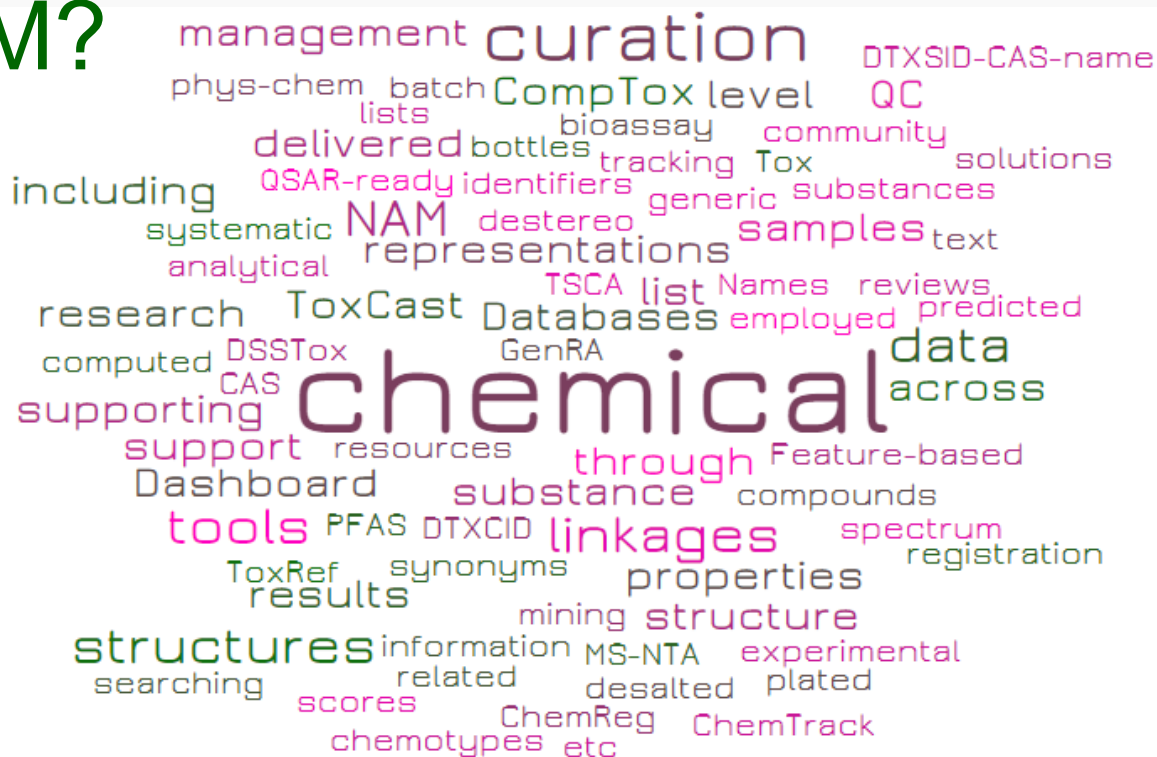


## What's in a NAM?

*Why chemistry,  
of course!*



*Ann Richard*

*Computational Chemistry & Cheminformatics Branch*

*Chemical Characterization & Exposure Division*

*CCCB/ CCED/ CCTE*

# Challenge: Linking data resources

- ToxCast (EPA) & Tox21 (Multi-Agency)
  - screening >4000 (ToxCast) to >10K (Tox21) environmentally relevant chemicals across 10's to 100's of HTS assays
- ACToR, ExpoCast, CPCat, ToxRef DB, etc
  - meshed CAS lists, product-use database, *in vivo* reference DB
- *In Silico* models
  - exposure models, ER/AR binding, physchem properties, ADME
- Public-facing ComTox dashboard
  - facilitate access to & utility of EPA data

*Chemical  
databases*

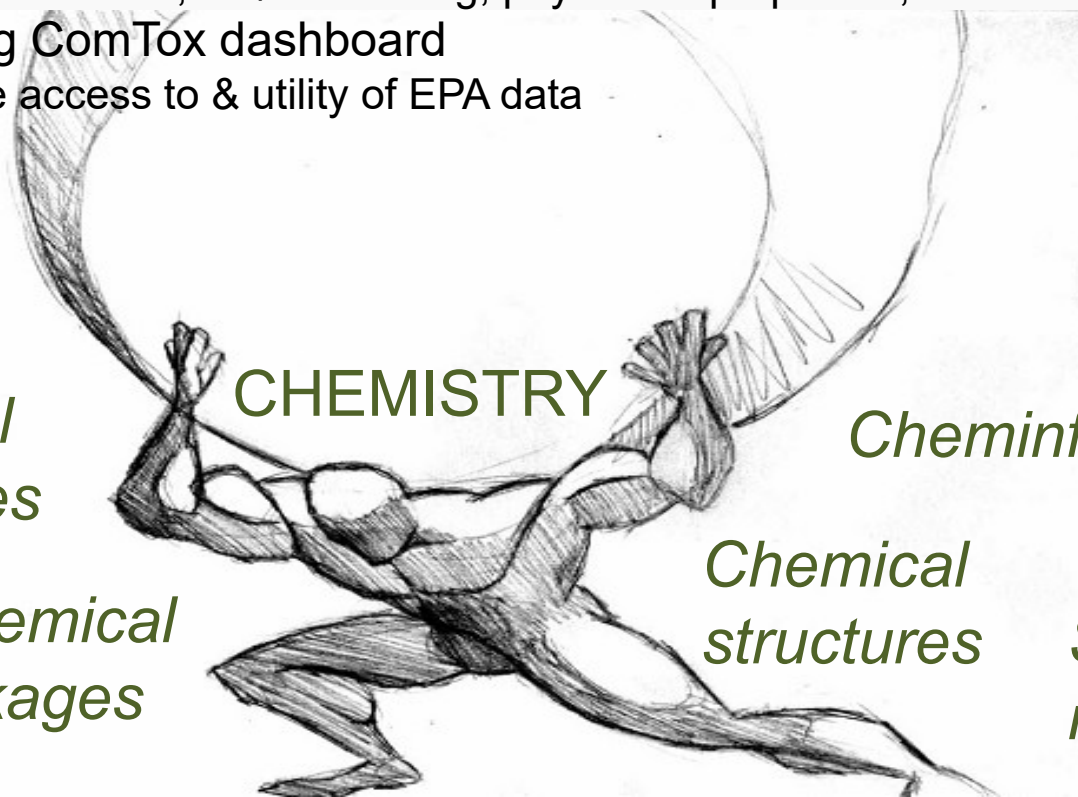
**CHEMISTRY**

*Cheminformatics*

*Chemical  
linkages*

*Chemical  
structures*

*SAR/QSAR  
models*



# Chemistry in NAM Research & Applications

## WHY?

Robust chemical assessments & systematic reviews require access to data with a clear relationship to the actual chemical(s) of concern

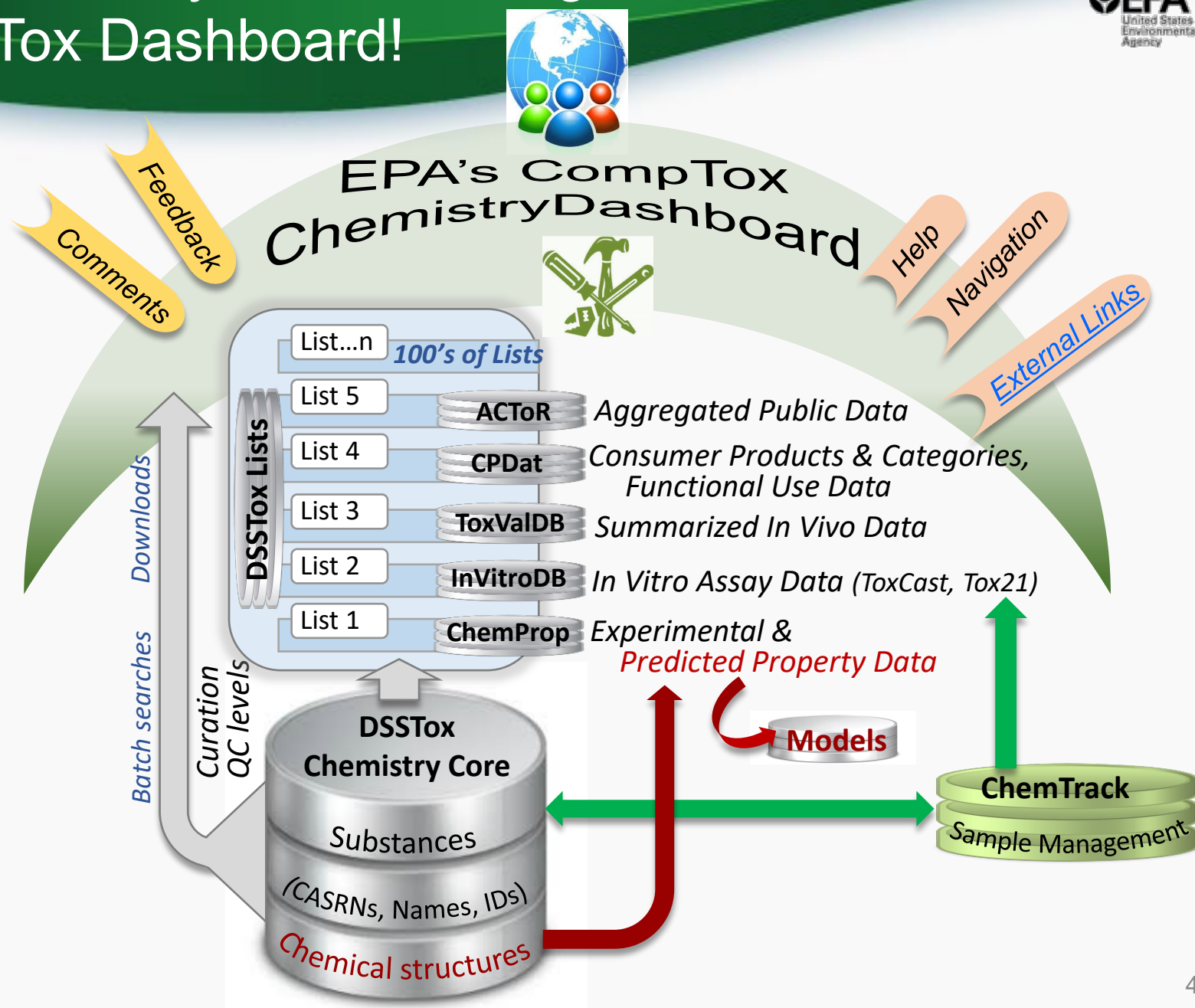
## WHAT?

Critical role of chemical curation and chemically indexed databases for providing accurate associations between a chemical and its associated data

## HOW?

Databases and tools supporting chemical management, chemical registration, chemical list curation, and chemical-data linkages across NAM resources

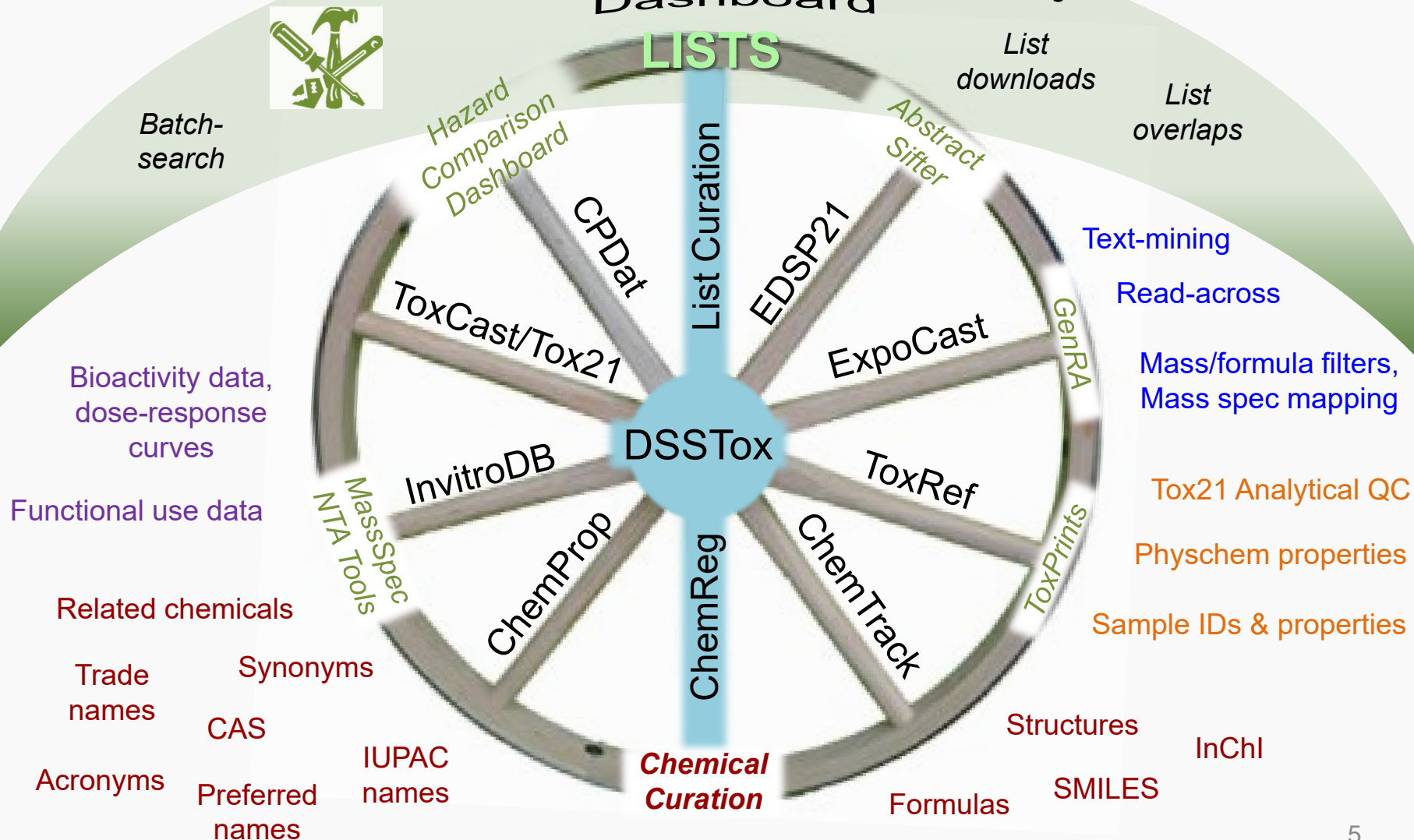
# The Chemistry beast feeding the CompTox Dashboard!





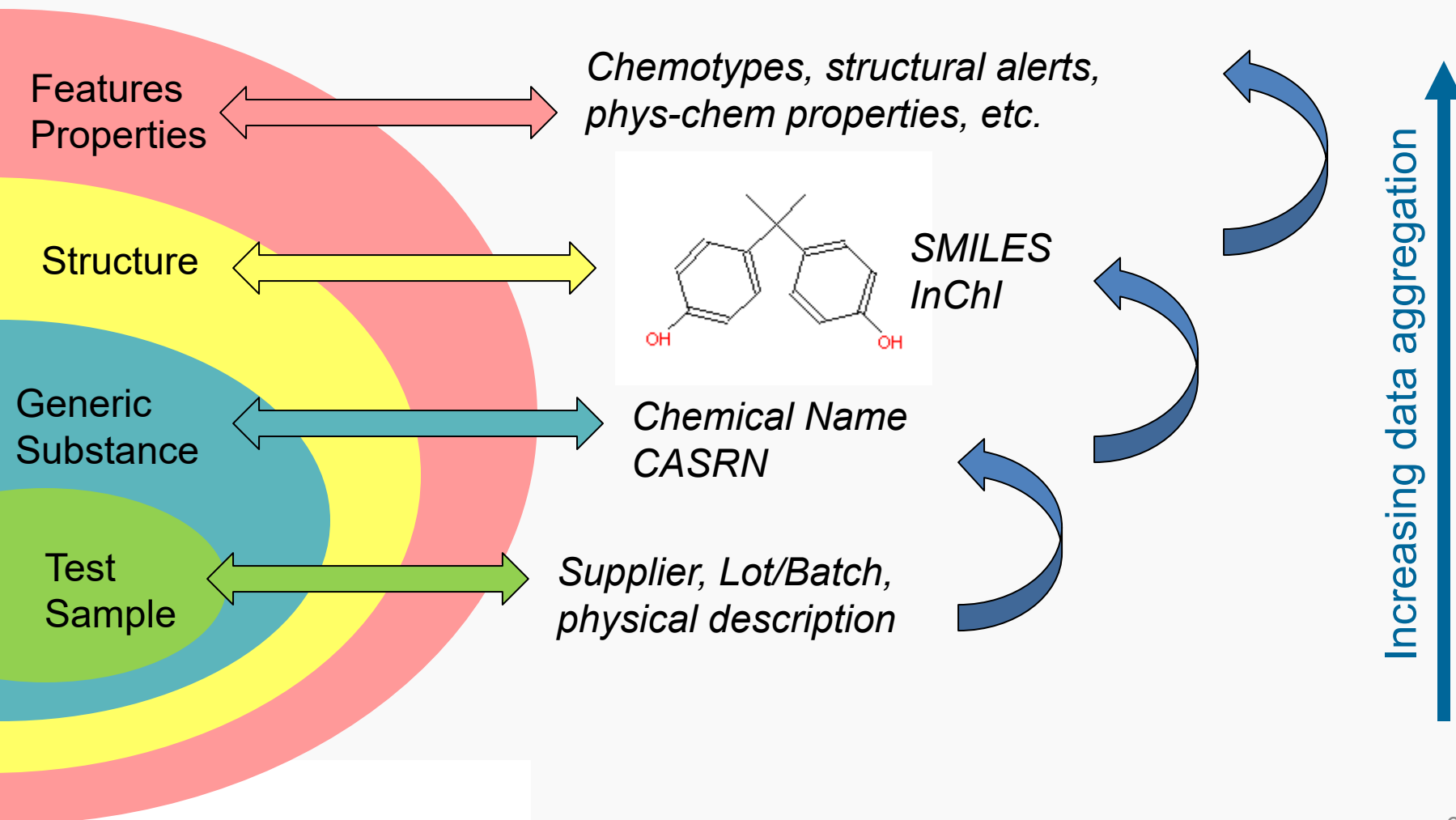
# DSSTox Chemical Hub

## EPA's CompTox Chemistry Dashboard

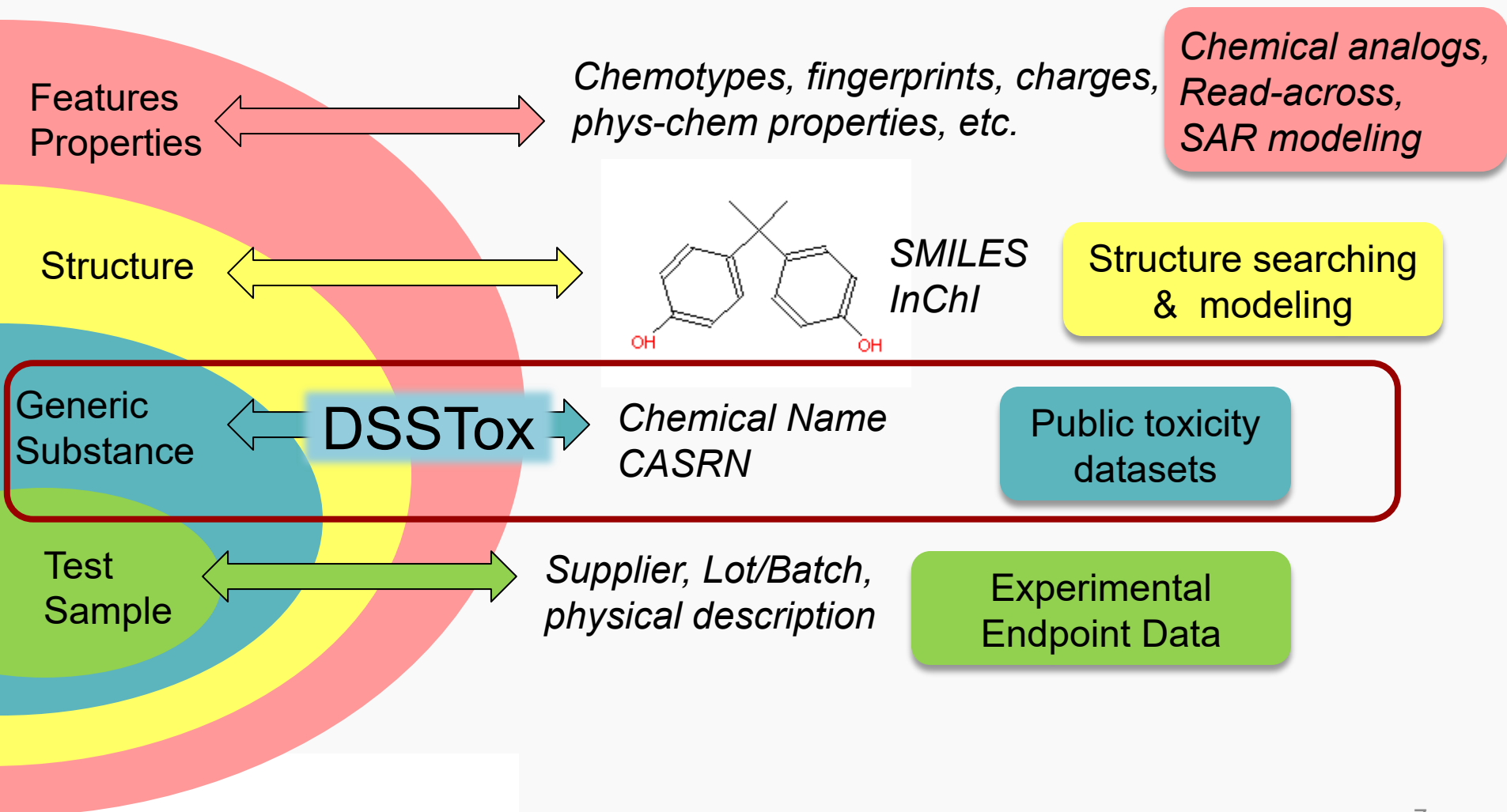


# Chemical Elements to Data Integration:

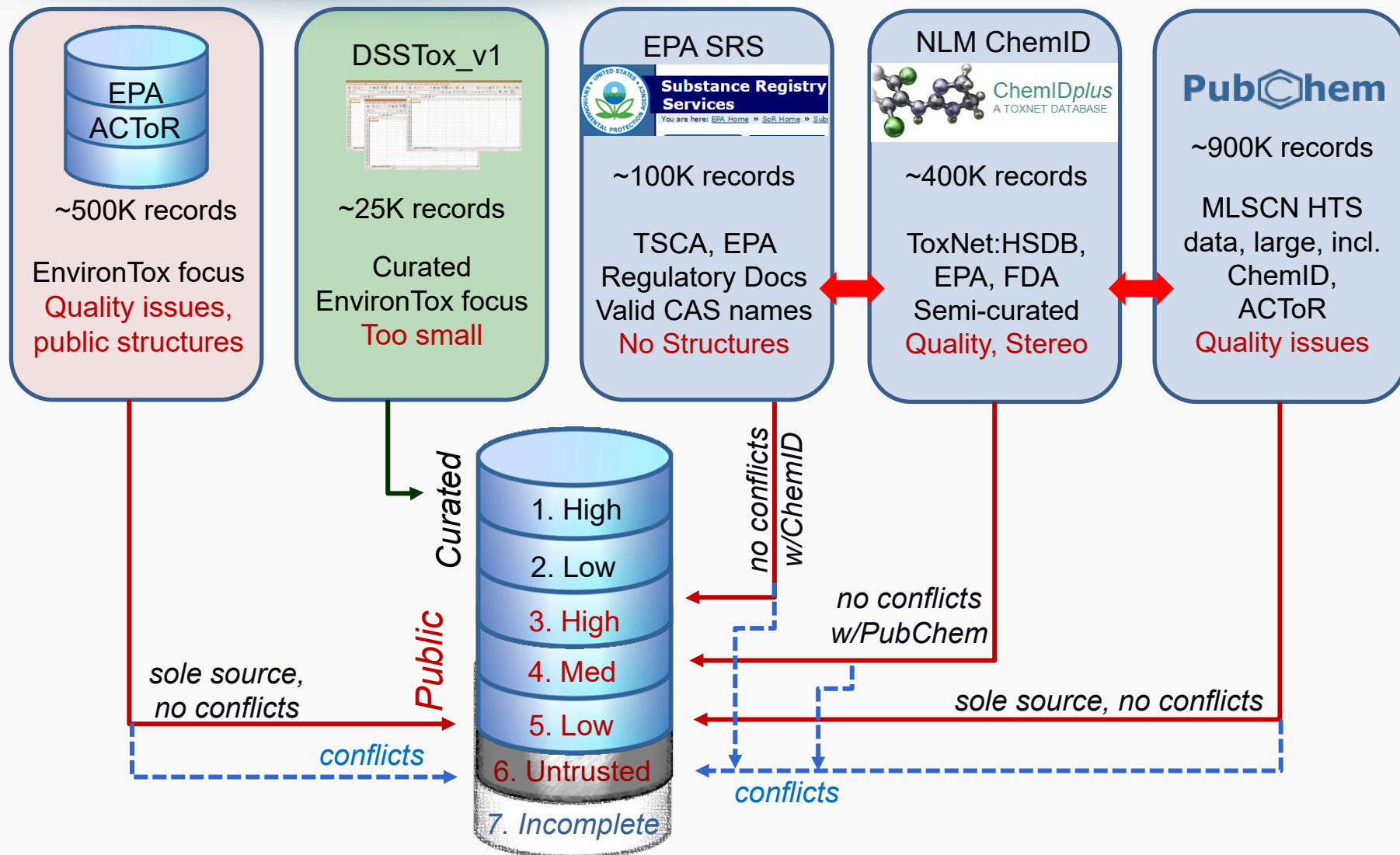
## *Chemical representations*



# Chemical Elements to Data Integration: *Chemical representations*

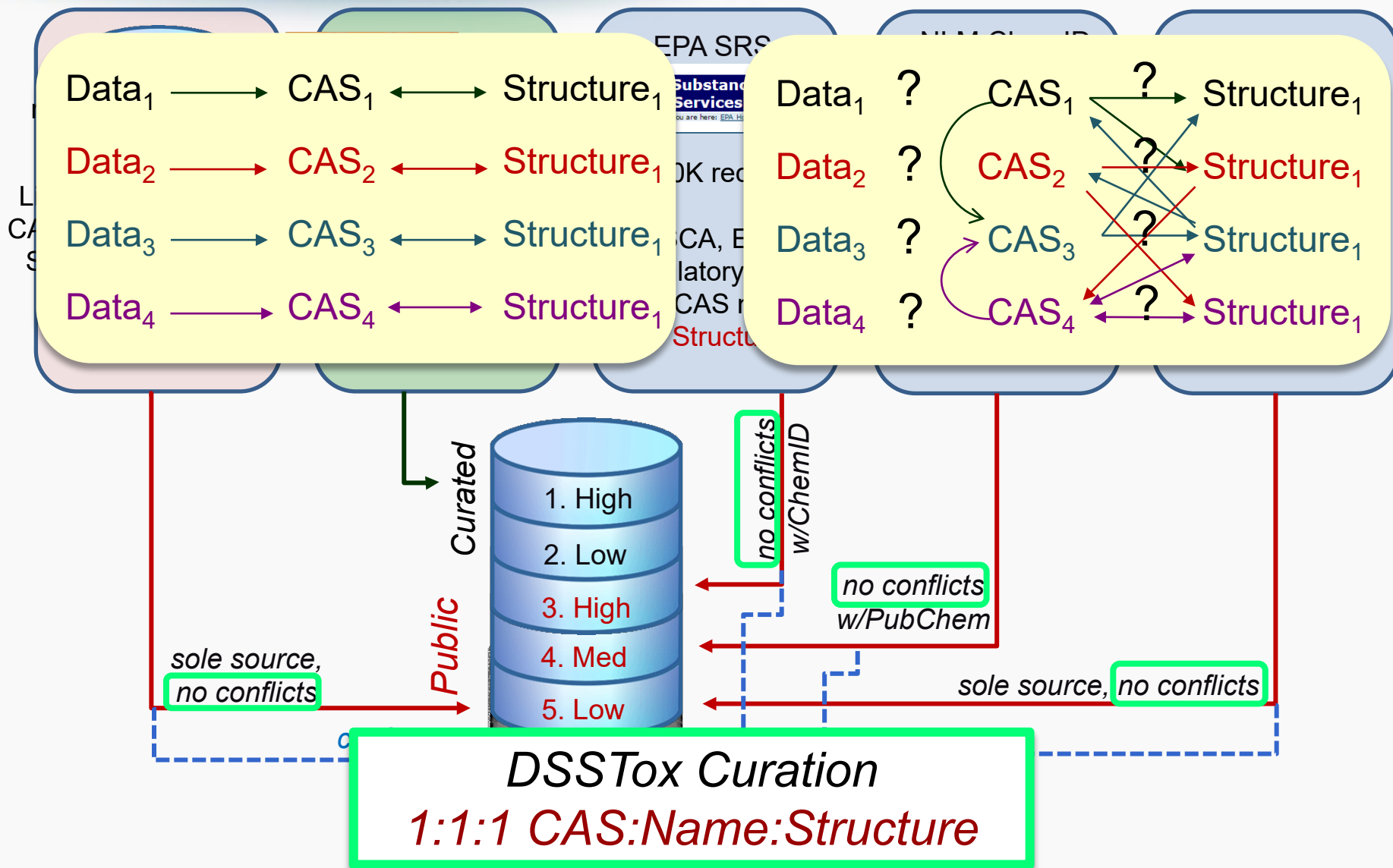


# DSSTox\_v2 Main Sources: Substance QC levels

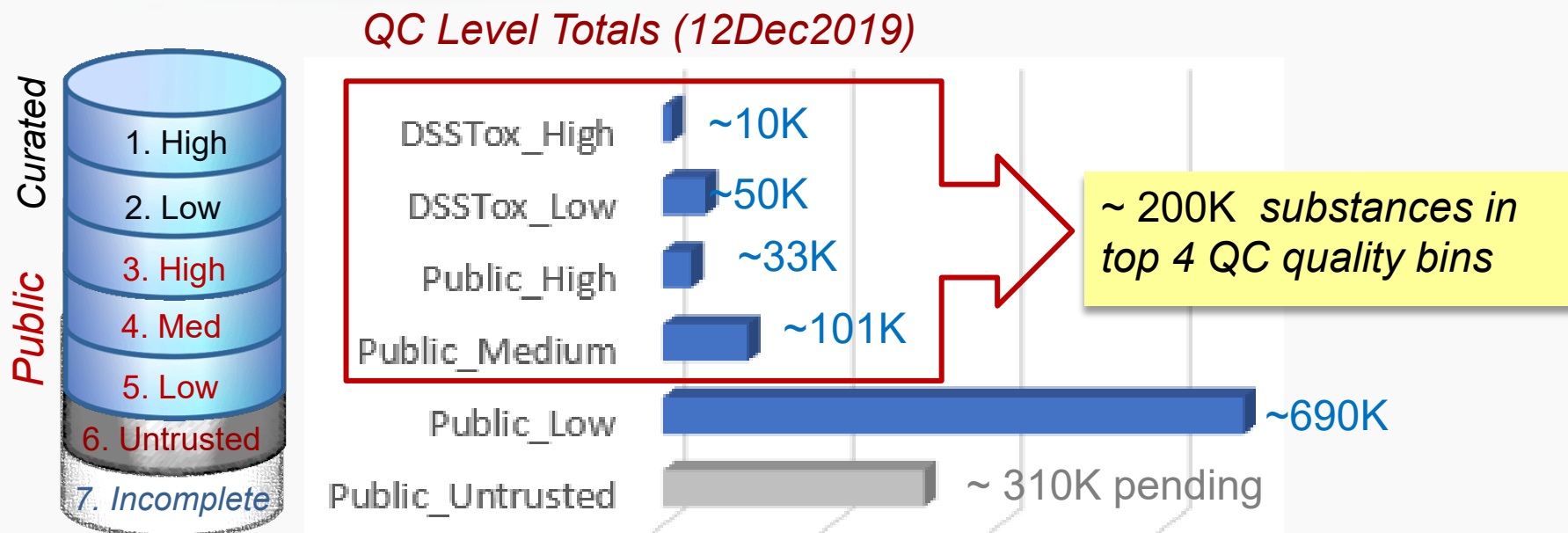




# DSSTox\_v2 Main Sources: Substance QC levels



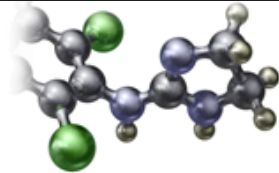
# DSSTox\_v2 QC Levels



## QC Levels

DSSTox_High:	Hand curated - highest confidence from definitive source
DSSTox_Low:	Hand curated and confirmed using multiple public sources
Public_High:	Extracted from EPA SRS and confirmed to have no conflicts in ChemID and PubChem
Public_Medium:	Extracted from ChemID and confirmed to have no conflicts in PubChem
Public_Low:	Extracted from ACToR or PubChem (single source, no conflicts)
Public_Untrusted:	Postulated, but found to have conflicts in public sources

# Substance-structure ambiguity



ChemIDplus  
A TOXNET DATABASE

Start New Query   Modify Query   Search History   Show Query

Switch to Summary View

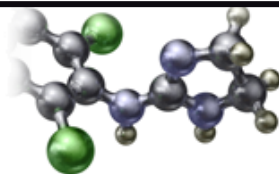
Substance Name: Hexyne  
RN: 26856-30-4  
InChIKey: CGHIBGNXEGJPQZ-UHFFFAOYSA-N

Molecular Formula

HC≡C-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>3</sub>

Navigation: Back, Home, Na+, Search, 3D

**DSSTox Curation**  
**1:1:1 CAS:Name:Structure**



ChemIDplus  
A TOXNET DATABASE

Start New Query   Modify Query   Search History   Show Query

Switch to Summary View

Go to summary view

Substance Name: 1-Hexyne  
RN: 693-02-7  
InChIKey: CGHIBGNXEGJPQZ-UHFFFAOYSA-N

Molecular Formula  
C<sub>6</sub>H<sub>10</sub>

Molecular Weight  
82.145

HC≡C-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>3</sub>

Navigation: Back, Home, Na+, Search, 3D

# ChemReg: Substance Registration

## ACToR-DSSTox Chemical Register

View/Edit a Single Record   Structure Search   Browse/Curate Records

Ambiguous Synonym matched <b>null</b>  
You are viewing the record associated with  
DTXSID3031864  
CASRN: 1763-23-1

PFOS

### Other Possible Records

CAS	Reason
DTXSID80108992	Ambiguous Synonym matched <b>null</b>

Systematic Name:  
MolFormula:  
MolWeight:  
InChI Key:  
Smiles:  
DTXSID:

Calculate from

Substance\_ID:  
CAS:

Name:

Substance Type:

QC Level:

Data Source:

QC Notes:

### Synonyms (20)

### Other CAS (1)

	CAS-RN	Relationship	Source	Comments
<input type="radio"/>	<input type="text" value="132324-11-9"/>	<input type="text" value="Deleted"/>	<input type="text" value="STN(DSSTox)"/>	<input type="text"/>
<input type="button" value="Delete Selected"/> <input type="button" value="Add Other Cas"/>				

### Successor Substances (8)

	CAS-RN	Relationship	Source	Struc	Casrn	Comments
<input type="radio"/>	<input type="text" value="45298-90-6"/>	<input type="text" value="Component"/>	<input type="text" value="STN(DSSTox)"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="text" value="Sulfonate"/>
<input type="radio"/>	<input type="text" value="2795-39-3"/>	<input type="text" value="Salt Form"/>	<input type="text" value="STN(DSSTox)"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="text" value="Potassium Salt"/>
<input type="radio"/>	<input type="text" value="29457-72-5"/>	<input type="text" value="Salt Form"/>	<input type="text" value="STN(DSSTox)"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="text" value="Lithium Salt"/>
<input type="radio"/>	<input type="text" value="56773-42-3"/>	<input type="text" value="Salt Form"/>	<input type="text" value="STN(DSSTox)"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="text" value="Tetraethylammonium Salt"/>
<input type="radio"/>	<input type="text" value="29081-56-9"/>	<input type="text" value="Salt Form"/>	<input type="text" value="STN(DSSTox)"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="text" value="NH4+ salt"/>
<input type="radio"/>	<input type="text" value="4021-47-0"/>	<input type="text" value="Salt Form"/>	<input type="text" value="STN(DSSTox)"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="text" value="Sodium Salt"/>
<input type="radio"/>	<input type="text" value="111873-33-7"/>	<input type="text" value="Salt Form"/>	<input type="text" value="STN(DSSTox)"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="text" value="N,N,N-Tributylbutylammon"/>
<input type="radio"/>	<input type="text" value="91036-71-4"/>	<input type="text" value="Salt Form"/>	<input type="text" value="STN(DSSTox)"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="text" value="Magnesium salt"/>
<input type="button" value="Delete Selected"/> <input type="button" value="Add Related Cas"/>						

### Predecessor Substances (2)

Relationship	DTXSID	CAS-RN	Source	Comments
Predecessor: Component	<a href="#">DTXSID20872963</a>	NOCAS_872963	STN(DSSTox)	<input type="text" value="PFOS"/>
Predecessor: Component	<a href="#">DTXSID40880545</a>	64202-77-3	STN(DSSTox)	<input type="text"/>

### Associated Lists (290)

DTXRID	Source Identifier	Inventory Code
<a href="#">DTXRID8031865</a>	Perfluorooctane Sulfonate, PFOS	NTPBSI
<a href="#">DTXRID0040753</a>	Perfluorooctane sulfonic acid	TOXCAST

# ChemReg: *List Curation*

## ACToR-DSSTox Chemical Registration

View/Edit a Single Record   Structure Search   Browse/Curate Records   Export DSSTox   Chemotypes   **Manage Chemical Lists**   Manage Property Data   Add Deleted Casrns   Welcome, Ann   [Logout](#)

Welcome aricha02

Editing Listname: NCCTCPP\_LOGP

Duplicates:

### External Check Results

Description	Records
Unique Synonym matched <b>NAME</b> CAS-RN matched <b>CASRN</b>	1
Structure matched <b>Smiles</b> Structure matched <b>MolBlock</b> Ambiguous Synonym matched <b>NAME</b> CAS-RN matched <b>CASRN</b> Preferred Name matched other record: <b>NAME</b>	1
Structure matched <b>Smiles</b> Structure matched <b>MolBlock</b> CAS-RN matched <b>CASRN</b> Unique Synonym matched other record: <b>NAME</b>	12
Structure matched <b>Smiles</b> Structure matched <b>MolBlock</b> Mapped Identifier matched <b>NAME</b>	6

### Substance Mapping

(1 of 1)

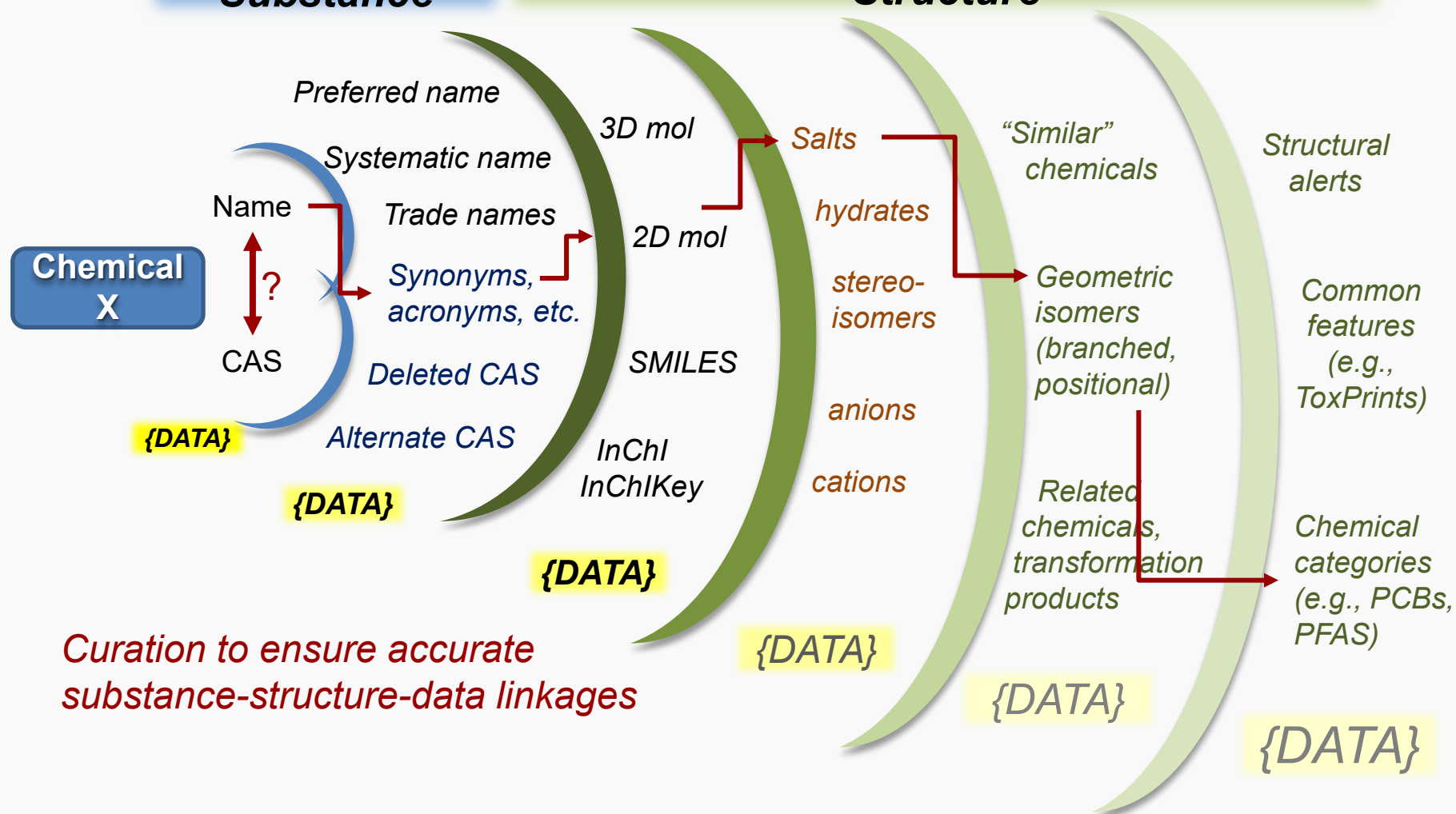
	Source Casrn	Source Name	Hit Substance_ID	Hit Casrn	Hit Name	
	59-92-7	DOPA	<a href="#">DTXSID9023209</a>	59-92-7	Levodopa	<a href="#">Other Hits</a>
	104-14-3	NORTRON	<a href="#">DTXSID7043873</a>	104-14-3	Octopamine	<a href="#">Other Hits</a>
	224-53-3	3,4,5,6-Dibenzacridine	<a href="#">DTXSID30176929</a>	224-53-3	Dibenz(c,h)acridine	<a href="#">Other Hits</a>
	226-36-8	DIBENZ(A,H)ACRIDINE	<a href="#">DTXSID3059761</a>	226-36-8	Dibenz[acridine	<a href="#">Other Hits</a>
	524-12-4	N,N'-	<a href="#">DTXSID2042101</a>	524-12-4	N,N'-	<a href="#">Other Hits</a>
Hits						
	ssCAS-RN	ssName	Hit Desc	Hit Substance_ID	Hit Casrn	Hit Name
	224-53-3	3,4,5,6-Dibenzacridine	Structure matched <b>Smiles</b> Structure matched <b>MolBlock</b> CAS-RN matched <b>CASRN</b>	<a href="#">DTXSID30176929</a>	224-53-3	Dibenz(c,h)acridine
	224-53-3	3,4,5,6-Dibenzacridine	Unique Synonym matched <b>NAME</b>	<a href="#">DTXSID4059758</a>	224-42-0	Dibenz[a,j]acridine
<a href="#">Map hit</a> <a href="#">Cancel</a>						
	3001-72-7	DBN	<a href="#">DTXSID10184087</a>	3001-72-7	1,5-Diazabicyclo(4.3.0)non-5-ene	<a href="#">Other Hits</a>
	13533-05-6	DEGA	<a href="#">DTXSID5050397</a>	13533-05-6	2-Propenoic acid, 2-(2-hydroxyethoxy)ethyl ester	<a href="#">Other Hits</a>
	39700-44-2	G-THIOBUTYROLACTONE	<a href="#">DTXSID30454118</a>	39700-44-2	THIOBUTYROLACTONE	<a href="#">Other Hits</a>



# Chemical-data gathering for systematic reviews

## Substance

## Structure



# Chemical-data gathering for systematic reviews: e.g., PFOS

**EPA** United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

## CompTox Chemicals Dashboard

883 Thousand Chemicals

Chemicals Product/Use Categories Assay/Gene

Q PFOS

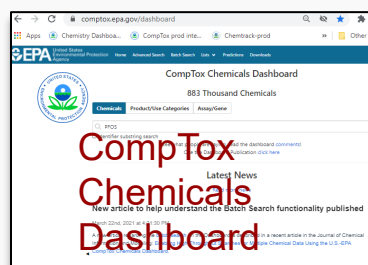
Select all Download Send to Batch Search Default DTXSID CASRN TOXCAST

*PFOS is ambiguous acronym*

Perfluorooctanesulfonic acid  
DTXSID:DTXSID3031864  
CASRN:1763-23-1  
TOXCAST:267/1129

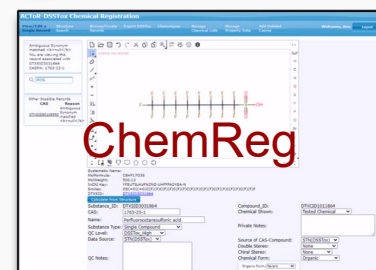
Perfluorooctanesulfonate  
DTXSID:DTXSID80108992  
CASRN:45298-90-6  
TOXCAST:-

# Chemical-data gathering for systematic reviews: e.g., PFOS



**CompTox Chemicals Dashboard**

Curated QC Level Lists  
Synonyms  
Similar cmpds  
Related cmpds



Perfluorooctanesulfonic acid

Perfluorooctanesulfonic acid  
1763-23-1 | DTXSID3031864  
Searched by Synonym from Valid Source.

13 chemicals

Select all Download Send to Batch Search Relationships DTGSD CASRN TOXCAT

Hide chemicals that are: Select by format or layout

Searched Chemical	Markush Parent	Markush Parent	Precursor: Component	Precursor: Component
 Perfluorooctanesulfonic acid DTXSID:DTXSID3031864 CASRN:1763-23-1 TOXCAT:1763-23-1	 Perfluorooctanesulfonate DTXSID:DTXSID3031864 CASRN:1763-23-1 TOXCAT:1763-23-1	 Perfluorooctanesulfonate DTXSID:DTXSID3031864 CASRN:1763-23-1 TOXCAT:1763-23-1	3 related chemical structures with this substance Mixture of PFOA and PFOS DTXSID:DTXSID3031864 CASRN:1763-23-1 TOXCAT:1763-23-1	3 related chemical structures with this substance 1-Octanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8,8,18,18,18-octadecafluoro- DTXSID:DTXSID3031864 CASRN:1763-23-1 TOXCAT:1763-23-1
 Perfluorooctanesulfonate DTXSID:DTXSID3031864 CASRN:1763-23-1 TOXCAT:1763-23-1	 Lithium perfluorooctanesulfonate DTXSID:DTXSID3031864 CASRN:1763-23-1 TOXCAT:1763-23-1	 Potassium perfluorooctanesulfonate DTXSID:DTXSID3031864 CASRN:1763-23-1 TOXCAT:1763-23-1	 Ammonium perfluorooctanesulfonate DTXSID:DTXSID3031864 CASRN:1763-23-1 TOXCAT:1763-23-1	 Tetraethylammonium perfluorooctanesulfonate DTXSID:DTXSID3031864 CASRN:1763-23-1 TOXCAT:1763-23-1
 Tetraethylammonium perfluorooctanesulfonate DTXSID:DTXSID3031864 CASRN:1763-23-1 TOXCAT:1763-23-1	 Sodium perfluorooctanesulfonate DTXSID:DTXSID3031864 CASRN:1763-23-1 TOXCAT:1763-23-1	 Magnesium bis(perfluorooctanesulfonate) DTXSID:DTXSID3031864 CASRN:1763-23-1 TOXCAT:1763-23-1		

13 Related substances, incl. Markush categories

# Curated Lists: e.g., PFAS

*Curated substance*

## PFAS|EPA: PFAS structures in DSSTox (update August 2020)

☐ Identifier substring search

PFAS structure file:

8163 substances with structures

Download

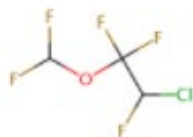
Columns

### List Details

**Description:** List consists of all DTXSID records with a structure assigned, and using a set of substructural filters based on community input. The substructural filters ([visible here](#)) are designed to be simple, reproducible and transparent, yet general enough to encompass the largest set of structures having sufficient levels of fluorination to potentially impart PFAS-type properties.

**Number of Chemicals:** 8163

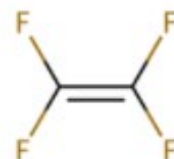
List Acronym	List Name
PFASNORDIC	PFAS: Nordic PFAS
PFASNTREV19	PFAS: PFAS in Nov 2019)
PFASOECD	PFAS: Listed in OECD
PFASOECDNA	NORMAN: List of PFAS
PFASSTRUCT	PFAS EPA: PFAS structures in DSSTox (update August 2020)
PFASTRI	PFAS: PFAS to the TRI Program by the Na
PFASTRIER	PFAS Community-
TONYPFASDASH	TONY'S Mockup of



Enflurane  
DTXSID:DTXSID1020562  
CASRN:13838-16-9  
TOXCAST:0/235



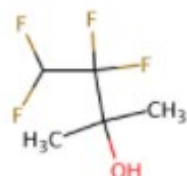
1,1,1,2-Tetrafluoroethane  
DTXSID:DTXSID1021324  
CASRN:811-97-2  
TOXCAST:-



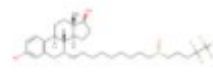
Tetrafluoroethylene  
DTXSID:DTXSID6021325  
CASRN:116-14-3  
TOXCAST:-



2H-Perfluoro-2-propanol  
DTXSID:DTXSID1022134  
CASRN:920-66-1  
TOXCAST:-



2-Methyl-3,3,4,4-tetrafluoro-2-butanol  
DTXSID:DTXSID9022283  
CASRN:29553-26-2  
TOXCAST:-



Fulvestrant  
DTXSID:DTXSID4022369  
CASRN:129453-61-8  
TOXCAST:157/924

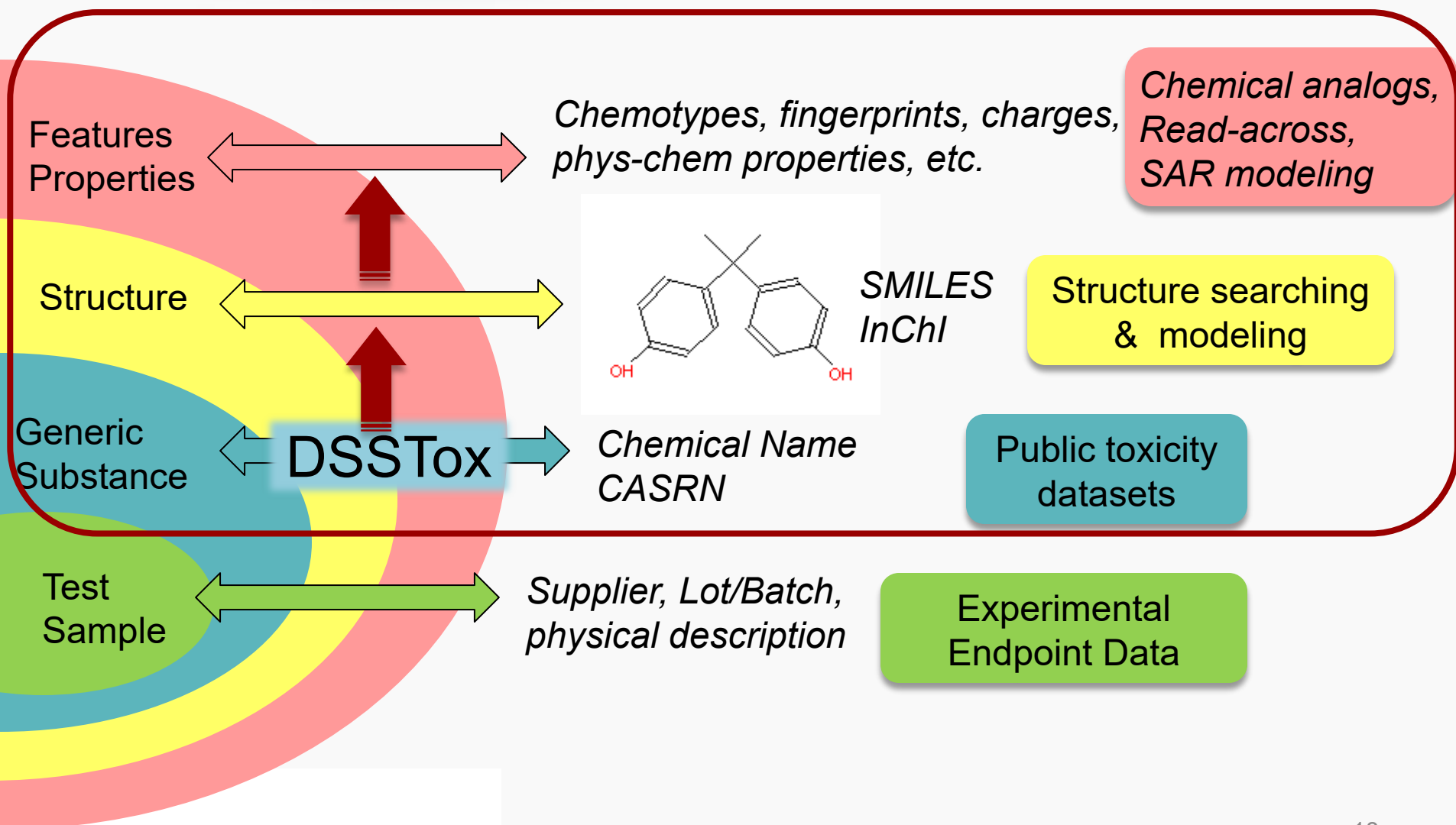


Pentafluoroethane  
DTXSID:DTXSID1024251  
CASRN:354-33-6  
TOXCAST:-



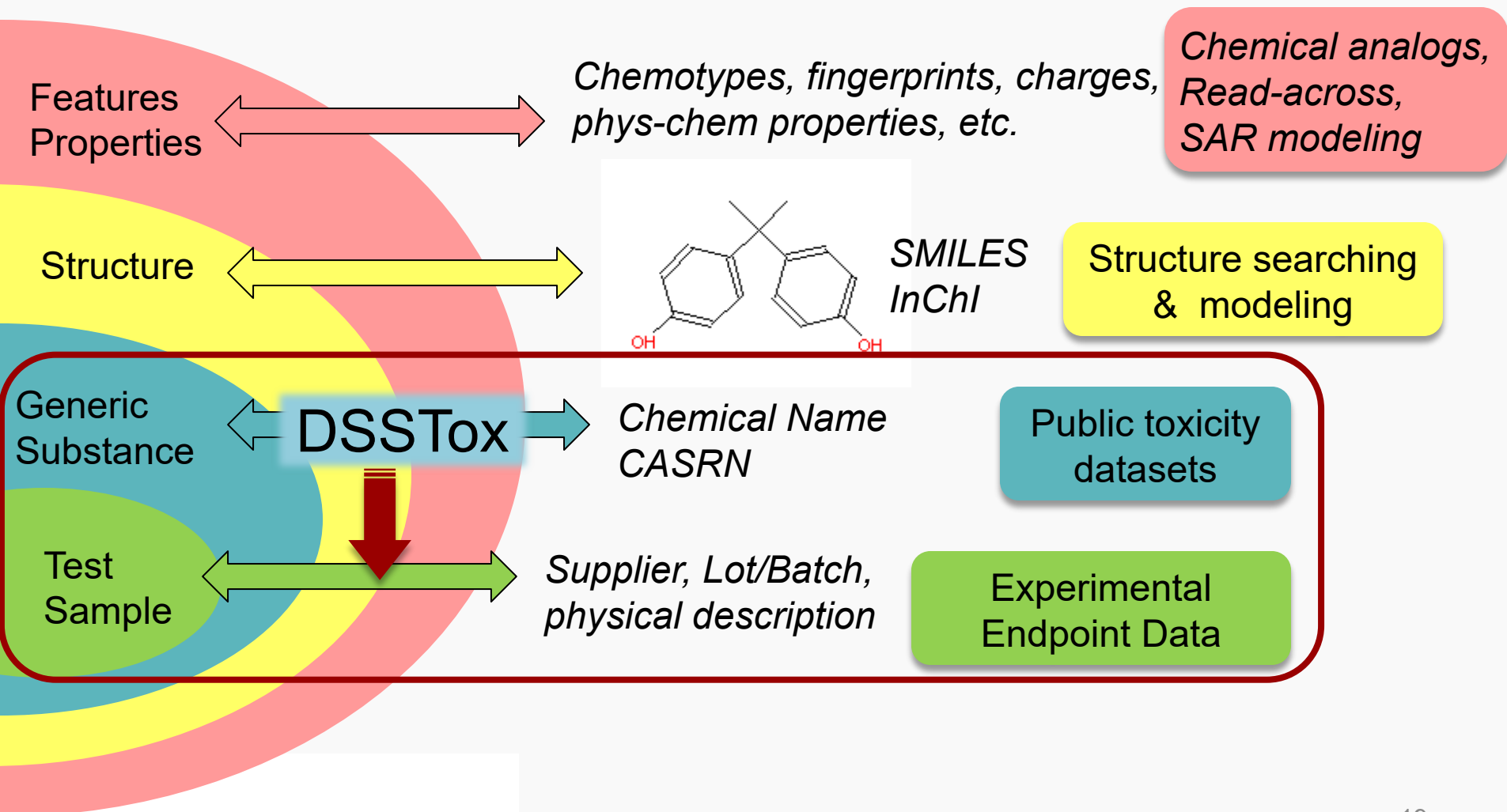
Hexafluoroacetone sesquihydrate  
DTXSID:DTXSID7025392  
CASRN:13098-39-0  
TOXCAST:-

# Chemical Elements to Data Integration: *Chemical representations*

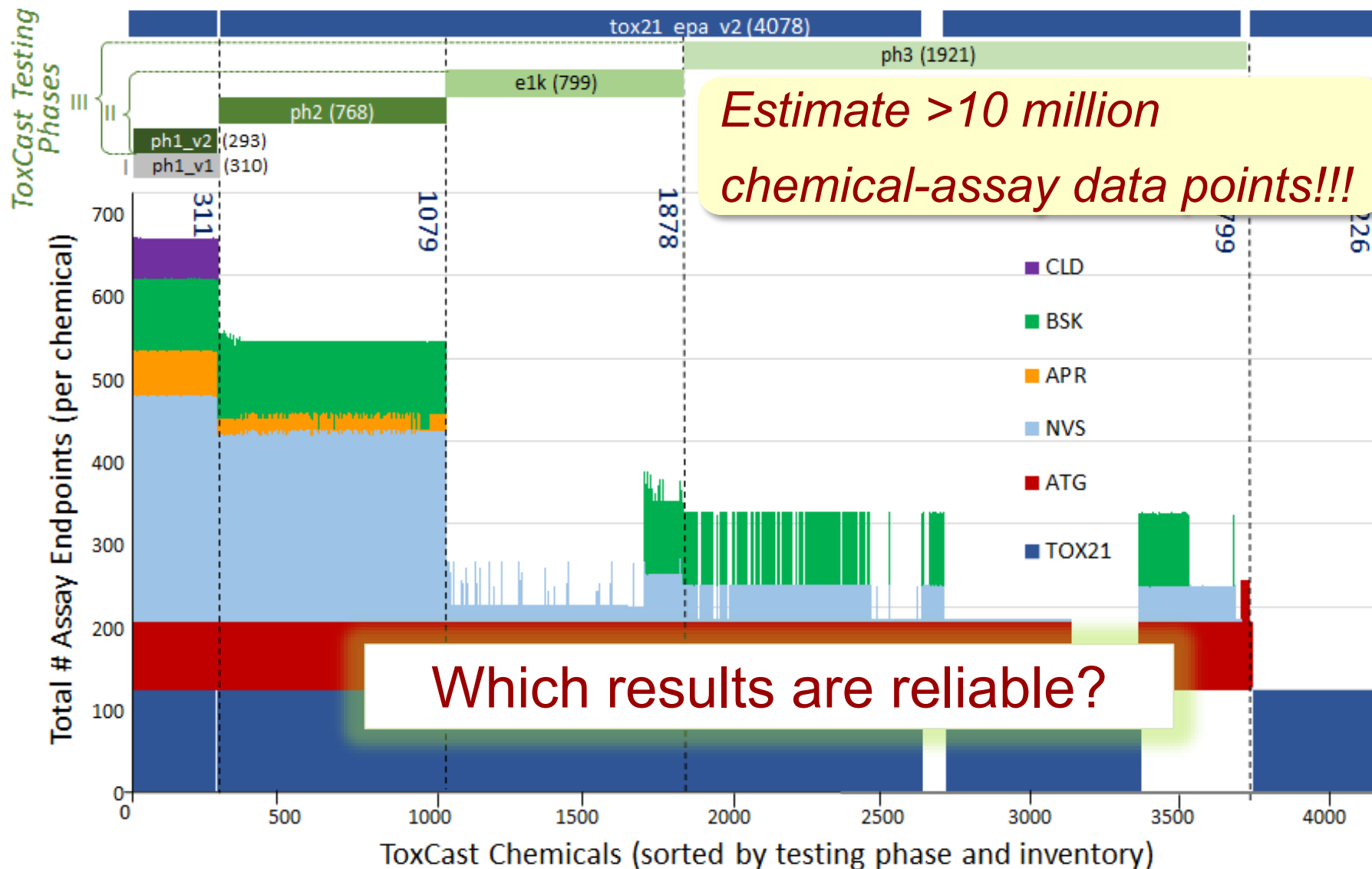




# Chemical Elements to Data Integration: *Chemical representations*



# ToxCast/To21 HTS data



# Chemical & Data Quality Issues

*Quality substance &  
structure annotations*

*ToxCast & Tox21  
Sample Database*

Solutions  
Bottles  
Supplier/Lot/Batch

**DSSTox**

**Compound  
Libraries**

Valid Structures

Accurate substance annotation:  
CAS – Name - Structure

Supplier-provided info  
(or lack thereof)

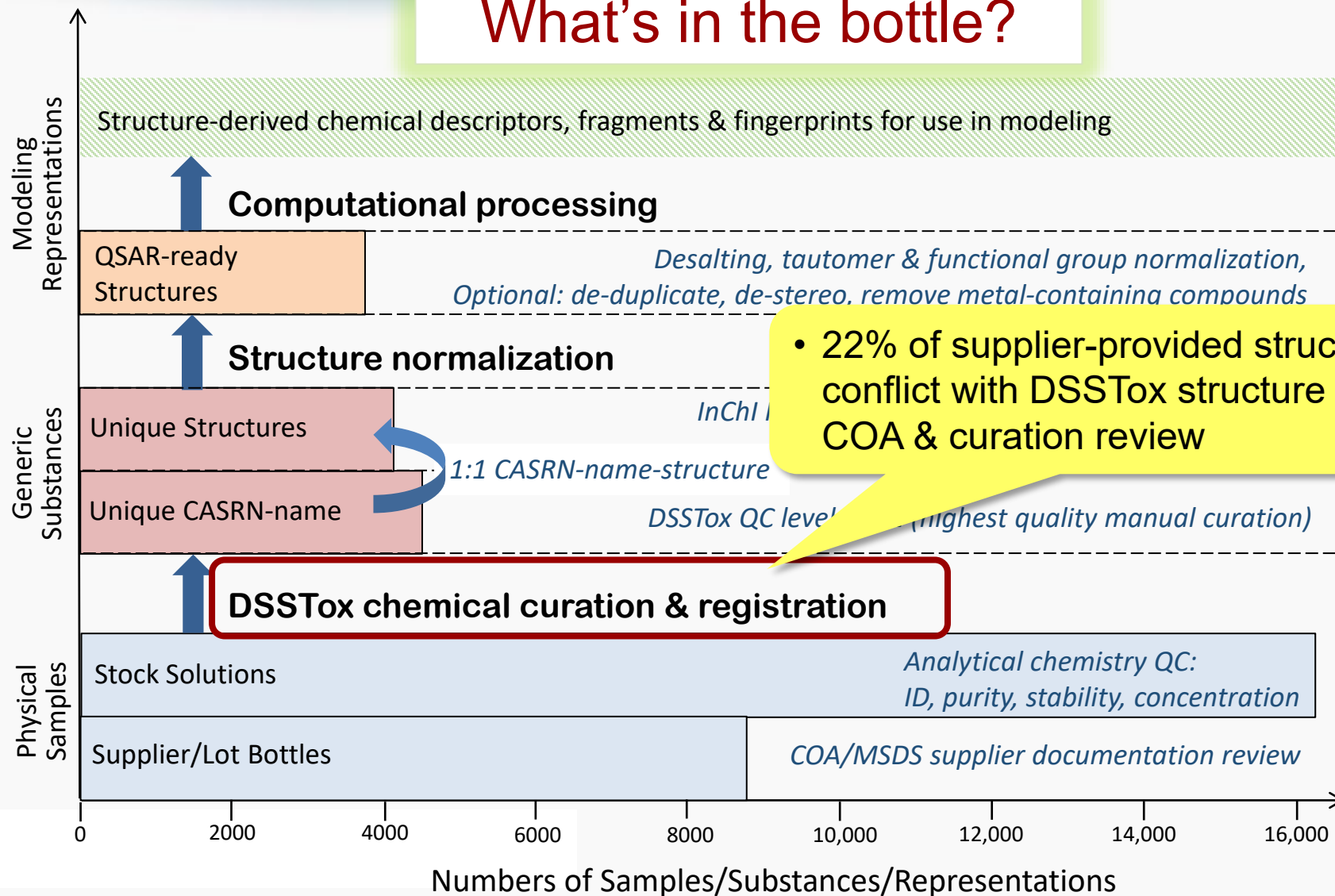
Reported (actual) purity

DMSO Soluble (or not)

Volatility  
(missing sample)

# ToxCast Chemical Library: Quality Control Steps

## What's in the bottle?



# ChemTrack:

## Chemical Sample Management

- Curators manually review COAs & MSDSs and map each original supplier bottle to a DTXSID
- Neat and solution tracking for >53K bottle codes!

 chemtrack

Inventory ▾

Partnerships ▾

Ordering ▾

### Bottle Inventory

Uploaded MOSAIC Files 48










Curated Bottles 53607

Uncurated Bottles 3360

Columns ▾

10 ▾

 Export

Barcode ▾	CoA Summary Id ▾	Barcode type ▾	DTXSID ▾	Compound name ▾	Casrn ▾	Qty available ▾	Concentration (mM) ▾	Vendor ▾
Filter by Barc	Filter by CoA	Filter by Barcode ty	Filter by DTXSI	Filter by Compou	Filter by Casrn	Filter by Qty	Filter by Concentration	Filter by Vendor
 0073019474	 7083	EPA_Vial_MLR96_(1.4mL)	 DTXSID2047648	3-PHENYLPROPYL ACETATE	122-72-5	1000ul	20	Sigma Chemical Company
 0073019475	 7065	EPA_Vial_MLR96_(1.4mL)	 DTXSID6047604	PHENETHYL BUTYRATE	103-52-6	955ul	20	Sigma Chemical Company
 0073019476	 7089	EPA_Vial_MLR96_(1.4mL)	 DTXSID5021621		116-53-0	1000ul	20	Sigma Chemical Company



# What can analytical QC data tell us?

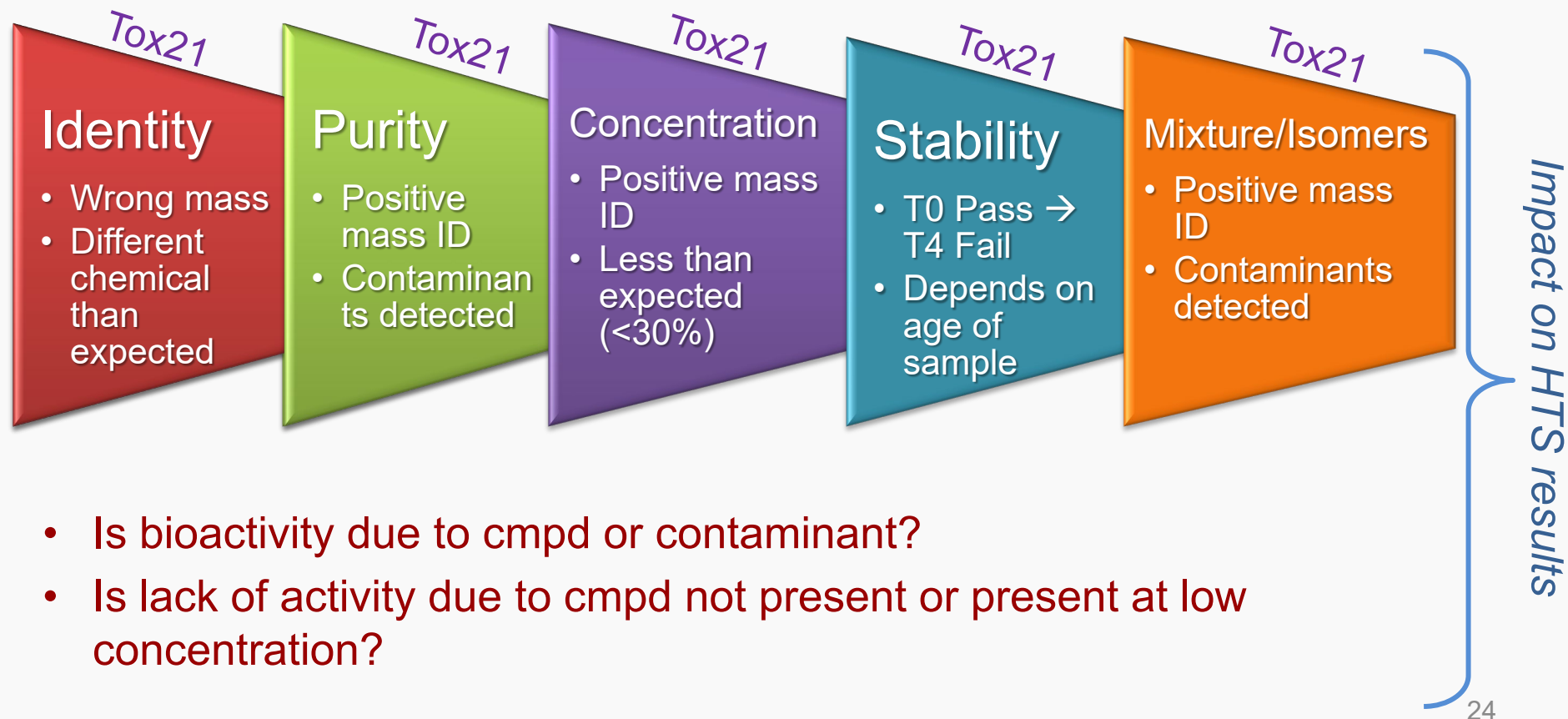
## *Sample-specific*

- purity
- age of sample
- supplier variability
- plating errors



## *Compound - specific*

- volatility
- reactivity
- limited solubility in DMSO
- adheres to plastic



- Is bioactivity due to cmpd or contaminant?
- Is lack of activity due to cmpd not present or present at low concentration?

# Some cmpds have QC data ...

## Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

### DETAILS

#### EXECUTIVE SUMMARY

#### PROPERTIES

#### ENV. FATE/TRANSPORT

#### HAZARD

##### ADME

##### EXPOSURE

##### BIOACTIVITY

#### SIMILAR COMPOUNDS

#### GENRA (BETA)

#### RELATED SUBSTANCES

#### SYNONYMS

##### LITERATURE

#### LINKS

#### COMMENTS

### General

[EPA Substance Registry Service](#)

[Household Products Database](#)

[Chemical Entities of Biological Interest \(ChEBI\)](#)

[PubChem](#)

[ChempSpider](#)

[CPCat](#)

[DrugBank](#)

[HMDB](#)

[Wikipedia](#)

[MSDS Lookup](#)

[ChEMBL](#)

[Chemical Vendors](#)

[CalEPA Office of Environmental Health Hazard Assessment](#)

[NIOSH Chemical Safety Cards](#)

[ToxPlanet](#)

[ACS Reagent Chemicals](#)

[Wikidata](#)

[ChemHat: Hazards and Alternatives Toolbox](#)

[Wolfram Alpha](#)

[ScrubChem](#)

[ECHA Brief Profile](#)

[ECHA Infocard](#)

[ChemAgora](#)

[Consumer Product Information Database \(CPID\)](#)

[ChEBI](#)

[Sigma-Aldrich Chemicals](#)

[NIST NIST Chemistry Webbook](#)

### Toxicology

[ACToR](#)

[DrugPortal](#)

[CCRIS](#)

[ChemView](#)

[CTD](#)

[eChemPortal](#)

[Gene-Tox](#)

[HSDB](#)

[ToxCast Dashboard 2](#)

[LactMed](#)

[International Toxicity Estimates for Risk](#)

[ATSDR Toxic Substances Portal](#)

[Superfund Chemical Data matrix](#)

[NIOSH IDLH Values](#)

[ACToR PDF Report](#)

[Toxics Release Inventory](#)

[CREST](#)

[National Air Toxics Assessment](#)

### Publications

[Toxline](#)

[Environmental Health Perspectives](#)

[NIEHS](#)

[National Toxicology Program](#)

[Google Books](#)

[Google Scholar](#)

[Google Patents](#)

[PPRTVWEB](#)

[PubMed](#)

[IRIS Assessments](#)

[EPA HERO](#)

[NIOSH Skin Notation Profiles](#)

[NIOSH Pocket Guide](#)

[RSC Publications](#)

[BioCaddie DataMed](#)

[Springer Materials](#)

[Federal Register](#)

[Regulations.gov](#)

[Bielefeld Academic Search Engine](#)

[CORE Literature Search](#)

### Analytical

[FOR-IDENT](#)

[NEMI: National Environmental Methods Index](#)

[RSC Analytical Abstracts](#)

[Tox21 analytical data](#)

[MONA: MassBank North America](#)

[mzCloud](#)

[NIST NIST IR Spectrum](#)

[NIST NIST MS Spectrum](#)

### Prediction

[2D NMR HSQC/HMBC Prediction](#)

[Carbon-13 NMR Prediction](#)

[Proton NMR Prediction](#)

[ChemRTP Predictor](#)

# At the Tox21 ID soln level...

Secure | <https://tripod.nih.gov/tox21/samples/80-05-7>

Apps Chemistry Dashboard CompTox (zn) Dashboard ChemReg\_v0.9.6 ChemTrack Confluence - NCCT K JIRA

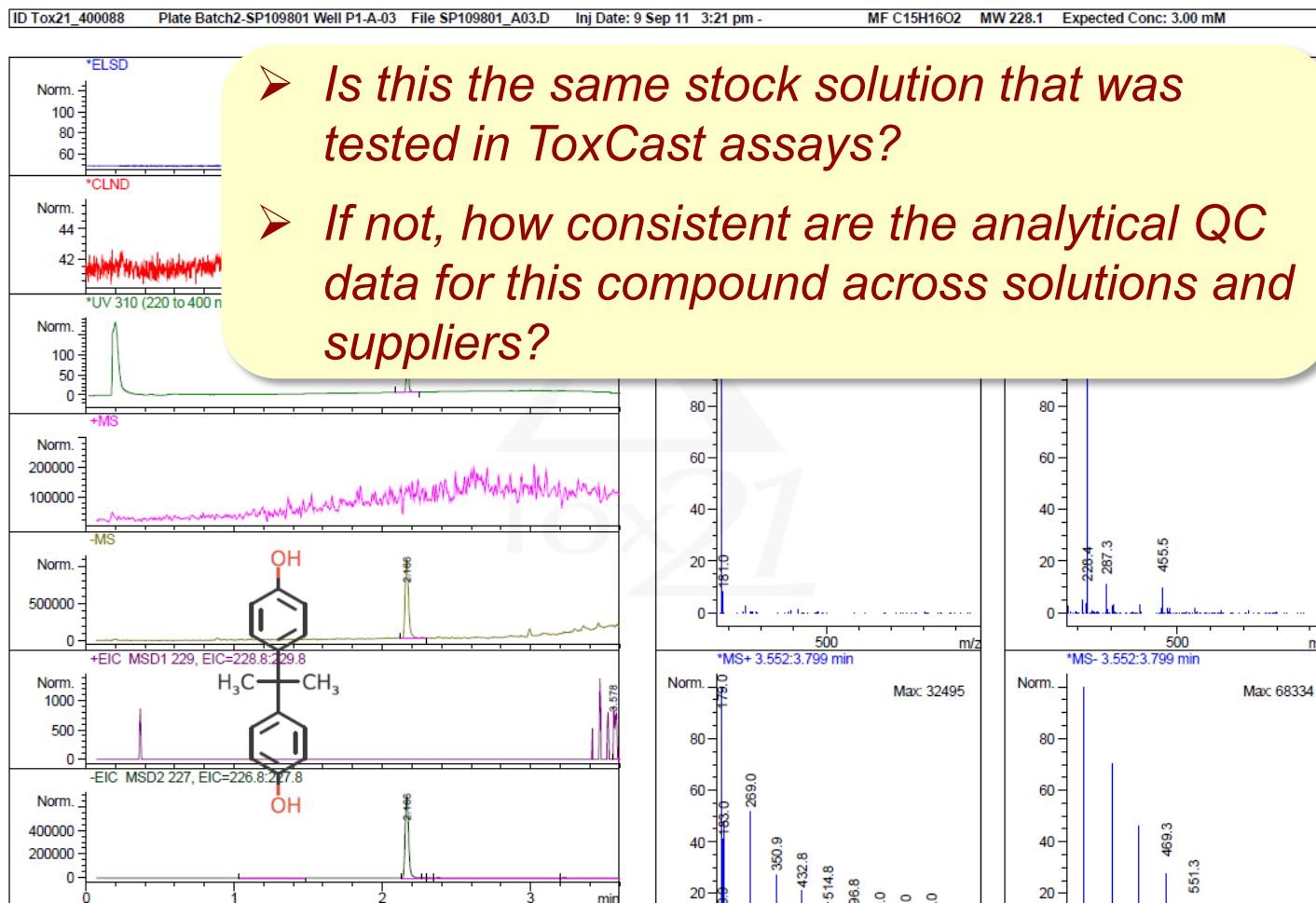
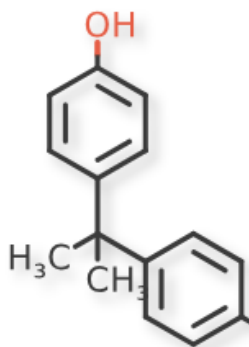
Other bookmark



Tox21

Home / Tox21 Samples / Tox21

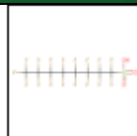
## Bisphenol A



MW Confirmed, Purity>90%

OpAns\_Process.MAC Version A.01.10 - Dec 9, 2010

# Some don't ...



Perfluorooctanesulfonic acid

1763-23-1 | DTXSID3031864

Searched by DSSTox Substance Id.

<https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID3031864#invitrodb-bioassays-toxcast-tox21>

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

SAFETY

ADME

EXPOSURE

BIOACTIVITY

TOXCAST: SUMMARY

EDSP21

TOXCAST/TOX21

PUBCHEM

TOXCAST: MODELS

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

LITERATURE

LINKS

COMMENTS

## ToxCast/Tox21

QC Data ID

Tox21\_400083

Grade

Not determined

Description

Analysis in progress

Assay Selection: 71 Selected

☒ Active ☐ Inactive ☐ All

Filter assays

A Single Assay Can Have Multiple Charts ☒

Representative Samples Only

Bioactivity Summary

Number of Charts: 271

Home / Tox21 Samples / Tox21\_400083

[https://tripod.nih.gov/tox21/samples/Tox21\\_400083](https://tripod.nih.gov/tox21/samples/Tox21_400083)

# PFOS



QC Grade

T0 ☐ Unknown/Inconclusive

T4 ☐ Unknown/Inconclusive

Identifiers

Tox21 Tox21\_400083

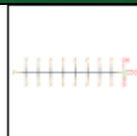
NCATS NCGC00164449-04

CAS 1763-23-1

PubChem 144214044

DTXSID DTXSID3031864

# But sometimes additional chemical knowledge is important ...



Perfluorooctanesulfonic acid

1763-23-1 | DTXSID3031864


Searched by DSSTox Substance Id.


<https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID3031864#invitrodb-bioassays-toxcast-tox21>

ToxCast/Tox21

- *PFOS (and other PFAS) are unusual in their properties often requiring customized analytical approaches*
- *Commercially available sources of PFOS contain 10-40% branched form (i.e., not pure!)*
- *Branched PFOS can have significantly different ADME properties from linear form!*



T0  Unknown/Inconclusive

T4  Unknown/Inconclusive

Tox21 Tox21\_400083

NCATS NCGC00164449-04

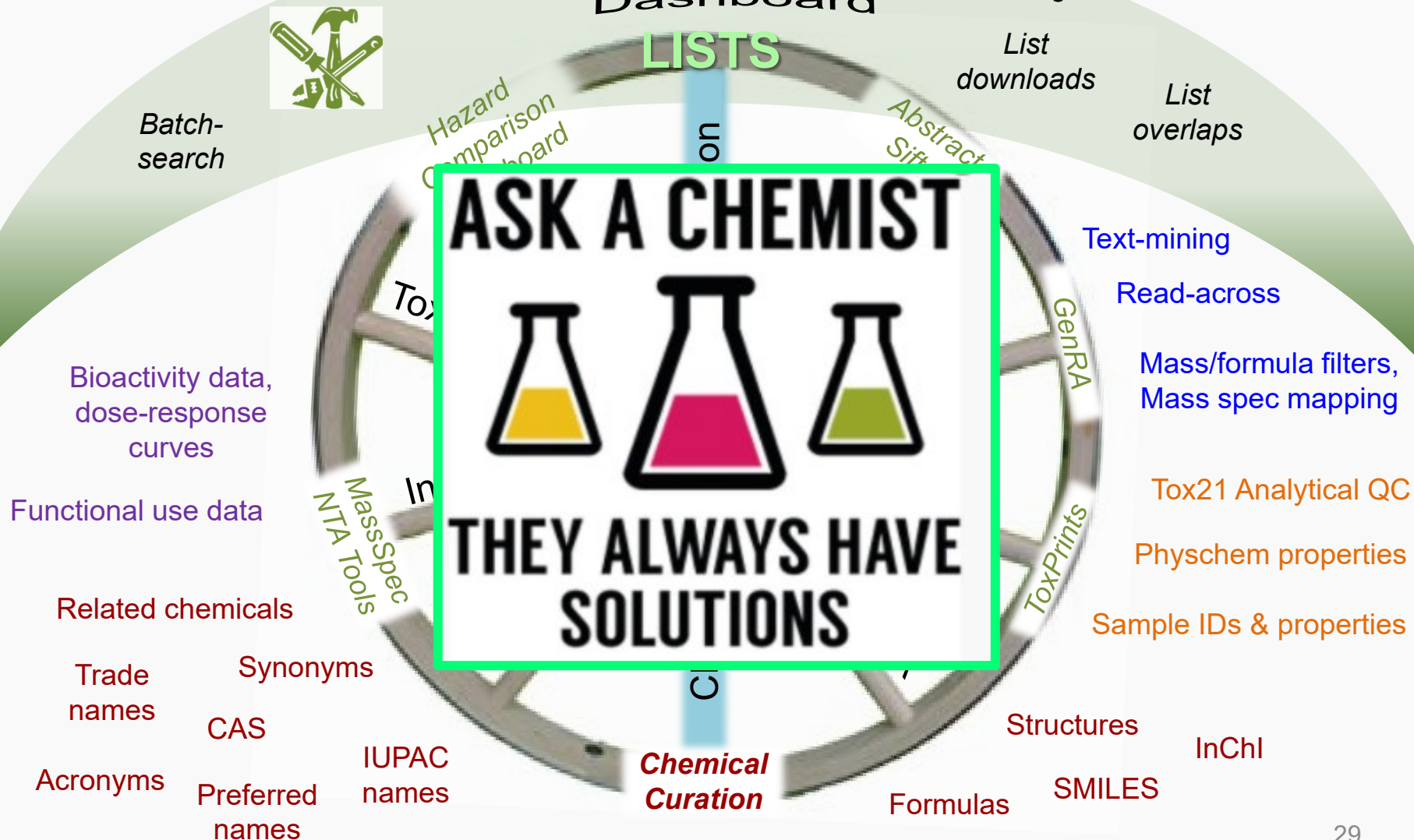
CAS 1763-23-1

PubChem 144214044

DTXSID DTXSID3031864



## EPA's CompTox Chemistry Dashboard



# Acknowledgements:

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## ✦ Chemistry Team & DSSTox Curators

Chris Grulke (ChemReg)

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Indira Thillainadarajah, Saku Sivasupramaniam, Brian Meyer, Vicente Samano, Linda Adams

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## ✦ ChemTrack

Kathy Coutros

## ✦ Tox21 Analytical Team (NCATS, NTP)

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*This work was reviewed by EPA and approved for publication but does not necessarily reflect official Agency policy.*