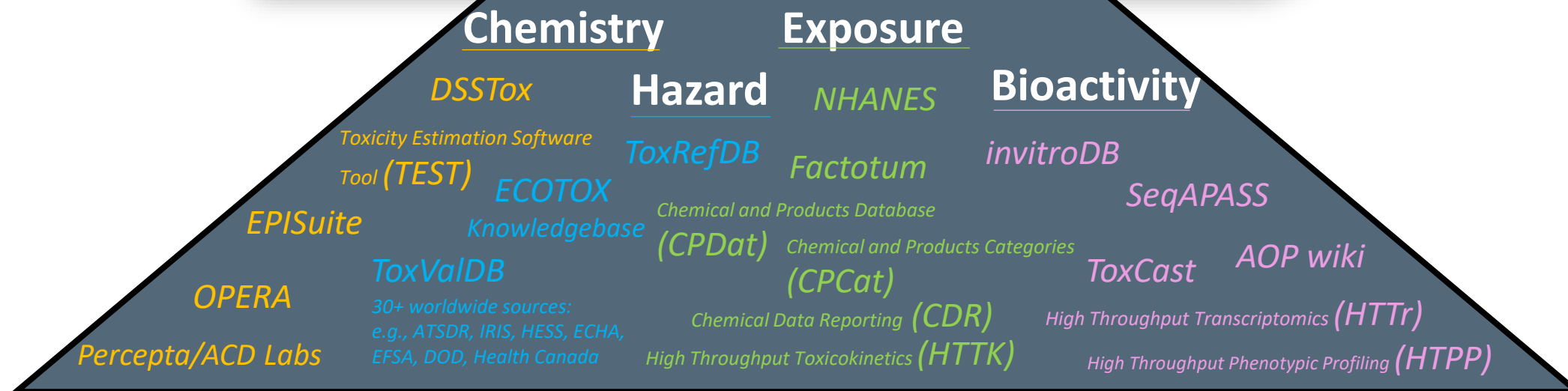
Links to websites



Links to EPA webtools

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

e.g., integrated data sources



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**

<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 <i>Related: Database, HTTP</i>
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 <i>Related: ToxRefDB, ToxValDB, Database</i>
					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](#)

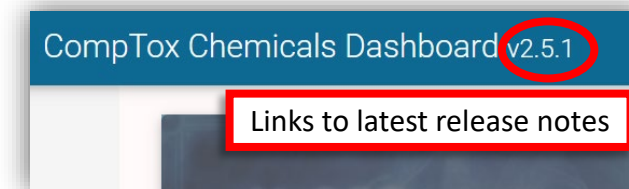
Related Resources

- [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>

CompTox Chemicals Dashboard v2.5.0 Home Search Lists About Tools Submit Comments PFOS DTXSID3031864

Perfluorooctanesulfonic acid

1763-23-1 | DTXSID3031864
Searched by Synonym

Bioactivity - HTPP Summary ⓘ

Assay Description

Assay Description

HTPP Bioactivity High-throughput phenotypic profiling (HTPP) with the Cell Painting assay Nyffeler et al. 2020, (PMID: 31899216) uses high content imaging of cells labeled with organelle-targeting fluorophores to profile chemical effects on cell morphology. The information displayed in this tab are results from global, category-level, and feature-level modeling of HTPP data as described in Nyffeler et al. 2021 (PMID: 32862757). Endpoints were subject to concentration-response modeling using the topleft2 package described in Sheffield et al. 2021 (PMID: 34791027).

Category Level Summary Points are plotted according to the potency (i.e. BMD, x-axis) and efficacy (i.e. Top/Cutoff, y-axis) determined from concentration-response modeling of global or category-level endpoints based on Mahalanobis distance modeling approaches described in Nyffeler et al. 2021. For each Sample ID × cell type × seeding density × exposure duration combination tested, up to 49 category-level endpoints and 1 global endpoint may be displayed on this plot if active (i.e. a hit). An example of a category-level endpoint is Mito_Texture_Cytoplasm, a latent variable measuring the texture of mitochondrial labeling in the cytoplasm compartment of the cells. If the global endpoint was active for a Sample ID × cell type × seeding density × exposure duration combination, the BMD is displayed as a large purple point. In addition, if category-level endpoint(s) for a Sample ID × cell type × seeding density × exposure duration combination were affected, the BMD of the most-sensitive category is also displayed as a large point color-coded to match the fluorescent channel / organelle from which it was derived. Points are shape coded based the compartment from which they were derived (i.e. cytoplasm, nuclei, membrane, ring or cell). Mouse over each point to display metadata and modeling results associated with that point. Click the cell type, exposure duration and/or seeding density checkboxes to display data associated with those conditions.

Feature Level Summary Points are plotted according to the potency (i.e. BMD, x-axis) and efficacy (i.e. Top/Cutoff, y-axis) determined from concentration-response modeling of normalized and z-scaled feature-level data. Up to 1300 feature-level endpoints may be displayed on this plot if active for each Sample ID × cell type × seeding density × exposure duration combination tested. If present on the graph, large purple points represent the global BMD and large not purple points represent the most sensitive category-level BMD for a given Sample ID × cell type × seeding density × exposure duration combination. Points are shape coded based the compartment from which they were derived (i.e. cytoplasm, nuclei, membrane, ring or cell). Mouse over each point to display metadata and modeling results associated with that point. Click the cell type, exposure duration and/or seeding density checkboxes to display data associated with those conditions.

Toggle Switches Set to No Filtering as the Default View

Global-, category-, and feature-level mapping information can be [found here](#)

Bioactivity

ToxCast: Summary

HTTr: Summary

HTPP: Summary

PubChem

ToxCast: Models

High Throughput Phenotypic Profiling (HTPP)

Bioactivity

ToxCast: Summary

HTTr: Summary

HTPP: Summary

PubChem

ToxCast: Models

New Toggle
Selections

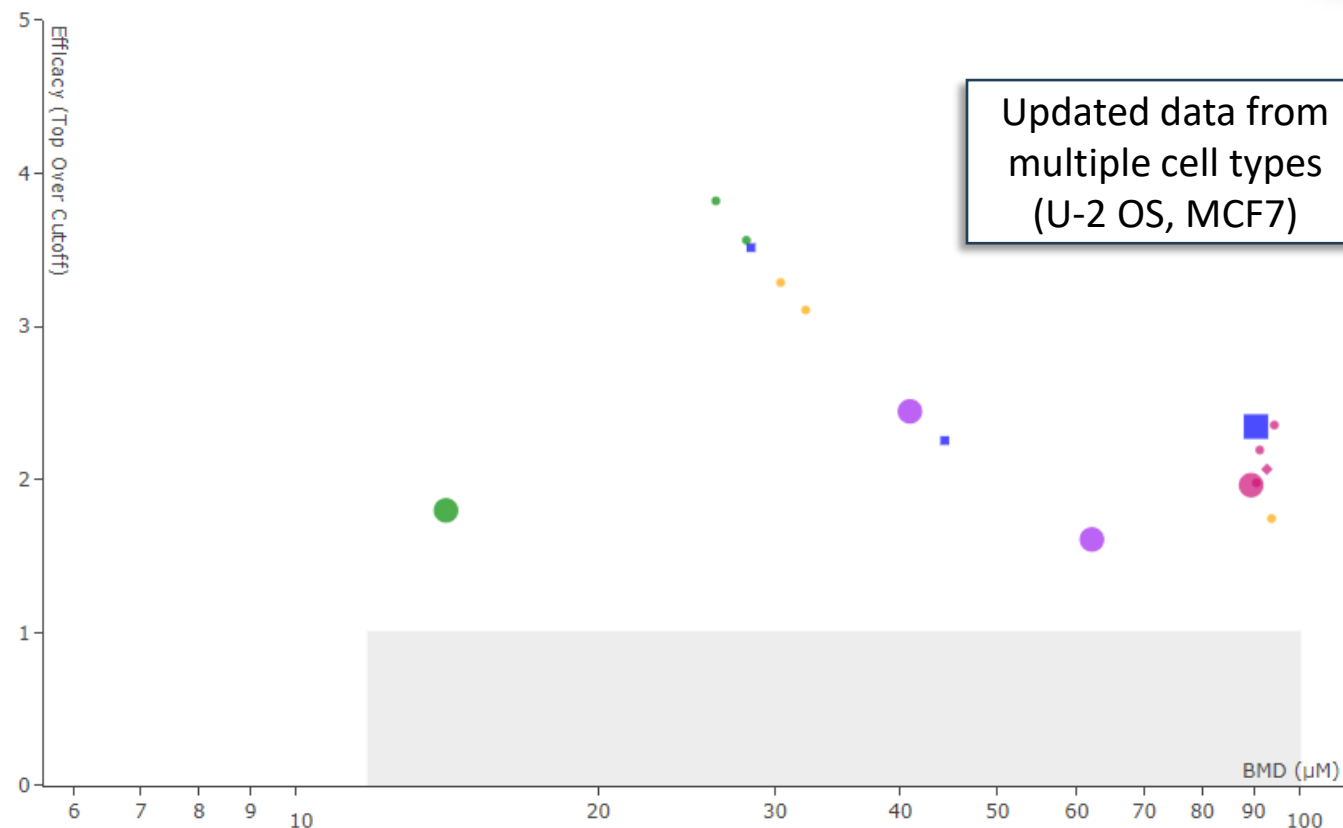
Updated
visuals

Cell Type
☐ MCF7 ☐ U-2 OS

Exposure Duration
☐ 24

Seeding Density
☐ 400 ☐ 2500 ☐ 3000

- AGP_Intensity_Cytoplasm
- AGP_Profile_Cytoplasm
- DNA_Profile_Nuclei
- DNA_Texture_Nuclei
- ER_Compactness_Cells
- ER_Intensity_Cytoplasm
- ER_Radial_Cells
- Mito_Intensity_Cytoplasm
- Mito_Profile_Cytoplasm
- Mito_Radial_Cells
- Mito_Texture_Cytoplasm
- Mito_Texture_Ring
- global



High Throughput Phenotypic Profiling (HTPP)

Bioactivity ▾

ToxCast: Summary

HTTr: Summary

HTPP: Summary

PubChem

ToxCast: Models


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

Factotum/CPDat/ChemExpoDB

CPDat 4.0.0-alpha.3 (March 2024)

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			

Exposure ▾

Product & Use Categories

Chemical Weight Fraction

Chemical Functional Use

New data

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)

Exposure

Product & Use Categories

Chemical Weight Fraction

Chemical Functional Use








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
<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	
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 Cleanse	Personal care:facial cleansing	Formulation	-	-	reported	Environme...	2

New data

Exposure - Collected and Predicted Data on Functional Use ⓘ

Search Reported

EXPORT

Collected Data On Functional Use ⓘ

Harmonized functional use ↓↑	Reported functional use ↓↑
Biocide	Antibacterial Agent
Biocide	antimicrobial
Biocide	biocide
Biocide	biocides > algicides & fungicides
Biocide	biocides / antimicrobial agents
Biocide	biocides > biocides, film protections
Biocide	cosmetic biocide
Deodorizer	deodorant
Deodorizer	Deodorant Agent

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>

Bioactivity

ToxCast: Summary

HTTr: Summary

HTPP: Summary

PubChem

ToxCast: Models

New data

Bioactivity Summary Grid										
<div>EXPORT</div> <div>Filter out non-representative sample (Repr.) results. Filter out 'background' from Intended Target Family.</div>										
	Name	Assay Lists	Details	SeqAPASS	Gene Symbol	AOP	Event	Repr. Plot	All Plots	Hit
										(1)
<input type="checkbox"/>	APR_HepG2_p53Act_24hr	-		NP_000537.3	TP53	-	-			Ac
<input type="checkbox"/>	CCTE_Shafer_MEA_acute_spik	-				-	-			Ac
<input type="checkbox"/>	ATG_chERa_XSP2	-			ESR1	-	-			Ac
<input type="checkbox"/>	TOX21_RORg_LUC_CHO_Anta	-		NP_005051.2	RORC	-	-			Ac
<input type="checkbox"/>	NVS_GPCR_hOpiate_mu	-		NP_000905.3	OPRM1	-	-			Ac
<input type="checkbox"/>	TOX21_SBE_BLA_Antagonist_c	-				-	-			Ac
<input type="checkbox"/>	TOX21_FXR_BLA_Antagonist_c	-				-	-			Ac
<input type="checkbox"/>	TOX21_RT_HEPG2_GLO_32hr	cytotoxicity burst				220	1393			Ac
<input type="checkbox"/>	TOX21_PR_BLA_Antagonist_vi	cytotoxicity burst				263	1771			Ac
<input type="checkbox"/>	LTEA_HepaRG_APOA5	-		NP_443200.2	APOA5	-	-			
<input type="checkbox"/>	BSK_LPS_MCSF	-		NP_000748.4	CSF1	-	-			
<input type="checkbox"/>	NVS_TR_gDAT	-			Slc6a3	-	-			Ac

Batch Search

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

Structures

☐ Mol File

☐ SMILES

☐ InChI String

☒ MS-Ready SMILES


☐ QSAR-Ready SMILES

Search ▾

Advanced Search

Batch Search

Structure Search (BETA)



	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	<chem>CC(C)(C1=CC=C(O)C=C1)C1=CC=C(O)C=C1</chem>	228.291	C15H16O2
3	atrazine	Approved Name	Atrazine	<chem>CCNC1=NC(NC(C)C)=NC(Cl)=N1</chem>	215.69	C8H14ClN5
4	triclosan	Approved Name	Triclosan	<chem>OC1=C(OC2=CC=C(Cl)C=C2Cl)C=CC(Cl)=C1</chem>	289.54	C12H7Cl3O2

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

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

1 Select Input Type(s)

☐ Substance Identifiers

☐ Chemical Name

☐ CASRN

☐ InChIKey

☐ DSSTox Substance ID

☐ DSSTox Compound ID

☒ InChIKey Skeleton

☐ MS-Ready Formula(e)

☐ Exact Formula(e)

☐ Monoisotopic Mass

Metadata

☐ Curation Level Details

☒ Safety Data

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

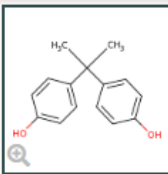
Hazard Data

Hazard

Cancer

Genotoxicity

Skin/Eye



Bisphenol A
80-05-7 | DTXSID7020182
Searched by Synonym

Hazard: Dose Response Summary Value ⓘ

Data Description

Categories have been updated

Dose Response Summary Value

Acute Exposure Guidelines

Mortality Response Summary Value

Media Exposure Guidelines

Dose Response Summary Value

Toxicity Value

Updated hover-over definitions

Submit Comments

Search all data

This toggle has been removed. Please refer to the ECOTOX Knowledge Base for ecology – relevant data <https://cfpub.epa.gov/ecotox>

☒ human ☐ eco

Updated metadata

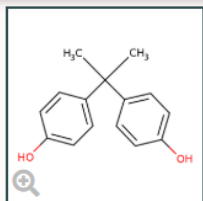
Human-Relevant Dose Response Summary Value Data

Source	Substance	Type	Subtype	Risk Assessment	Qualifier	Value	Units	Study Type	Exposure Route	Effect	Species	Year	Experimental	Stored Source Record	QC Level
EPA ECOTOX	EPA ORD	LOEL	-	-	=	200	mg/k...	subchronic	oral	Genetics: CYP19A1 mR...	Rat	2012	experimental	https://clowderedao-clus...	Data soun
EPA HAWC	-	LOEL	-	-	=	20.0	mg/k...	short-term	injection	uterus: uterine dry wei...	Rat	2002	experimental	https://clowderedao-clus...	Programm
EPA ECOTOX	EPA ORD	LOEL	-	-	=	0.500	mg	reproducti...	injection	Morphology: Weight	Rat	2003	experimental	https://clowderedao-clus...	Data soun
EPA ToxRefDB	-	LOAEL	-	-	=	160	mg/k...	reproducti...	oral	systemic: in life observa...	Rat	1985	experimental	https://clowderedao-clus...	Data soun

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



Bisphenol A

80-05-7 | DTXSID7020182

Searched by DTXSID7020182

Executive Summary

Quantitative Risk Assessment Values

- ✓ IRIS values available [link](#)
- ✗ No PPRTV values
- ✗ No EPA RSL values
- ✓ Minimum RfD:: 0.05 mg/kg-day [link](#)
- ✗ No RfC

Quantitative Hazard Values

- ✓ Minimum oral POD:: 0.609 mg/kg-day (-, oral) [link](#)
- ✗ No inhalation POD values

Cancer Information

- ✗ No cancer slope factor
- ✗ No cancer unit risk values
- ✗ No cancer data
- ✓ Genotoxicity:: negative [link](#)

Regional Screening ?

Class ↓↑	Risk Level	Value 2 ↑
screening level (tap water) (mg/L)	THQ = 0.1	7.70e-2
risk-based SSL, groundwater (mg/kg)	THQ = 0.1	5.80
screening level (residential soil) (mg/kg soil)	THQ = 0.1	320
screening level (industrial soil) (mg/kg soil)	THQ = 0.1	4.10e+3
screening level (tap water) (mg/L)	THQ = 1	0.770
risk-based SSL, groundwater (mg/kg)	THQ = 1	58.0
screening level (residential soil) (mg/kg soil)	THQ = 1	3.20e+3
screening level (industrial soil) (mg/kg soil)	THQ = 1	4.10e+4

Regional
Screening table

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

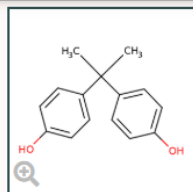
Hazard Data

Hazard

Cancer

Genotoxicity

Skin/Eye



Bisphenol A

80-05-7 | DTXSID7020182

Searched by DTXSID7020182

Hazard Data - Genotoxicity

New

EXPORT

Genotoxicity Summary

New

Reports Positive ↓↑	Reports Negative ↓↑	Reports Other ↓↑	Genotox Call ↓↑	AMES ↓↑	Micronucleus ↓↑
0	3	0	negative	false	negative

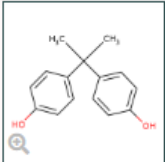
EXPORT

Genotoxicity Details

Source ↓↑	Assay Category ↓↑	Assay Type ↓↑	Metabolic Activation	Species ↓↑	Strain ↓↑	Assay Result ↓↑	Year ↓↑
NTP	in vivo	in vivo comet (rat) ma...		Not specified		negative	
NTP	in vitro	Ames bacterial revers...		Not specified		negative	

ToxValDBv9.5 (Skin/Eye data)

- New GLP and Authority columns
- Updated source link

 **Bisphenol A**
80-05-7 | DTXSID7020182
Searched by DTXSID7020182

Skin/Eye ⓘ

Search Skin/Eye

EXPORT

Skin/Eye **New**

Source	Study Type	Species	Reliability	GLP	Authority
<input type="checkbox"/> ECHA CLP	-	-	-		Authoritative
<input type="checkbox"/> ECHA CLP	-	-	-		Authoritative
<input type="checkbox"/> ECHA eChemPor...	skin sensitization	mouse	1 (reliable without restriction)	yes	Screening
<input type="checkbox"/> ECHA eChemPor...	skin sensitization	mouse	1 (reliable without restriction)	yes	Screening

Search...

- ☒ Source
- ☐ RECORD_URL
- ☒ Study Type
- ☒ Species
- ☒ Reliability
- ☒ GLP
- ☒ Authority
- ☒ Strain
- ☒ Endpoint

nmri skin sensitisation: in vivo (non-LLNA)

Hazard Data

- Hazard
- Cancer
- Genotoxicity
- Skin/Eye**

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



Efforts include many more than who are shown here

Many external collaborators provided data & links

EPA/ORD/Center for Computational Toxicology and Exposure

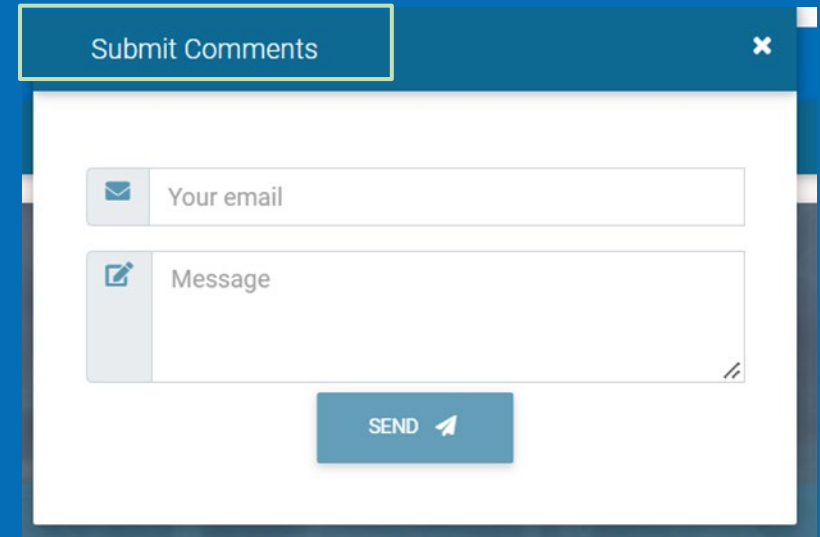
We value your feedback!

Nisha S. Sipes, PhD

Assistant Center Director

US EPA ORD Center for
Computational Toxicology and Exposure

sipes.nisha@epa.gov



The screenshot shows a 'Submit Comments' modal window. It has a title bar with the text 'Submit Comments' and a close button (X). The form contains two input fields: 'Your email' with an envelope icon and 'Message' with a pencil icon. Below the fields is a 'SEND' button with a paper plane icon.

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



Updates to the Toxicity Values Database, ToxValDB

Chelsea Weitekamp
US EPA, Office of Research and Development
Center for Computational Toxicology and Exposure

January 23, 2025
Computational Toxicology and Exposure Communities of Practice

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

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

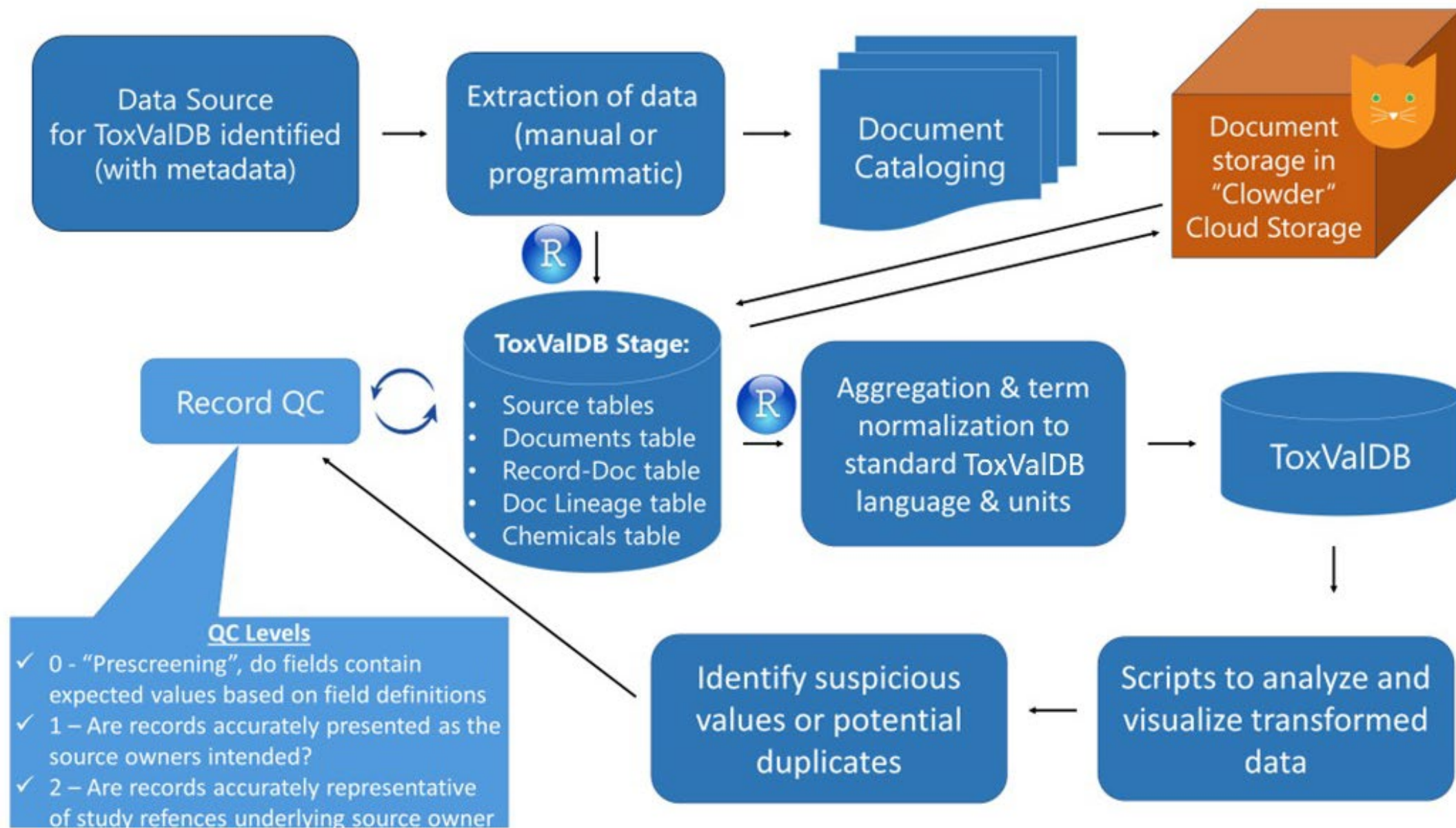
Major Updates in Version 9.5+

- 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



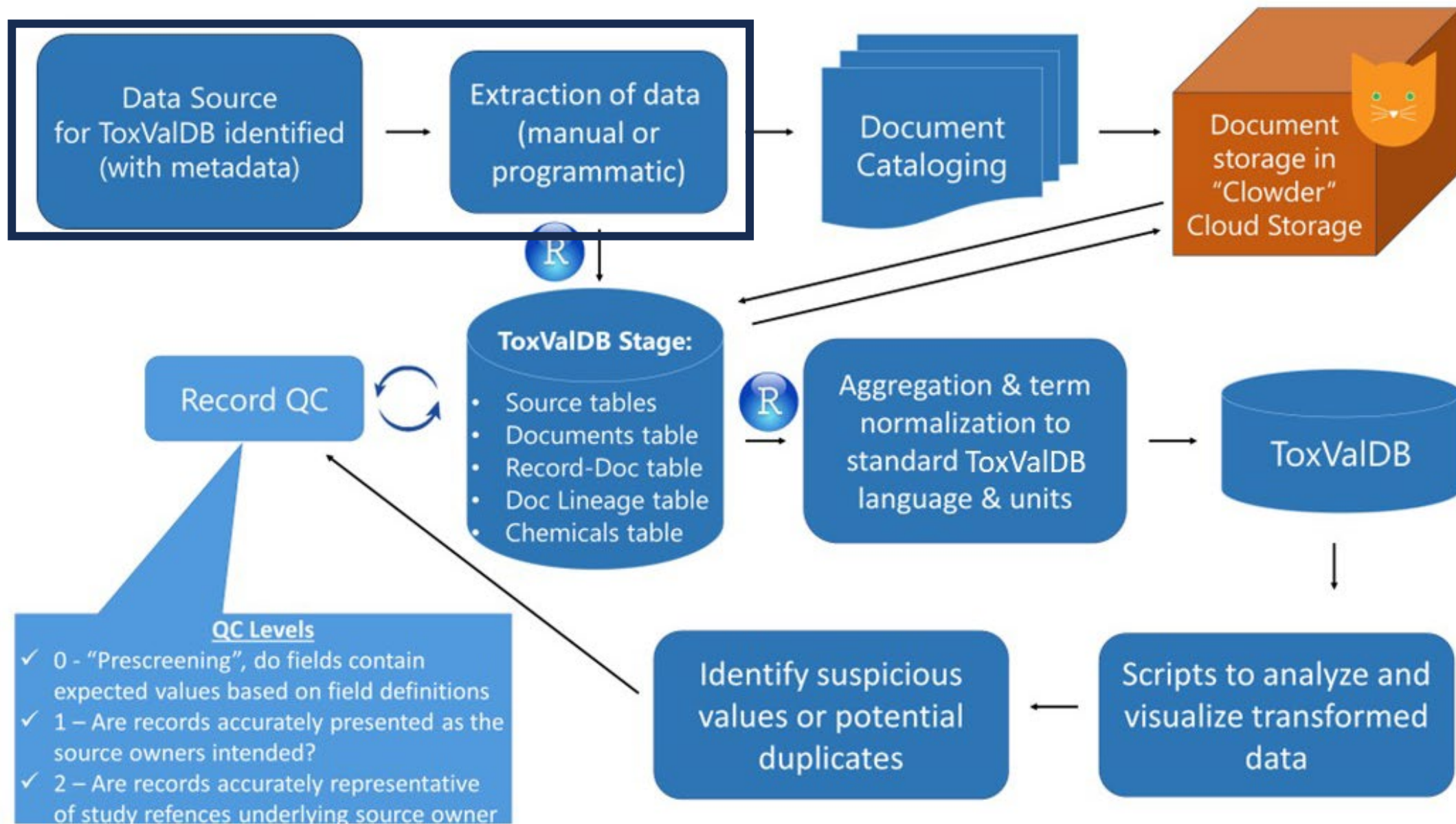
Database Development

- 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*

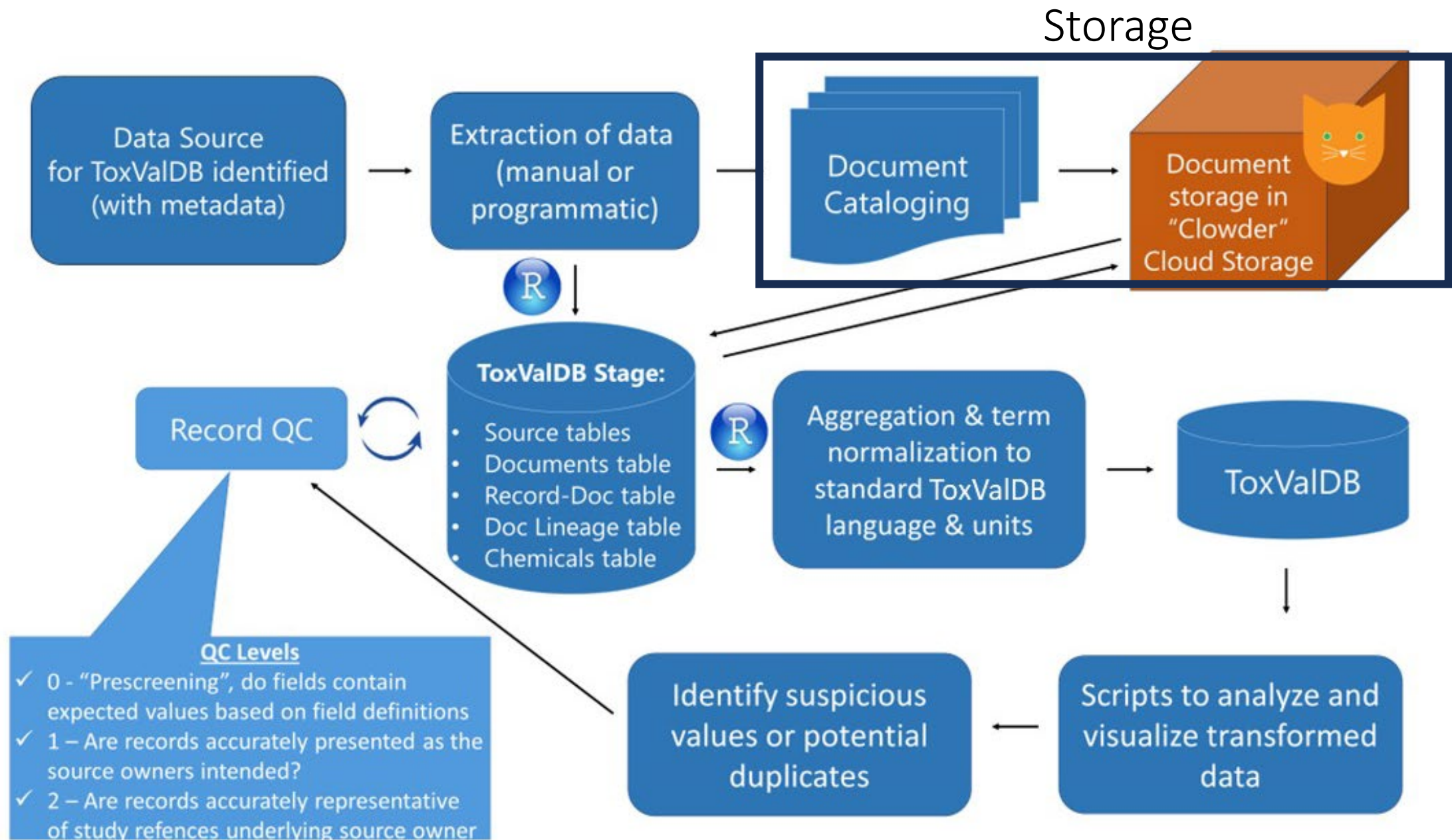
Data Curation – Source Identification

- 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

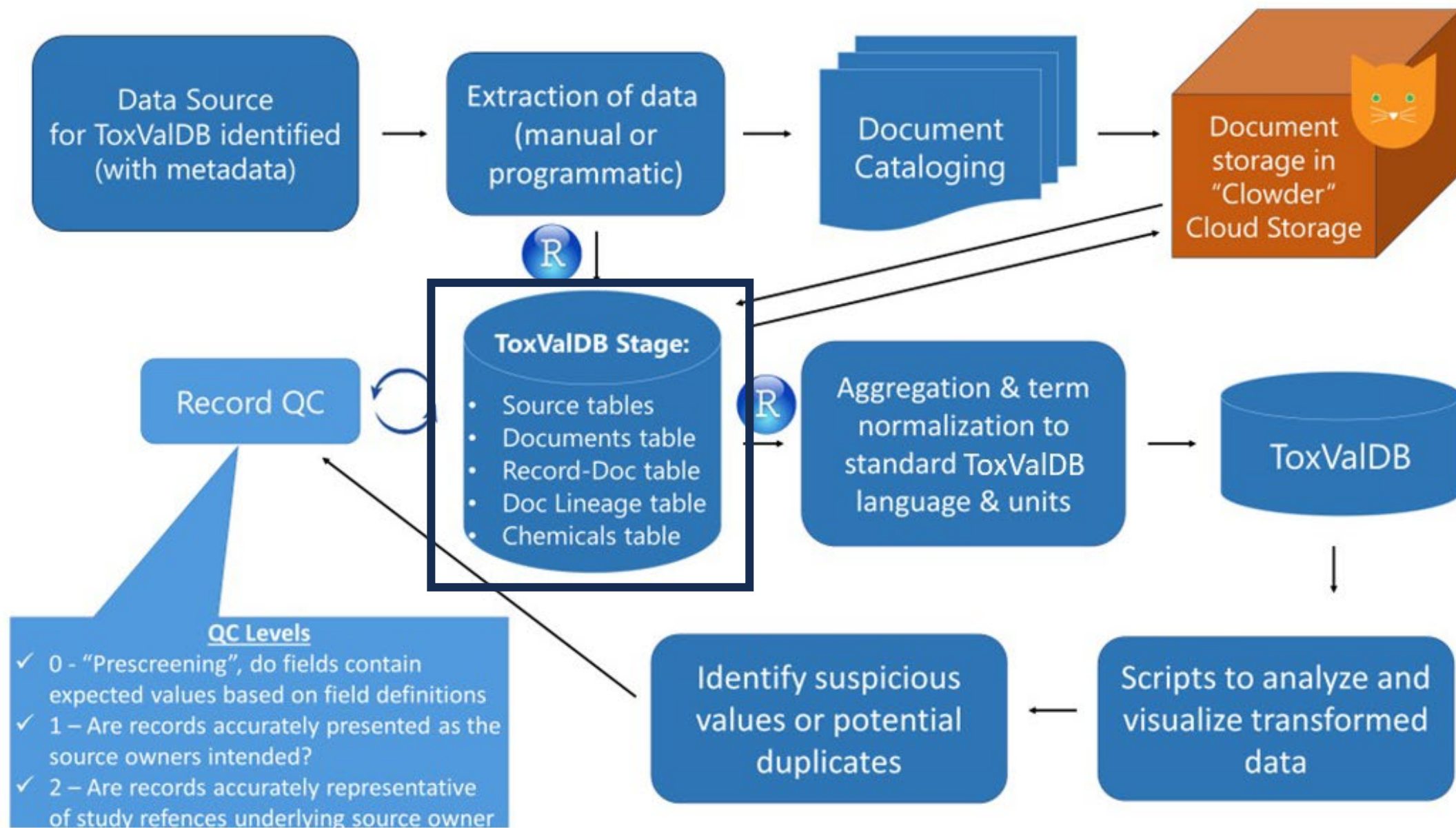
- Programmatically curated
 - Structured, machine-readable source data
 - Custom script is developed for each source that follows a standard template and uses common, generic functions when possible
- Manually curated
 - Complex, text-based, unstructured data
 - Expert and trained curators manually extract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



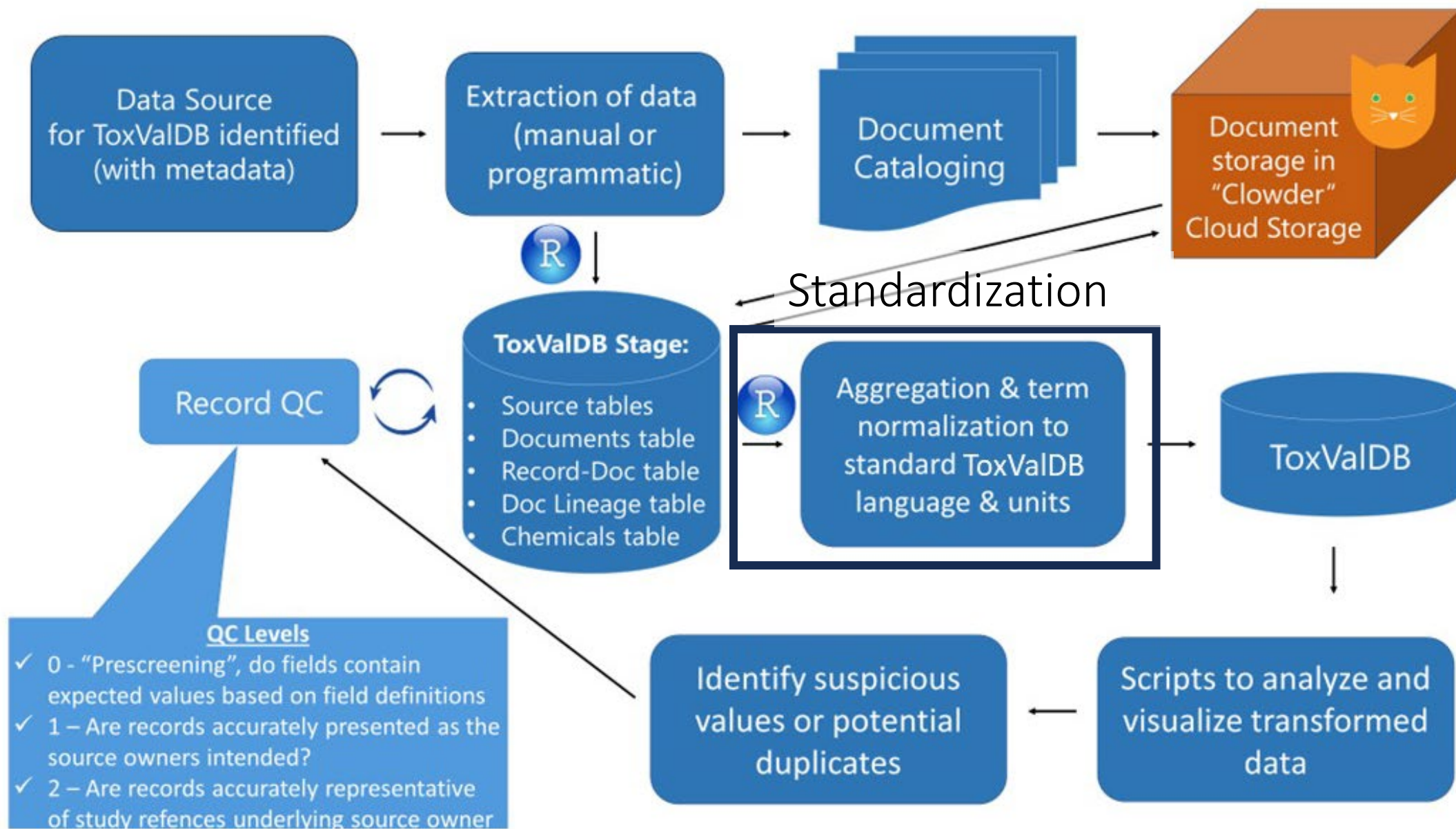
Wall et al., *in prep*

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



Wall et al., *in prep*



Wall et al., *in prep*

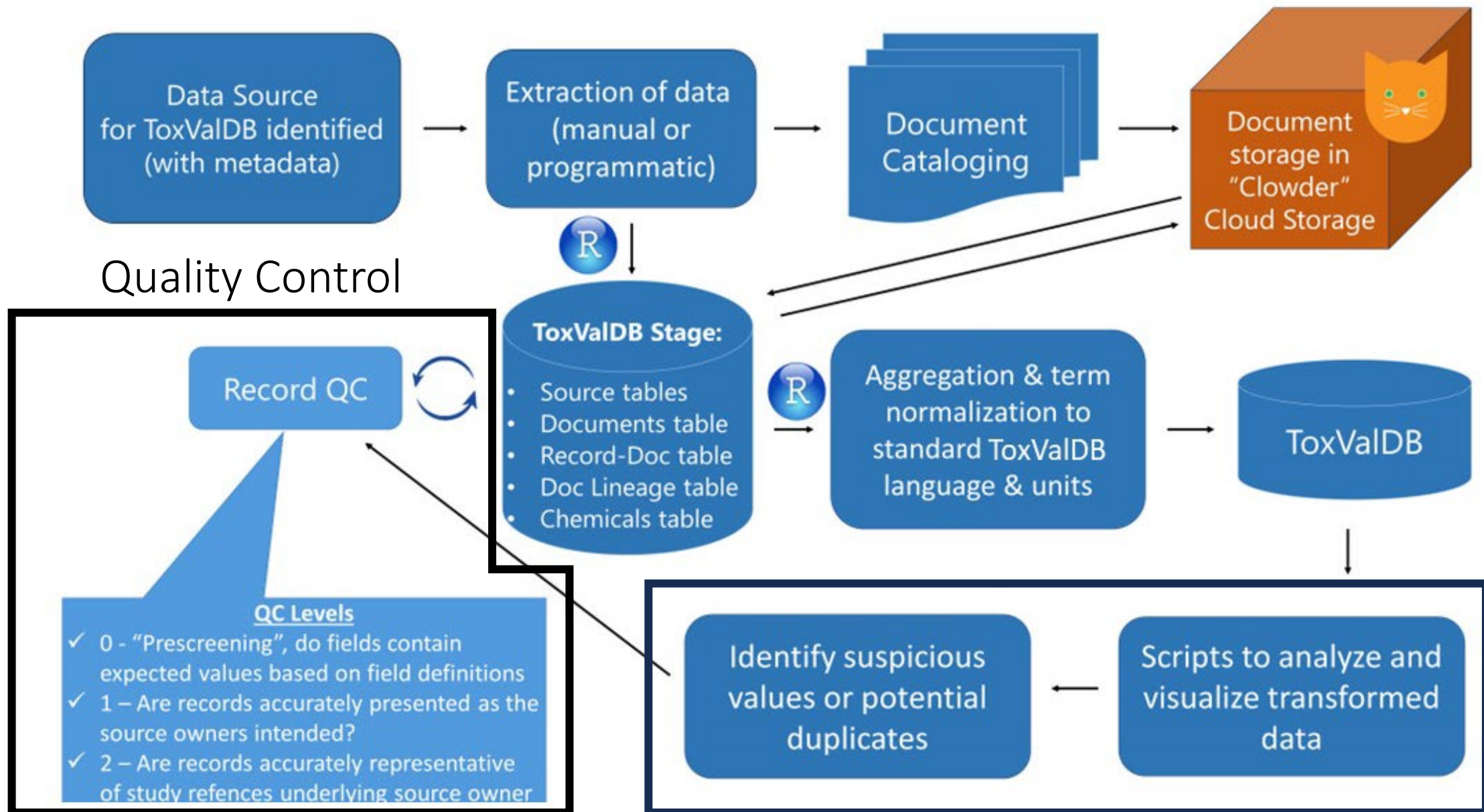
Standardization Steps

- 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/m³ 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

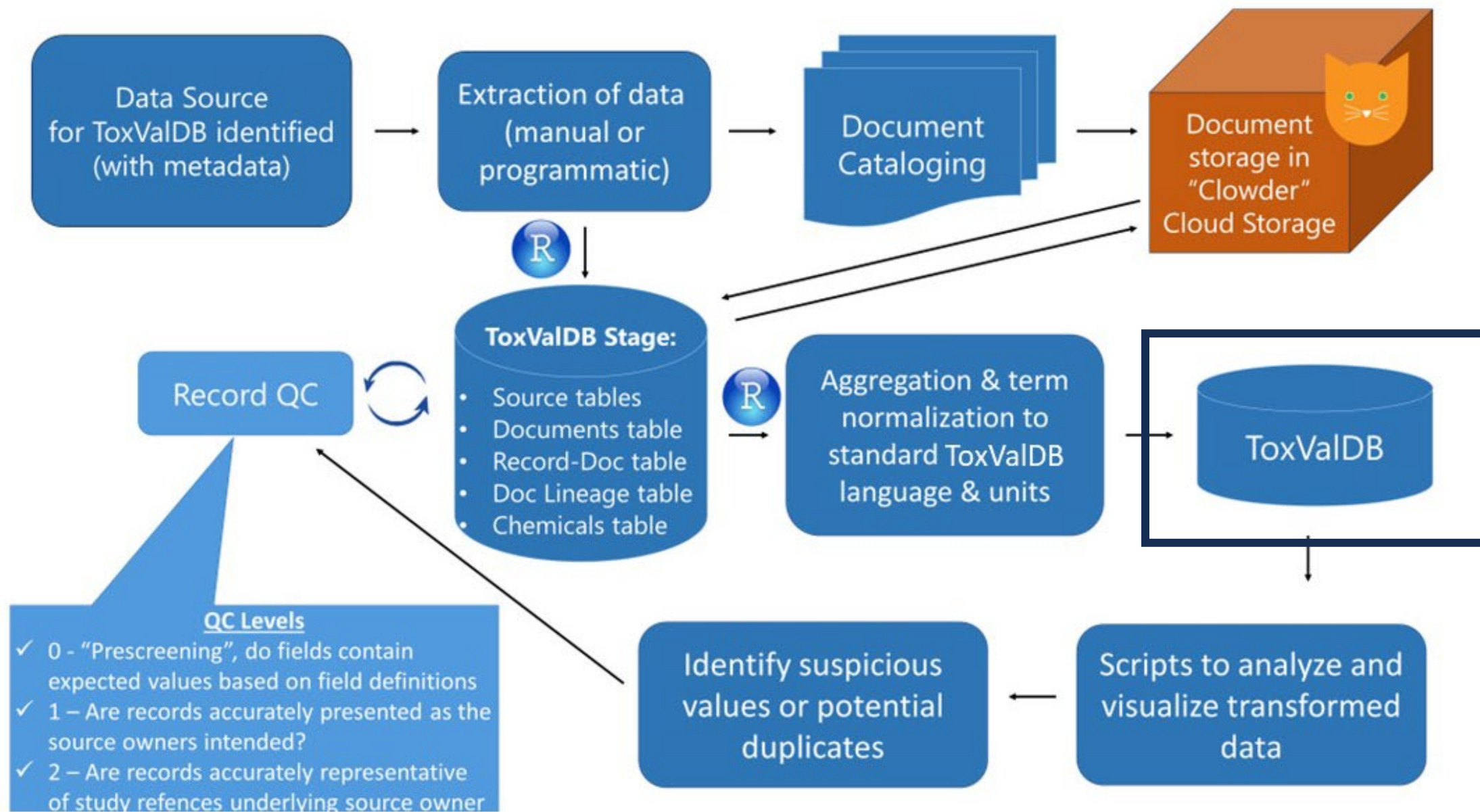
BMDL = Benchmark Dose Level; NOAEL = No Observed Adverse Effect Level; LD = Lethal Dose; RfD = Reference Dose; MRL = Minimal Risk Level; MCL = Maximum Contaminant Level; MEG = Military Exposure Guideline; AEGL = Acute Exposure Guideline Level; PAC = Protective Action Criteria



Wall et al., *in prep*

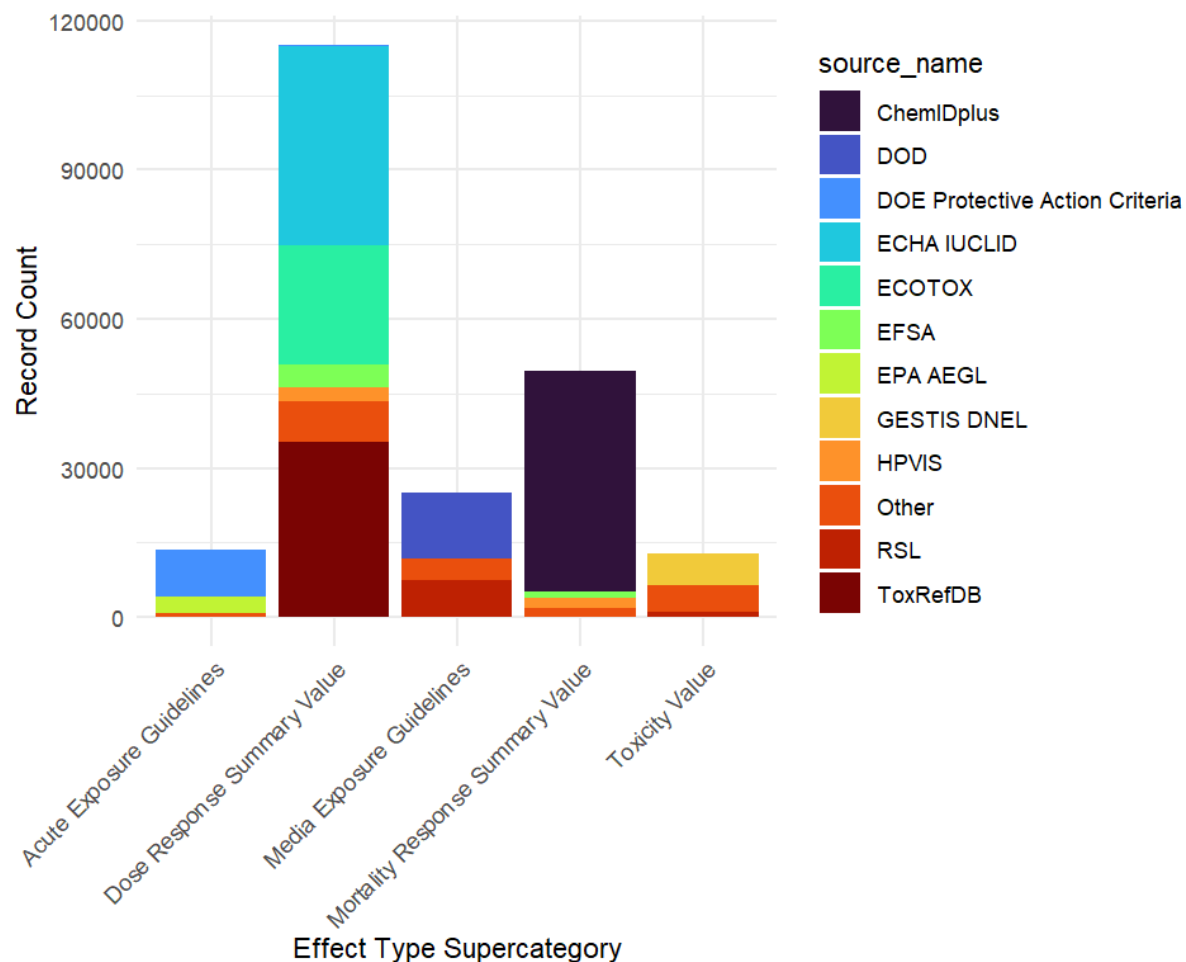
Quality Control

- 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: $\geq 10\%$ of records
 - Manually extracted sources: $\geq 20\%$ 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.



Wall et al., *in prep*

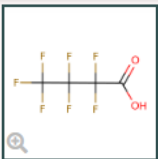
Sources in ToxValDB



- 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](#)



Perfluorobutanoic acid
375-22-4 | DTXSID4059916
Searched by Synonym

Hazard: Toxicity Value ⓘ

Data Description ▾

Toxicity Value ▾

EXPORT ▾

Human-Relevant Toxicity Value Data

More	Source	Subsource	Type	Subtype	Risk Assessment	Qualifier	Value	Units	Study Type	Exposure Route	Effect	Species	Year	Experimental	Stored Source Record	QC Level
	EPA IRIS	IRIS Summary	RfD	subchronic	Non-cancer	=	6.00e-3	mg/k...	Toxicity Val...	oral	Developmental dela...	Human	-	not experime...	https://clowderedap-clus...	Manually extracted f...
	EPA IRIS	IRIS Summary	RfD	chronic	Non-cancer	=	1.00e-3	mg/k...	Toxicity Val...	oral	Increased hepatocell...	Human	-	not experime...	https://clowderedap-clus...	Manually extracted f...

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

The screenshot displays the 'Batch Search' interface of the CompTox Chemicals Dashboard. It is organized into several sections with checkboxes for selecting search criteria:

- Chemical Identifiers:** Includes checkboxes for DTXSID, Chemical Name, DTXCID, CAS-RN, InChIKey, and IUPAC Name. 'Chemical Name' is selected.
- Structures:** Includes checkboxes for Mol File, SMILES, InChI String, MS-Ready SMILES, and QSAR-Ready SMILES.
- Intrinsic and Predicted Properties:** Includes checkboxes for Molecular Formula, Average Mass, Monoisotopic Mass, TEST Model Predictions, OPERA Model Predictions, ToxPrint fingerprints (separate columns), and ToxPrint fingerprints (tab delimited string).
- Metadata:** Includes checkboxes for Curation Level Details, Safety Data, NHANES/Predicted Exposure, Data Sources, Include ToxVal Data Availability (highlighted with a black box and selected), Assay Hit Count, IRIS, PPRTV, Wikipedia Article, and QC Notes.
- Enhanced Data Sheets:** Includes checkboxes for Abstract Sifter Input File, Synonyms and Identifiers, Related Substance relationships, ToxCast Assays: AC50, ToxValDB Details (selected), ToxRefDB Details, and Physicochemical Property Values.

Database Access – CompTox Chemicals Dashboard Batch Search

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

The screenshot displays the 'Batch Search' interface of the CompTox Chemicals Dashboard. It features several sections of filters, each with a title and a list of options, some of which are selected with a blue square icon.

- Chemical Identifiers**
 - ☒ DTXSID
 - ☒ Chemical Name
 - ☐ DTXCID
 - ☐ CAS-RN
 - ☐ InChIKey
 - ☐ IUPAC Name
- Structures**
 - ☐ Mol File
 - ☐ SMILES
 - ☐ InChI String
 - ☐ MS-Ready SMILES
 - ☐ QSAR-Ready SMILES
- Intrinsic and Predicted Properties**
 - ☐ Molecular Formula
 - ☐ Average Mass
 - ☐ Monoisotopic Mass
 - ☐ TEST Model Predictions
 - ☐ OPERA Model Predictions
 - ☐ ToxPrint fingerprints (separate columns)
 - ☐ ToxPrint fingerprints (tab delimited string)
- Metadata**
 - ☐ Curation Level Details
 - ☐ Safety Data
 - ☐ NHANES/Predicted Exposure
 - ☐ Data Sources
 - ☒ Include ToxVal Data Availability
 - ☐ Assay Hit Count
 - ☐ IRIS
 - ☐ PPRTV
 - ☐ Wikipedia Article
 - ☐ QC Notes
- Enhanced Data Sheets**
 - ☐ Abstract Sifter Input File
 - ☐ Synonyms and Identifiers
 - ☐ Related Substance relationships
 - ☐ ToxCast Assays: AC50
 - ☒ ToxValDB Details
 - ☐ ToxRefDB Details
 - ☐ Physicochemical Property Values

Database Access – CompTox Chemicals Dashboard Version Information

Environmental Topics Laws & Regulations About EPA Search EPA.gov

CompTox Chemicals Dashboard v2.5.1 Home Search Lists About Tools Submit Comments Search all data

Perfluorobutanoic acid
375-22-4 | DTXSID
Searched by Synonym.

Hazard: Dose Response Summary Value

Release Notes

Human-Relevant Dose Response Summary Value Data

More	Source	Subsource	Type	Subtype	Risk Assessment	Qualifier	Value	Units	Study Type	Exposure Route	Effect	Species	Year	Experimental	Stored Source Record	QC Level
	ATSDR	ATSDR TP 2021 Per	NOAEL	-	-	=	30.0	mg/k...	short-term	oral	Neurological: Delayed ...	Rat	2007	undetermined	https://download.epa.gov/...	Manual
	ATSDR	ATSDR TP 2021 Per	LOAEL	less serious	-	=	30.0	mg/k...	short-term	oral	Endocrine: Hyperplasia...	Rat	2007	undetermined	https://download.epa.gov/...	Manual

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](http://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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Rusty Thomas

Colleen Elonen

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