

# Expansion of DSSTox: Leveraging public data to create a semantic cheminformatics resource with quality annotations for support of U.S. EPA applications

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*This work was reviewed by the U.S. EPA and approved for presentation but does not necessarily reflect official Agency policy.*

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ACS Spring Meeting, San Diego, CA*

# EPA's National Center for Computational Toxicology (NCCT)



- ToxCast (EPA) & Tox21 (Multi-Agency)
  - screening >3800 (ToxCast) to >10K (Tox21) environmentally relevant chemicals across 10's to 100's of HTS assays
- ACToR, ExpoCast, CPCat, ToxRef DB
  - meshed CAS lists, product-use database, exposure models, guideline animal toxicity study reference DB
- Public-facing, web-dashboards (ToxCast, EDSP, ...)
  - facilitate access to & utility of EPA data

*Chemical  
databases*

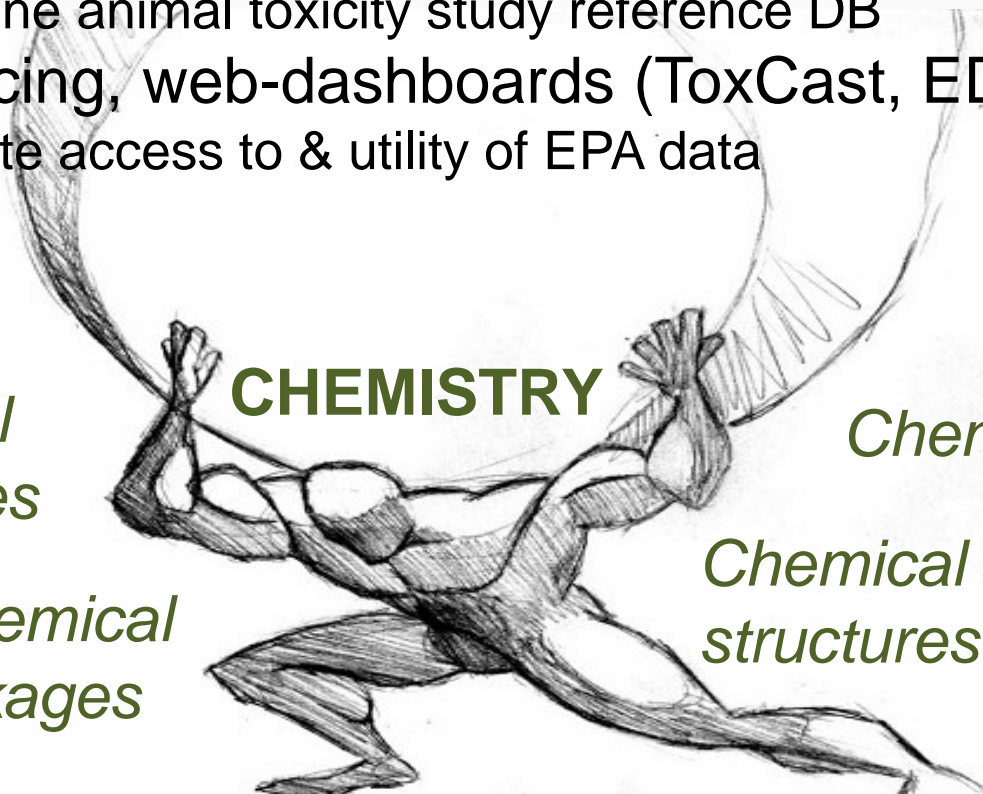
**CHEMISTRY**

*Cheminformatics*

*Chemical  
linkages*

*Chemical  
structures*

*SAR/QSAR  
models*



# Current NCCT activities



- Building a new cheminformatics architecture and public-facing chemical dashboard
- Aiming to be the host for curated chemistry across EPA
- Integrating NCCT and agency resources –both internal *and* external
- Designing tools and “services” to underpin other EPA research efforts
  - *Predictive modeling*
  - *Read-across*
  - *Non-targeted screening (linking to analytical data)*

Why build yet another public chemistry  
database and web-interface?

# Improve chemistry linkages across EPA Resources



- NCCT ToxCast / EDSP Dashboards
- NCCT ACToR, ExpoCast, CPCat
- EPA Chemical Safety & Sustainability (CSS) research
- EPA Substance Registry System (SRS)
- EPA Integrated Risk Information System (IRIS)
- EPA Office of Pesticides (Inerts, Active Ingredients)
- EPA Endocrine Disruption Screening Program (EDSP)
- EPA Office of Water's Chemical Contaminants List
- EPA Office of Pollution Prevention & Toxics ChemView
- EPA EcoTox, WebICE, etc.

*Lots of CAS-name lists !!*

# Using Chemistry to improve linkages across EPA Resources



Integrated Risk Information System

https://www.epa.gov/iris

EPA United States Environmental Protection Agency

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### RDX Public Comment Draft Toxicological Review Released in Advance of Public Science Meeting

- IRIS Toxicological Review of Hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) (Public Comment Draft)
- Meeting Details and Key Dates
- Register Now!

1 2 3 4

**Exact name/CAS match only**

### Staying Connected

- How IRIS connects with you
- How you can connect with IRIS

Get email alerts

sign up

### Search IRIS

By Chemical, CASRN, or Keyword

Search the IRIS database

Search

EPA's mission is to protect human health and the environment. EPA's IRIS Program supports this mission by identifying and characterizing the health hazards of chemicals found in the environment. Each IRIS assessment can cover a chemical, a group of related chemicals, or a complex mixture.



# Using Chemistry to improve linkages across EPA Resources



Integrated Risk Information System (IRIS) - U.S. Environmental Protection Agency

**A-Z List of Substances**

The substances in IRIS are listed in order alphabetically by the substance name. You can click on the Alphabetical letter corresponding to the chemicals beginning with that letter to list the relevant substances, or use your browser's "Find" command to search for a substance name or Chemical Abstracts Service Registry Number (CASRN).

The IRIS Program does not currently develop updated assessments for registered pesticides unless the registered pesticides also have non-pesticide uses. The IRIS user should consult OPP Reregistration Eligibility Decision (RED) documents prepared by the Office of Pesticide Programs for additional health assessment information (see link provided in the OPP Reregistration Eligibility Decision (RED) column below).

(To search the IRIS database, use [Advanced Search](#))

You will need Adobe Reader to view some of the files on this page. See [EPA's PDF page](#) to learn more.

\* Refers to the most recent statement of or change to a toxicity value [RfD, RfC, slope factor or unit risk], or most recent significant statement of or change to the basis or justification for the conclusions in the assessment. This column is provided for the convenience of the IRIS user. For specific information, see the Revision History for each substance.

- [A-Z List of Substances](#)
- [Substances Sorted by Date](#)

**Example:**

EPA's mission is to protect human health and the environment. EPA's IRIS Program supports this mission by identifying and characterizing the risks to human health from chemicals found in the environment. IRIS assessment can cover a chemical, a mixture of chemicals, or a complex mixture.

# Using Chemistry to improve linkages across EPA Resources



https://ofmpub.epa.gov/sor\_internet/registry/substreg/home/overview/home.do

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Substance Registry Services (SRS)

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You are here: [EPA Home](#) > [System of Registries](#) > [SRS](#) > [About](#)

## About

About Search & Retrieve Automated Services References

### Overview

#### Providing Quality Substance Identification Information

Substance Registry Services (SRS) is the Environmental Protection Agency's (EPA) central system for information about substances that are tracked or regulated by EPA or other sources. It is the authoritative resource for basic information about chemicals, biological organisms, and other substances of interest to EPA and its state and tribal partners.

The SRS makes it possible to identify which EPA data systems, environmental statutes, or other sources have information about a substance and which synonym is used by that system or statute. It becomes possible therefore to map substance data across EPA programs regardless of synonym.

The system provides a common basis for identification of, and information about:

- Chemicals

#### System of Registries

- [Registry of EPA Applications, Models and Databases \(READ\)](#)
- [Data Element Registry Services \(DERS\)](#)
- [Terminology Services \(TS\)](#)
- [Reusable Component Services \(RCS\)](#)
- [Facility Registry Services \(FRS\)](#)
- [Environmental Dataset Gateway \(EDG\)](#)



# Using Chemistry to improve linkages across EPA Resources



Browser address bar: [https://ofmpub.epa.gov/sor\\_internet/registry/substreg/home/overview/home.do](https://ofmpub.epa.gov/sor_internet/registry/substreg/home/overview/home.do)

Browser tabs: About SRS

Browser menu: File Edit View Favorites Tools Help

Browser toolbar: Adobe Connect Central L... US EPA Computational Toxicolog... US EPA Computational Toxicolog... Convert

Navigation bar: Learn the Issues Science & Technology Laws & Regulations About EPA Search EPA.gov

## Substance Registry Services (SRS)

You are here: EPA Home > System of Registries > S

### About

About **Search & Retrieve** Autom

### Search and Retrieve

About **Search & Retrieve** Automated Services References

#### Substance Search

**Search by Substance Information**

**Synonym** Please enter a CAS Name, Biological Name, EPA Registry Name or other Synonym  
  
☒ Contains ☐ Begins With ☐ Exact Match

**Substance Identifier** Please enter a CAS Number, TSN, EPA Identifier, Internal Tracking Number, or Alternate Identifier

**Substance Type** Narrow your Search by identifying whether the Substance is a Chemical, Biological Organism, Physical Property, Miscellaneous Object, or Not Known  
All

**Overview**

**Providing Quality Substance Ident**

Substance Registry Services (SRS) is the authoritative resource for basic information about substances that are of interest to EPA and its state and tribal partners.

The SRS makes it possible to identify substances and have information about a substance and its properties, making it possible therefore to map substance data across various EPA systems.

The system provides a common basis for:

- Chemicals

# EPA ACToR – CAS List Meshing



**EPA** United States Environmental Protection Agency

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## ACToR

You are here: EPA Home » Computational Toxicology Research » ACToR » Home

[ACToR](#) | [ToxCast Data](#) | [Exposure Data](#) | [DSSTox](#) | [CSS Dashboards](#) | [CPCat](#) | [EDSP21](#)

[Home](#) | [Basic Info](#) | [Data Collections](#) | [Structure Search](#) | [Assays By Toxicity](#) | [Assays By Category](#) | [External Links](#) | [Download](#) | [Help](#)

ACToR (Aggregated Computational Toxicology Resource) is EPA's online warehouse of all publicly available chemical toxicity data and can be used to find all publicly available data about risks to human health and the environment. ACToR aggregates data from over 1,000 public sources on over 500,000 chemicals and is searchable by chemical name and other identifiers. The data warehouse:

- Allows users to search and query data from other EPA chemical toxicity data collections including:
  - ToxCastDB (data from screening 1,800 chemicals in over 700 high-throughput assays)
  - Exposure Data (consolidate and link human exposure and exposure factor data with chemical identification)
  - DSSTox (provides high quality chemical structures and annotations).
- Includes chemical structure, physico-chemical values, in vitro assay data and toxicity data
- Includes, but not limited to, high and medium production volume industrial chemicals

Chemical Name Parameters

☒ Search on Chemical Names ☐ Search on CAS Numbers

Match by

☐ exact ☒ any

Enter Chemical Name:

- Structures retrieved from DSSTox by CAS, if available, by PubChem, if not
- No curation, same data quality as public sources
- Original DSSTox (25K) → ACToR (500K)

## Why build yet another public chemistry database and web-interface?

- Focus on environmental chemicals
- Focus on data quality
- Better support EPA research & chemical regulatory programs

# DSSTox Update

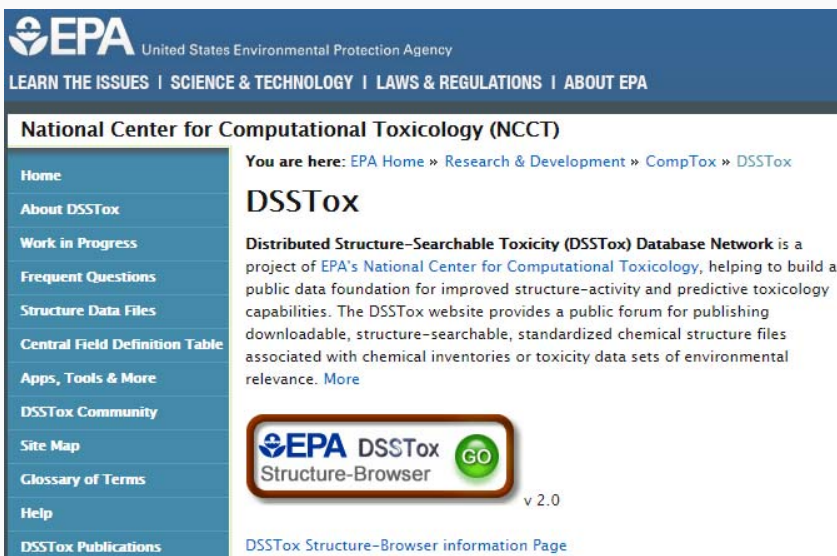


## DSSTox\_v1



## DSSTox\_v2

- Convert DSSTox tables to MySQL
- Develop curation interface & cheminformatics workflow
- Expand chemical content
- Web-services & Dashboard access



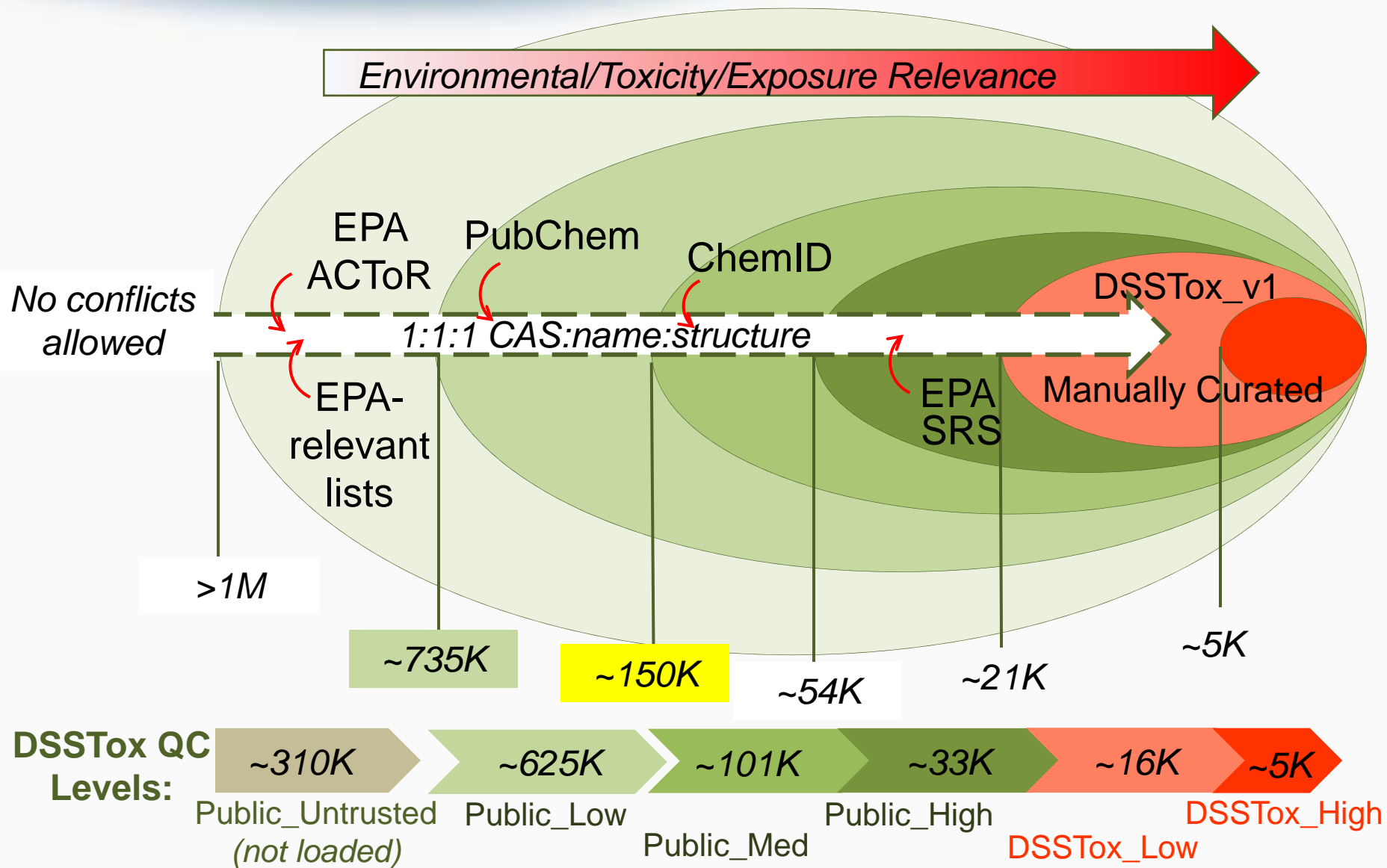
- Manually curated 25K substance records
- EPA-focus, environmental tox datasets
- Emphasis on accurate CAS-name-structure annotations
- Public resource for high-quality structure-data files (SDF)



How did we go from 25K to 735K  
chemicals while addressing EPA's  
needs & quality concerns?



# Building DSSTox\_v2



Why the concerns for data quality?

# Chemical errors associated with toxicity information (ACS, 2009)

## Chemical Annotation of Public resources

Generic  
Chemical of  
Toxicological  
Interest

- ✓ Name is misspelled or incorrect
- ✓ CAS is invalid or retired
- ✓ CAS and name do not agree
- ✓ Name and structure do not agree
- ✓ Name is insufficient for structure assignment
- ✓ Insufficient description of substance

## Sample Annotation & QC

Procure  
from  
Chemical  
Supplier

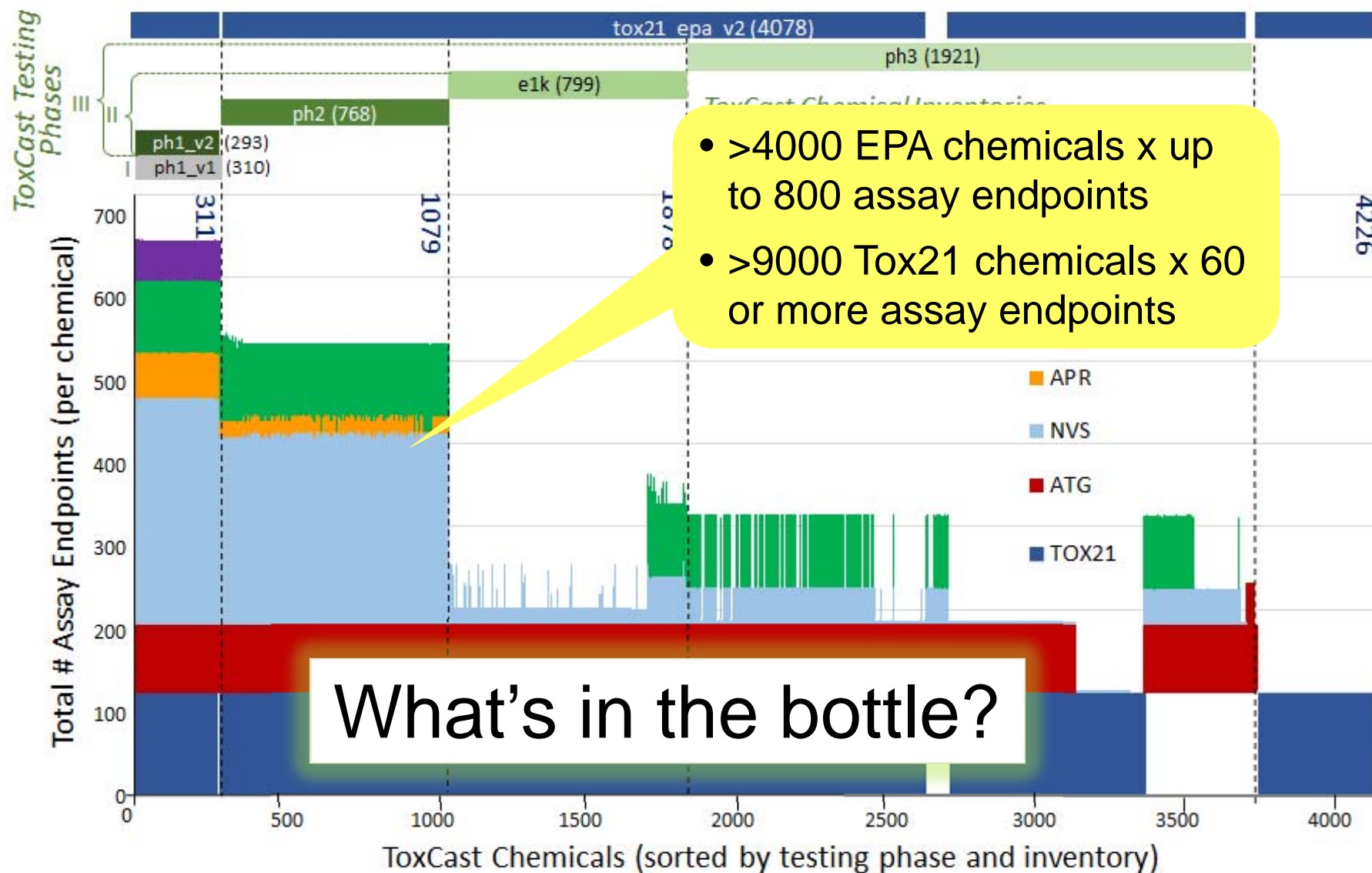
Name, CAS,  
purity (COA)

MW, dose

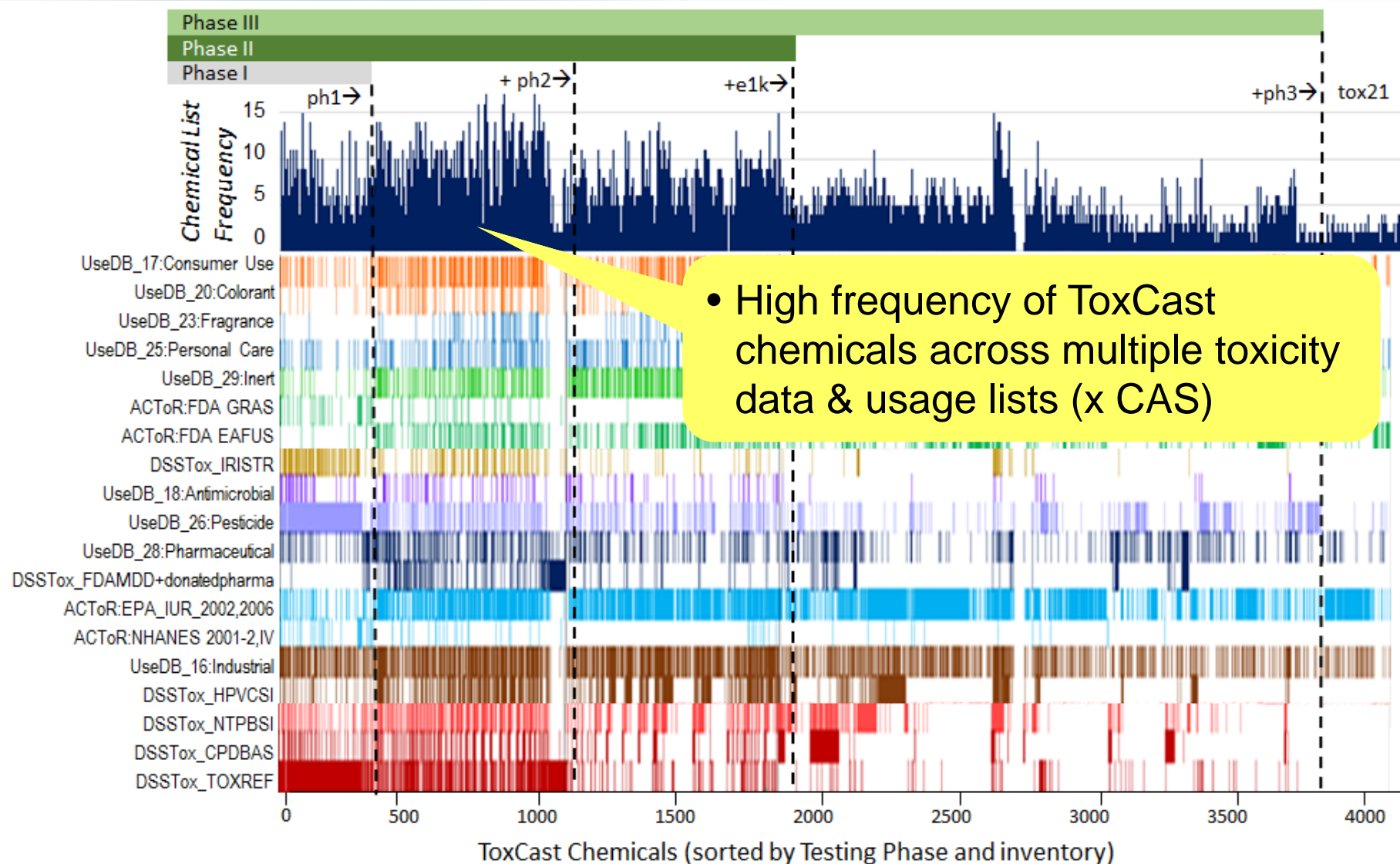
IC 50

- ✓ Not same as generic chemical  
*Salt, isomer, ...*
- ✓ Name does not match COA  
*hydrate, stereo*
- ✓ Wrong MW, dose
- ✓ COA purity <90%
- ✓ Purity <90%
- ✓ Active impurities
- ✓ Sample degrades
- ✓ Rxn with solvent

# ToxCast chemical x assay counts summary (Jan 2016)



# Tox Data & Use List Coverage of ToxCast Chemicals

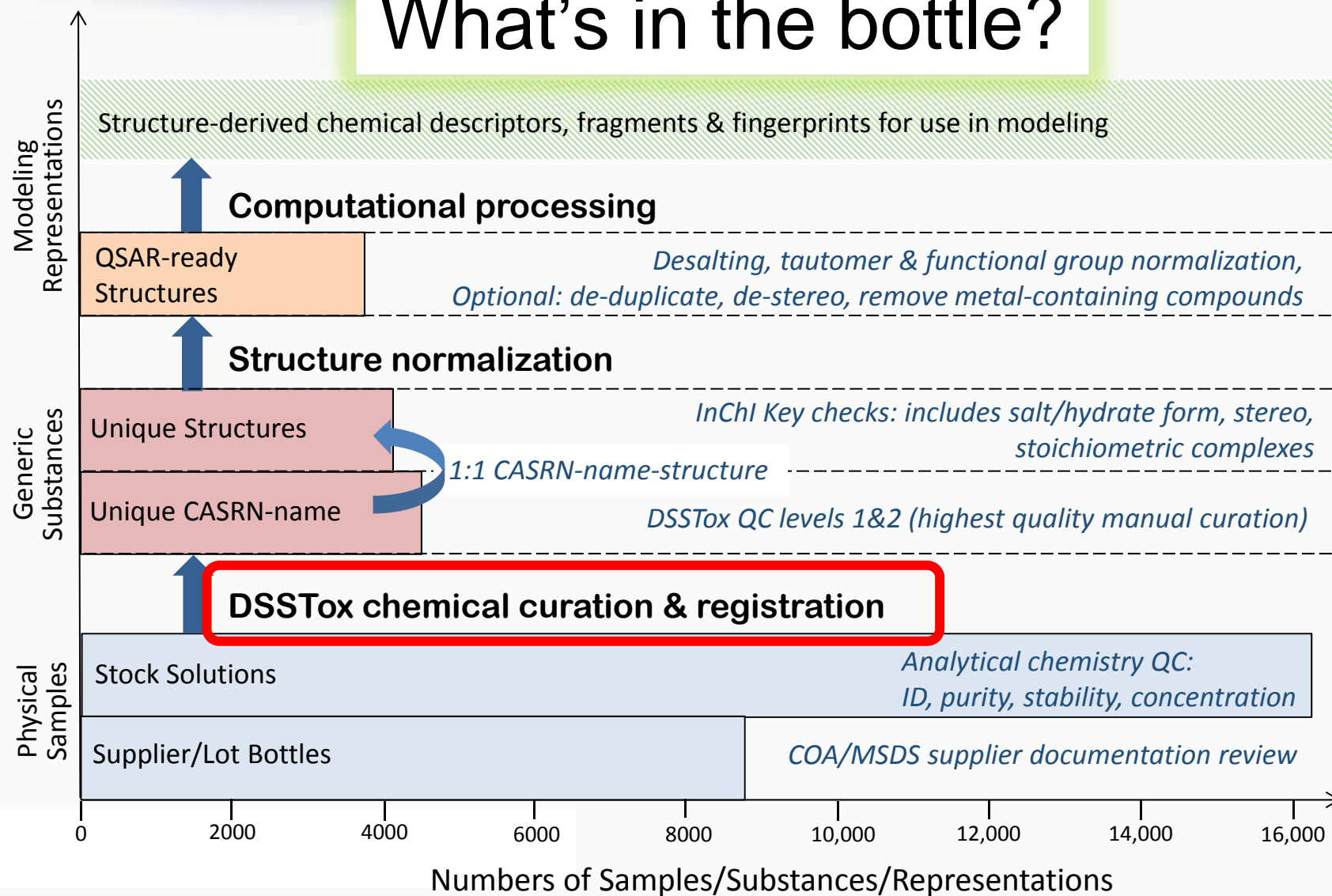




# ToxCast Chemical Library: Quality Control Steps



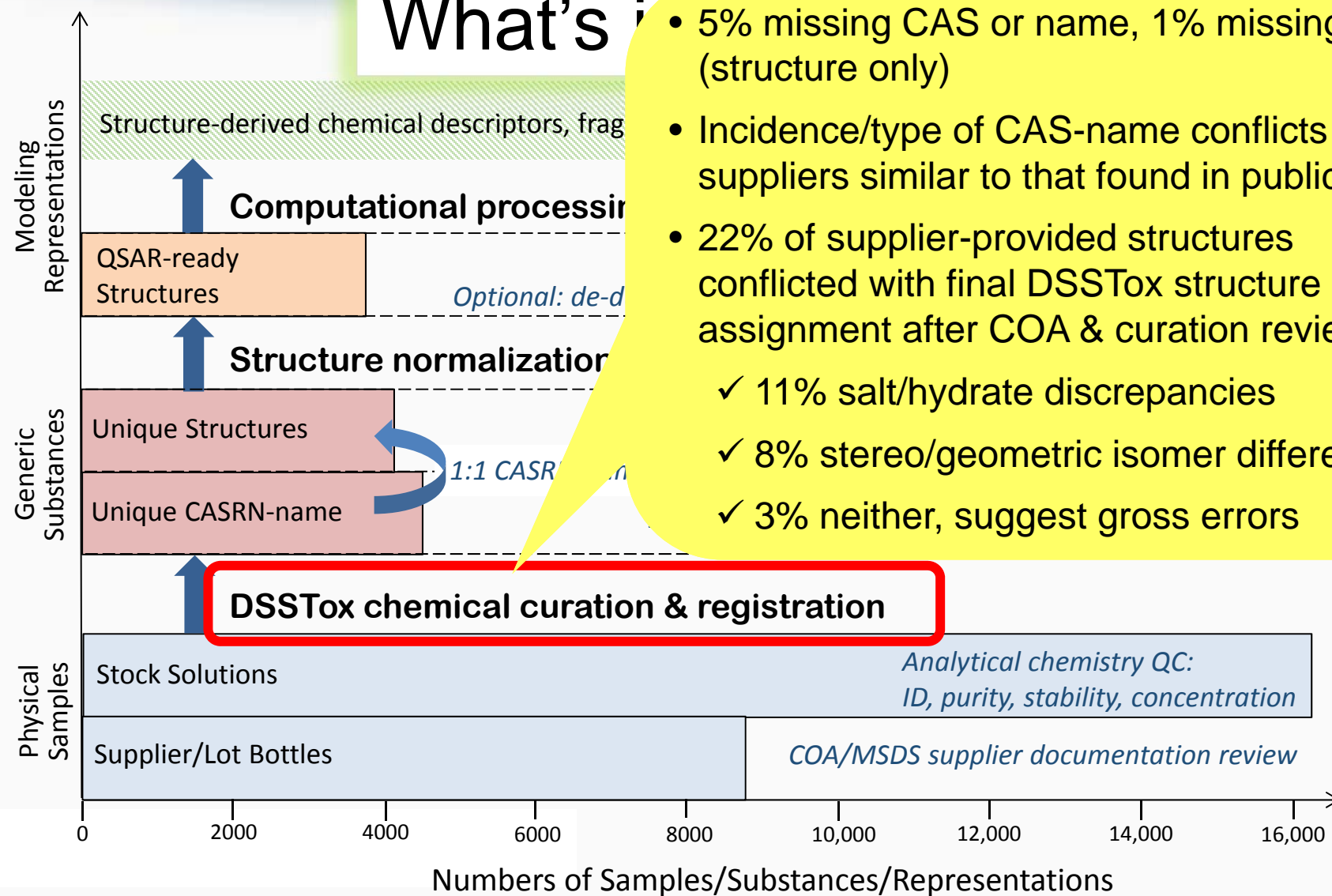
## What's in the bottle?



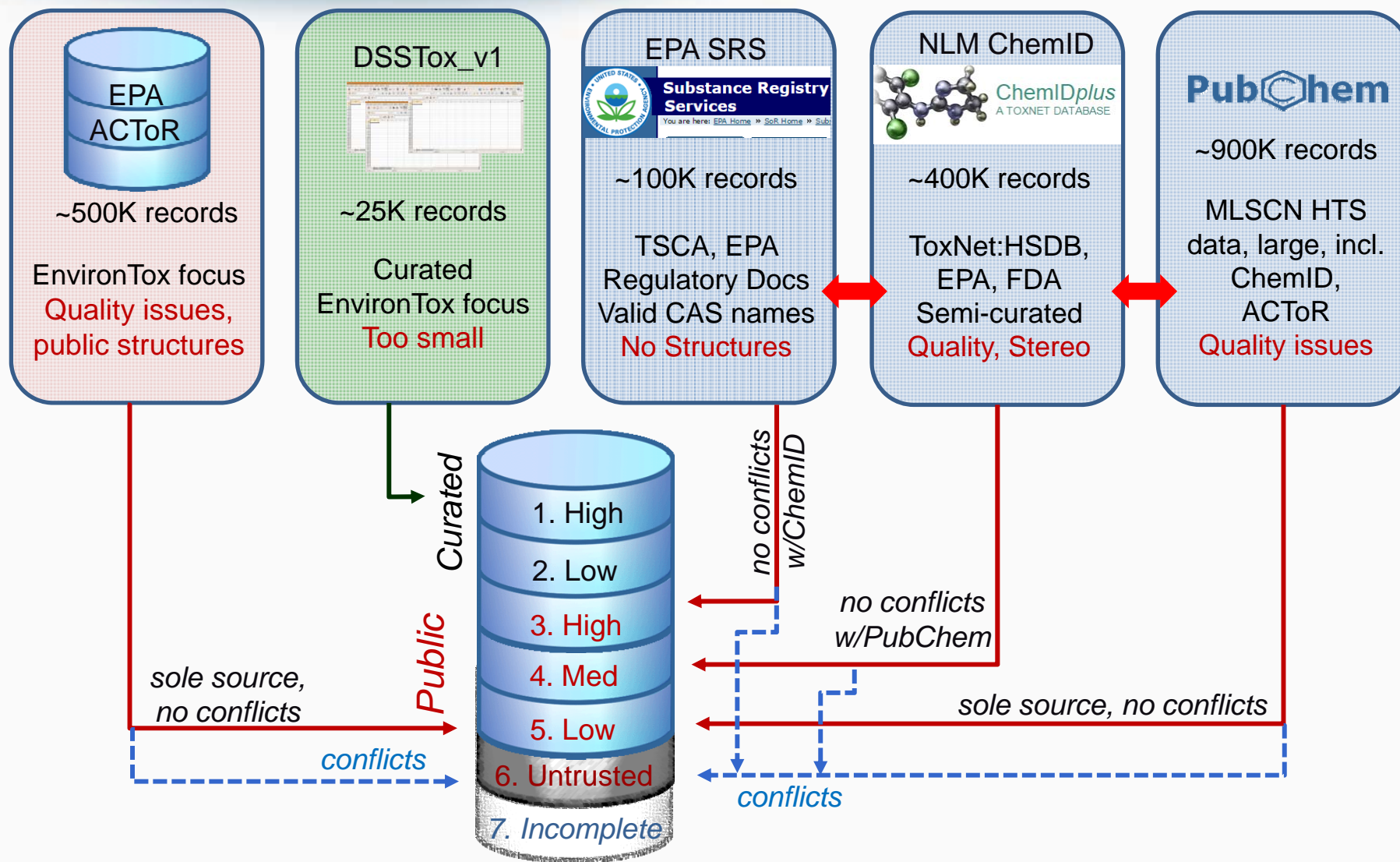
# ToxCast Chemical Library: Quality Control Steps



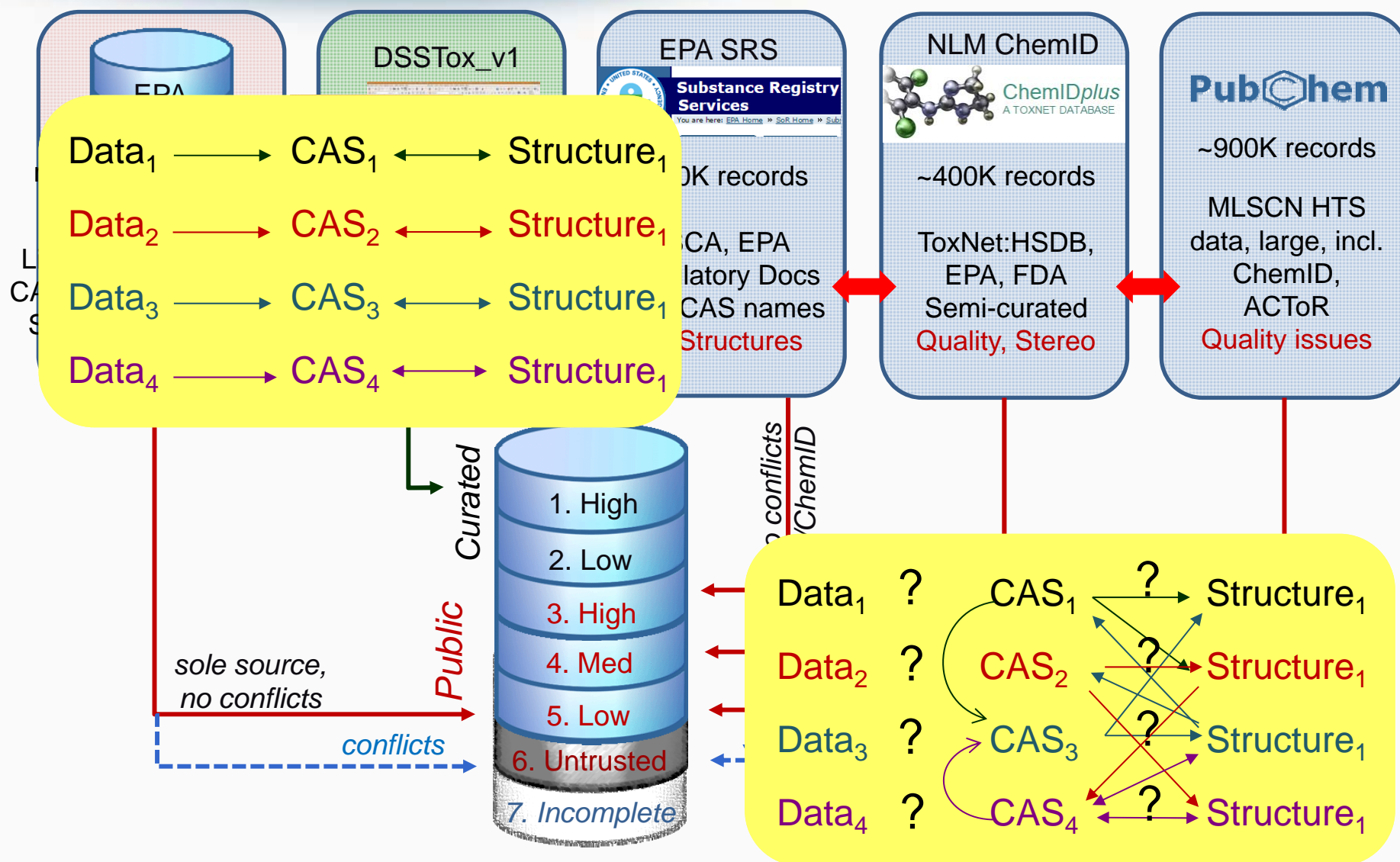
## What's i



# DSSTox\_v2 CAS-Structure Sources: QC levels



# DSSTox\_v2 CAS-Structure Sources: QC levels





# DSSTox\_v2 Construction



## *Data source load order:*

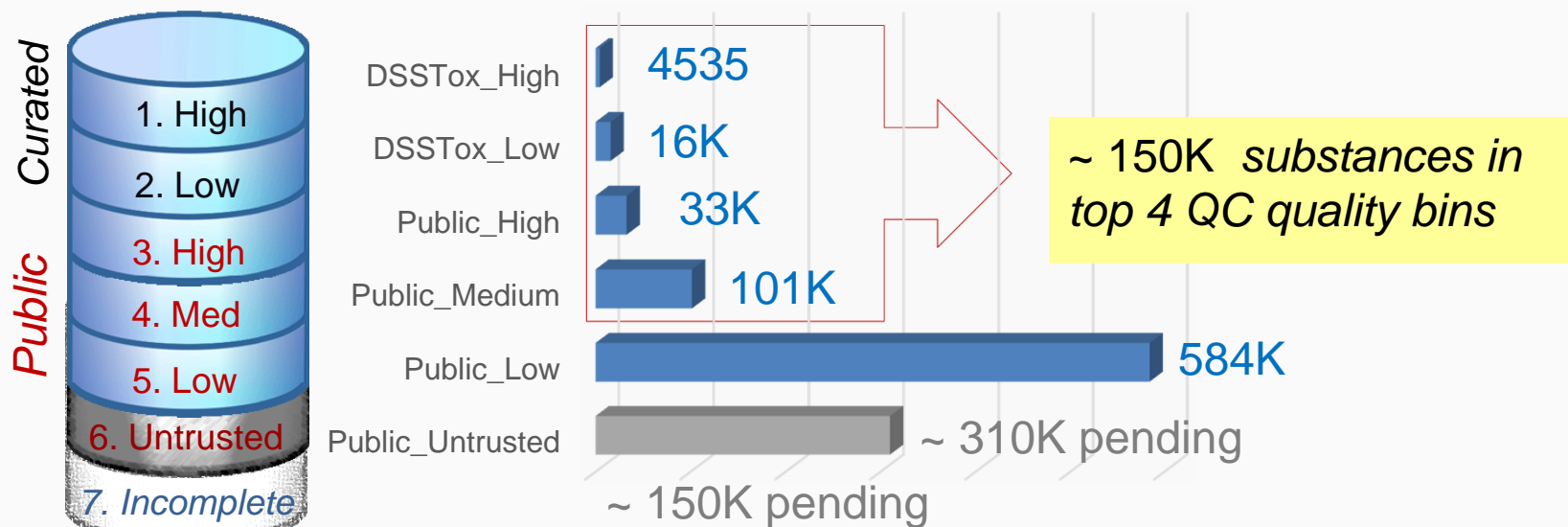
- 1) DSSTox\_v1 (~22K)
  - ✓ 1:1 CAS-structure mappings
  - ✓ Assign NOCAS\_GSID
  - ✓ Related CAS & structure mappings (e.g., NOCAS, mixtures)
- 2) EPA SRS (~77K)
  - ✓ *systematic name* → *structure conversion*
  - ✓ *internal CAS-structure conflicts (12.5%)*
  - ✓ *ChemID conflicts (24% of 30K overlaps)*
  - ✓ *DSSTox conflicts (8% of 6200 overlaps) → queue for curation*
- 3) ChemID (~400K)
  - ✓ *internal CAS-structure conflicts (4.5%)*
  - ✓ *PubChem conflicts (45% of 225K overlaps) ... OUCH!!*
  - ✓ *DSSTox conflicts (11% of 2300 overlaps) → queue for curation*
- 4) And so on ...



# DSSTox\_v2 Totals



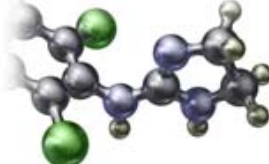
## QC Level Totals (12Jun2015)



### QC Levels

DSSTox_High:	Hand curated - highest confidence
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)
Public_Untrusted:	Postulated, but found to have conflicts in public sources

e.g., structure mapping collision

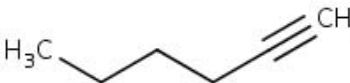



**ChemIDplus**  
A TOXNET DATABASE

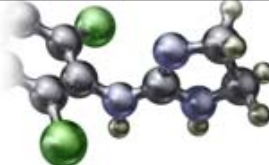
[Start New Query](#) [Modify Query](#) [Search History](#) [Show Query](#)  
[Switch to Summary View](#)

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

**Molecular Formula**  
C<sub>6</sub>H<sub>10</sub>  
**Molecular Weight**  
82.145





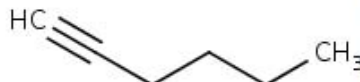


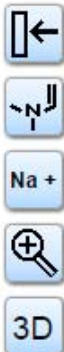
**ChemIDplus**  
A TOXNET DATABASE

[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





# e.g., list curation problems



Raw file → Initial manual review, clean-up → store source CAS-names  
curator checks mapping  
curator registers 32

*Functional  
Use DB:*

List of 176 CAS  
chemicals  
indicated for  
use as  
“Flame  
Retardants”

17 CAS, no  
name

9 invalid CAS  
(manual fix)

10 duplicate  
names,  
different CAS

23 duplicate  
CAS, different  
names

152 cleaned  
list, no  
duplicates

121 CAS map  
to DSSTox\_v2

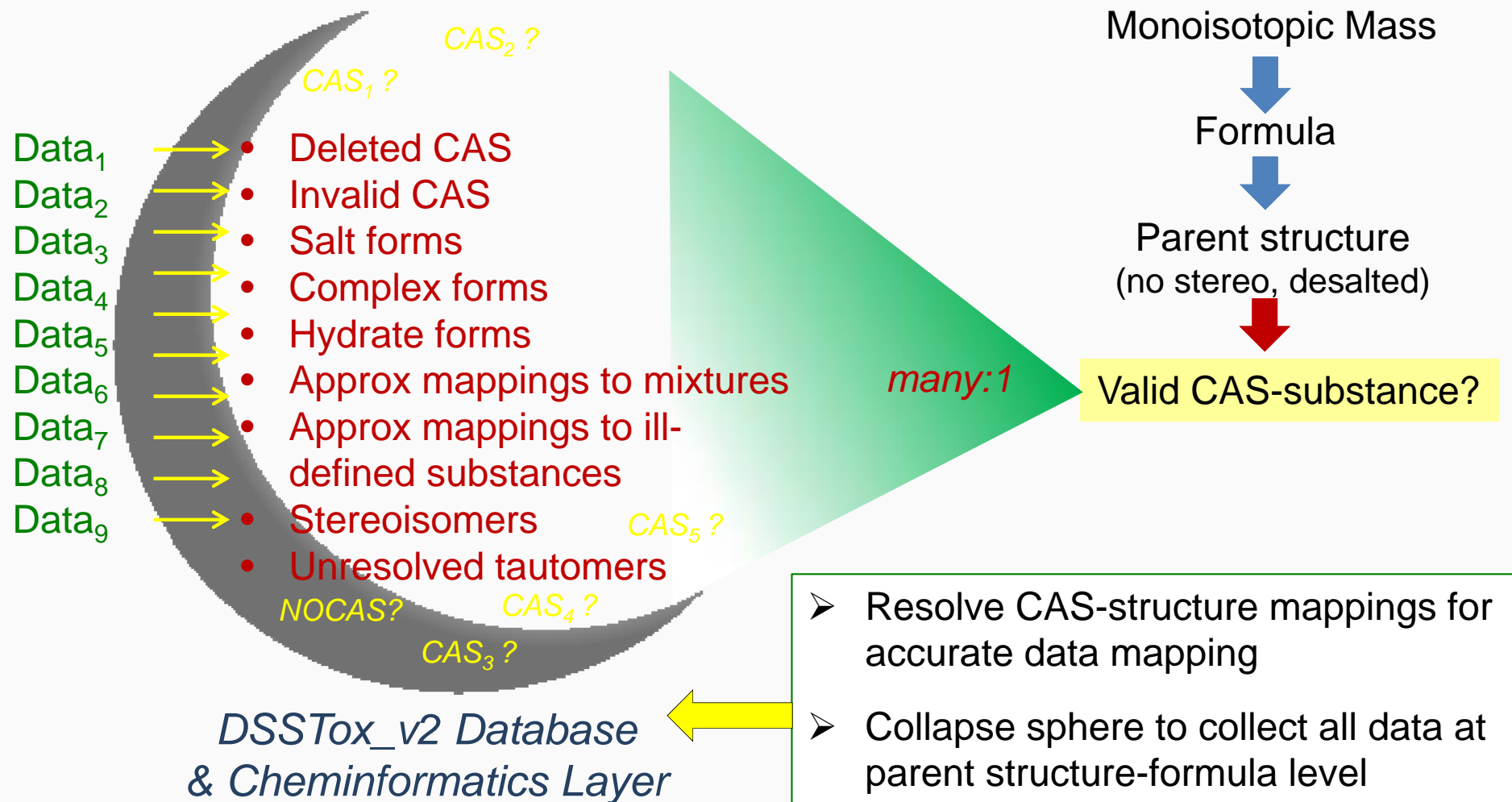
32 CAS not  
found

15% CAS error or no name, 19% conflicts, 18% CAS not found,  
80% of cleaned list map to existing DSSTox\_v2 content

# e.g., non-targeted MS screening of environmental samples



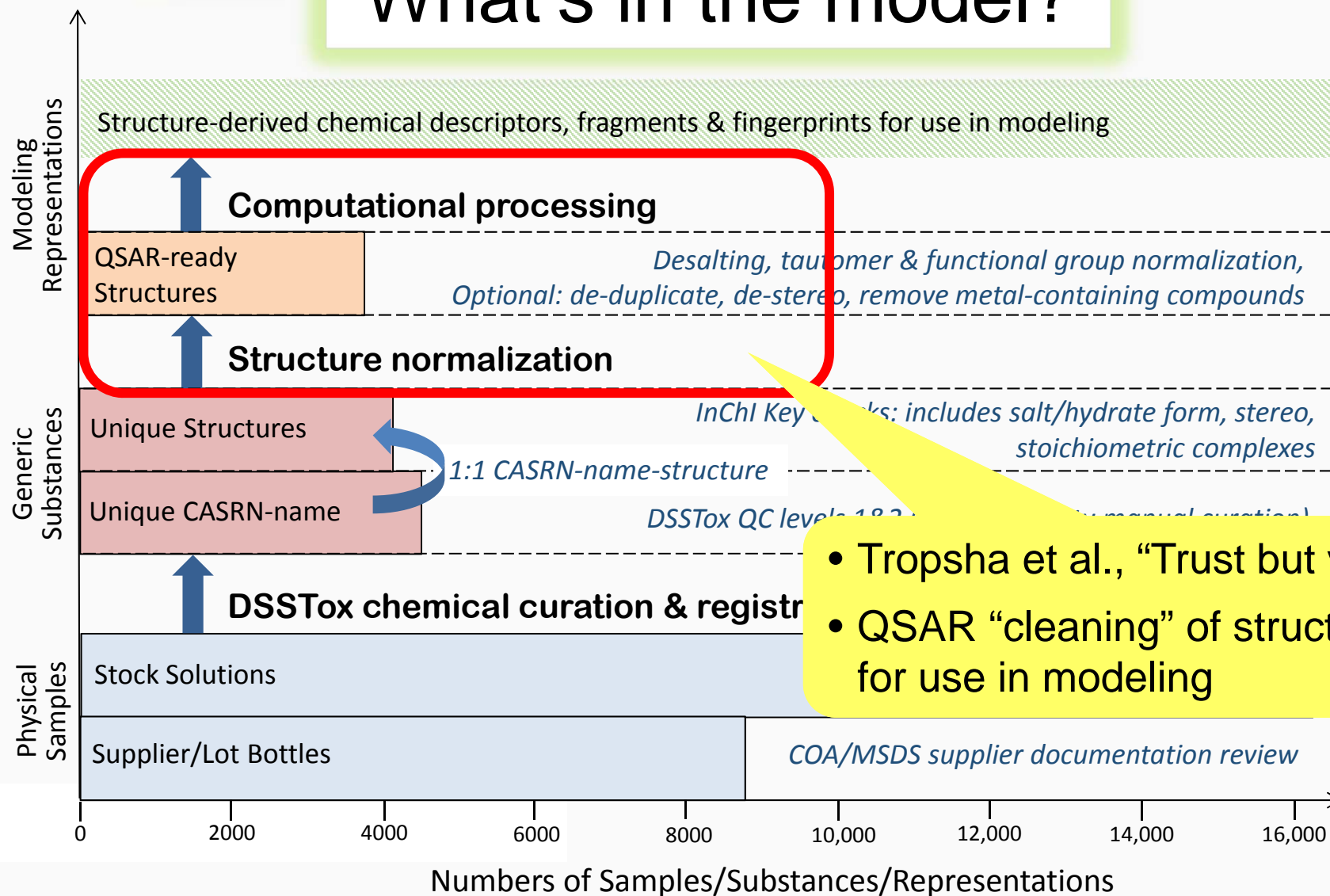
## CAS-Name-Structure “Sphere of Confusion”



# ToxCast Chemical Library: Quality Control Steps



## What's in the model?



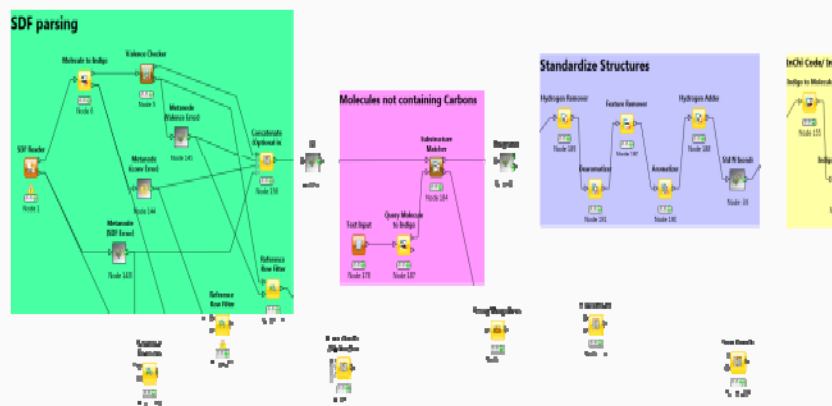
- Tropsha et al., "Trust but verify"
- QSAR "cleaning" of structures for use in modeling



# KNIME structure-“cleaning” workflow

<https://www.knime.org/knime>

- Combine community approaches to structure processing
- Develop a flexible workflow to be used by EPA and shared publicly
- Process DSSTox files to create “QSAR-ready” structures



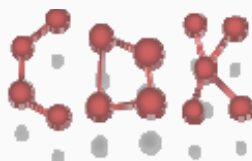
- ✓ Parse SDF, remove fragments
- ✓ Explicit hydrogen removed
- ✓ Dearomatization
- ✓ Removal of chirality info, isotopes and pseudo-atoms
- ✓ Aromatization + add explicit hydrogen atoms
- ✓ Standardize Nitro groups
- ✓ Other tautomerize/mesomerization
- ✓ Neutralize (when possible)

*Publicly available cheminformatics toolkits in KNIME:*

Indigo



Open Source Cheminformatics and Molecular Modeling



Pharmaceutical Data  
Exploration Laboratory

*Slide courtesy of K. Mansouri*

# DSSTox Chemical Registration Tool



## ACToR-DSSTox Chemical Registration

Search/Edit a  
Single Record

Add Deleted  
Cas

Browse/Curate  
Records

Manage  
Chemical Lists

Export  
DSSTox

Structure  
Search

Welcome aricha02

Matched Name.

You are editing the  
record associated with

GSID: 20182

CASRN: 80-05-7

GSID

or

DTXID

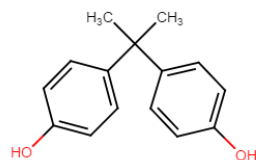
or

CAS

or

Name bisphenol a

search



### Calculate from Structure

Substance\_ID: [DTXSID7020182](#)

CAS: 80-05-7

Name: Bisphenol A

Substance  
Type: Single Compound

QC Level: DSSTox High

Data Source: STN(DSSTox)

QC Notes:

Compound\_ID: DTXCID30182

Chemical Shown: Tested Chemical

CAS-Compound  
Relationship  
Notes:

Source of CAS-  
Compound:

STN(DSSTox)

Double Stereo:

None

Chiral Stereo:

None

Chemical Form:

Organic

Organic Form:

Parent

► Synonyms (73)

► Other Cas (5)

► More Specific Cas (0)

► Less Specific Cas (0)

Update Record

# DSSTox List Curation Tool



ChemReg\_v0.8.0 x ChemReg\_v0.8.0 x

ag.epa.gov:8502/ChemRegJSF/pickChemicalList.jsf

Yahoo Mail 16 Google Calendar Gmail Inbox Gmail Contacts Dropbox Evernote ChemReg\_v0.7.7 EPA TO Tracking Go... DSSToxViewer\_v0.2.1 JIRA » Other bookmarks

## ACToR-DSSTox Chemical Registration

Search/Edit a Single Record Add Deleted Cas Browse/Curate Records Manage Chemical Lists Export DSSTox Structure Search

Welcome aricha02

Editing Listname: RUSYN\_ORDER

External Check Results	
Description	Records
Matched CASRN. Matched NAME.	104
CASRN matched other record. Matched NAME.	1
Matched CASRN. Matched NAME2STRUCT.	2
Matched CASRN.	32
Matched CASRN. NAME2STRUCT matched other record.	1
No Hits	10

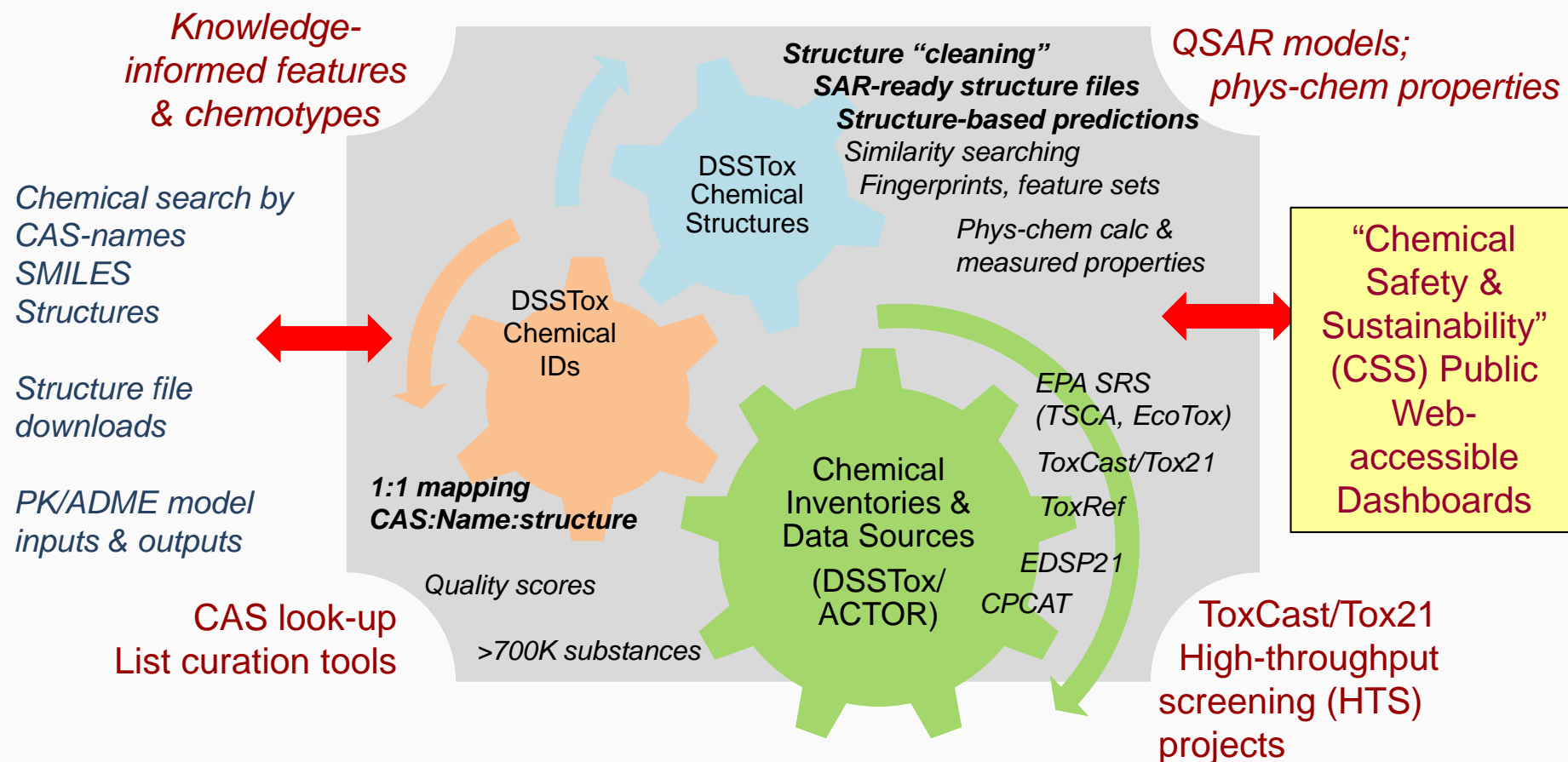
### Substance Mapping

(1 of 5) 1 2 3 4 5 25

Source Casrn	Source Name	Hit Substance_ID	Hit Casrn	Hit Name	
183133-96-2	cabazitaxel	<a href="#">DTXSID40171389</a>	183133-96-2	Cabazitaxel	<a href="#">Validate Mapping</a>
59729-33-8	citalopram	<a href="#">DTXSID8022826</a>	59729-33-8	Citalopram	<a href="#">Validate Mapping</a>
115256-11-6	dofetilide	<a href="#">DTXSID5046433</a>	115256-11-6	Dofetilide	<a href="#">Validate Mapping</a>
54143-56-5	flecainide acetate	<a href="#">DTXSID8020626</a>	54143-56-5	Flecainide acetate	<a href="#">Validate Mapping</a>
161967-81-3	grepafloxacin hydrochloride	<a href="#">DTXSID0046692</a>	161967-81-3	Grepafloxacin hydrochloride	<a href="#">Validate Mapping</a>
84057-84-1	lamotrigine	<a href="#">DTXSID2023195</a>	84057-84-1	Lamotrigine	<a href="#">Validate Mapping</a>
84371-65-3	mifepristone	<a href="#">DTXSID5023322</a>	84371-65-3	Mifepristone	<a href="#">Validate Mapping</a>
186826-86-8	moxifloxacin hydrochloride	<a href="#">DTXSID4045921</a>	186826-86-8	Moxifloxacin hydrochloride	<a href="#">Validate Mapping</a>

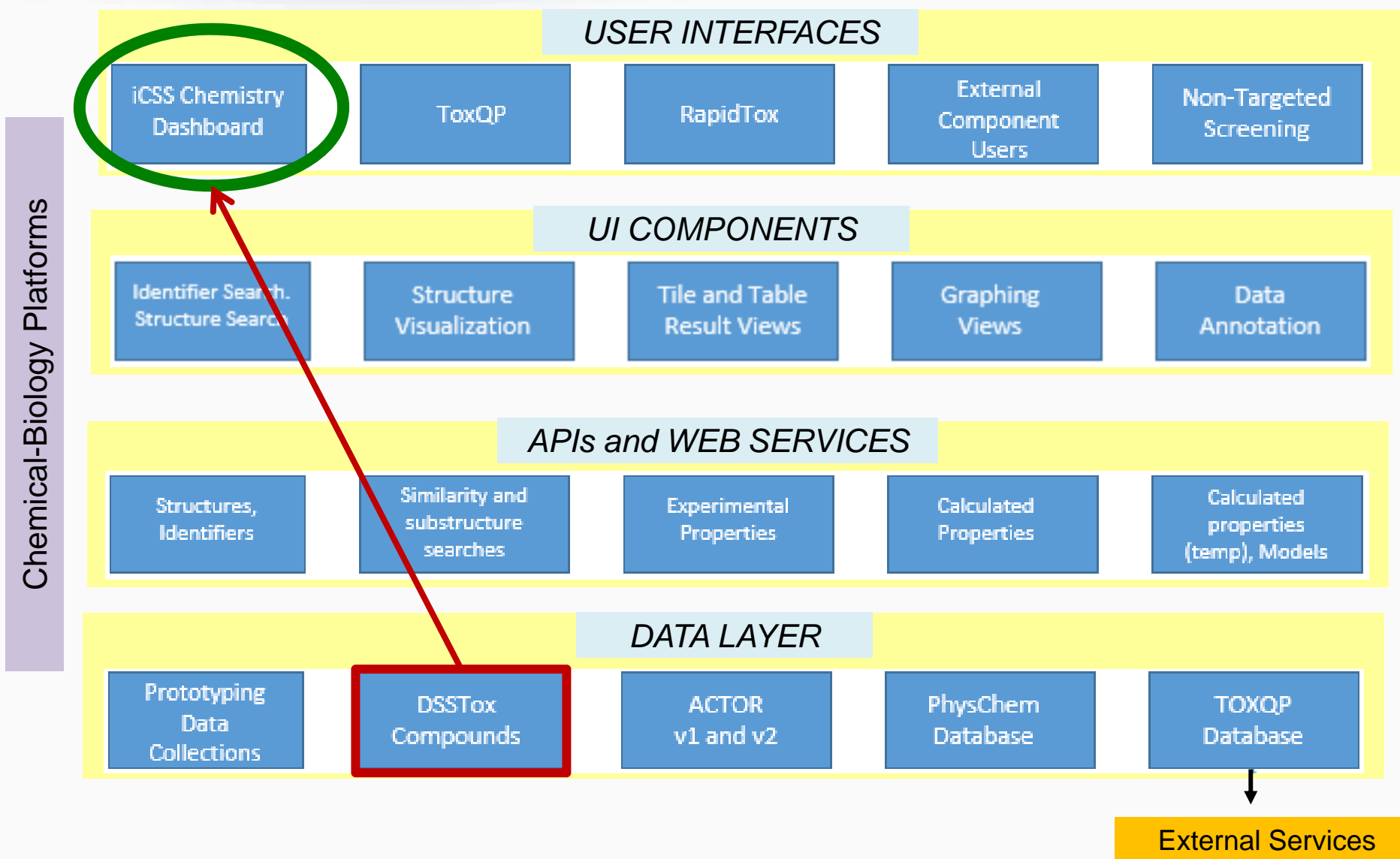
Conflicts binned to facilitate curation

# Chemistry Foundation to Support Multiple NCCT & EPA Projects





# Building the Chemistry Software Architecture





# iCSS Chemistry Dashboard



D  
E  
V  
E  
L  
O  
P  
M  
E  
N  
T

- Web interface supporting EPA's Chemical Safety & Sustainability research (iCSS)
- To be released April 2016
- Will provide public access to DSSTox db
- Initially name/ID-based searching only ...but



## Chemistry Dashboard

Search a chemical by systematic name, synonym, CAS number, or InChIKey



☐ Single component search ☐ Ignore isotopes

Need more? Use [advanced search](#).

734 Thousand Chemicals

# Componentizing API for Resolving Chemical Names/IDs



Search a chemical by systematic name, synonym, CAS number, or InChIKey



- Look familiar?
  - *ChemSpider, PubChem, ChEMBL, NCI Resolver ...*
- ONE reusable EPA component API that searches for Names and CAS Registry Numbers...
- ... and SMILES, and InChIKeys, and recognizes invalid CAS Numbers, and converts SMILES when they aren't in DB, etc. etc.

# iCSS Chemistry Dashboard Releasing in April 2016



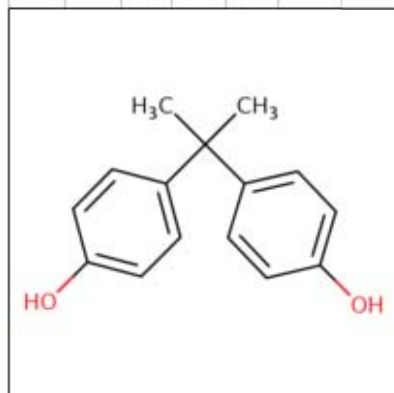
## Bisphenol A

80-05-7 **DTXSID7020182**

*Formerly DSSTox GSID, new unique public substance ID, essential for RDF/semantic web applications*

? Searched by Synonym: Found 1 result for 'bisphenol A'.

2D 3D



### Intrinsic Properties

Molecular Formula: C<sub>15</sub>H<sub>16</sub>O<sub>2</sub>

Average Mass: 228.291 g/mol



Monoisotopic Mass: 228.11503 g/mol



### Structural Identifiers

### Citation

Chemical  
Properties

External Links

Synonyms

PubChem  
Biological Activities

PubChem Articles

PubChem Patents

Comments

CSV Excel

Property	Average (Exp.)	Range (Exp.)	Average (Pred.)	Range (Pred.)
<a href="#">Solubility</a>	0.001 (1)	0.0005257 to 0.0005257	0.38 (2)	0.003675 to 0.7565
<a href="#">Melting Point</a>	154.929 (7)	153.0 to 158.0	144.033 (3)	131.8 to 158.0
<a href="#">Boiling Point</a>	200.0 (1)	200.0 to 200.0	348.95 (2)	334.4 to 363.5
<a href="#">LogP</a>	3.357 (3)	3.32 to 3.431	3.524 (3)	3.205 to 3.727
<a href="#">Atmospheric Hydroxylation Rate</a>	N/A	N/A	0.0 (1)	4.237e-11 to 4.237e-11

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DSSTox

Privacy

Accessibility

Help

# Build once, use many times

Chemical Input:

(Retrieved using standard InChIKey)

Chemical Input:

(Retrieved using numeric identifier)

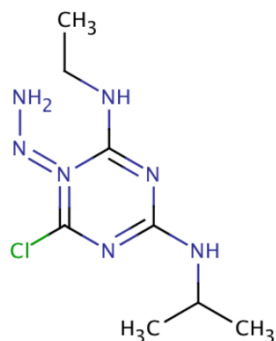
Warnings: Leading zeros stripped

Chemical Input:

Warnings: Identifier not found in DSSTox, Unable to resolve identifier

Chemical Input:

Warnings: Identifier not found in DSSTox



Chemical Input:

(Retrieved using standard InChIKey)

- Componentizing functionality for reuse
- Adopting a common development framework

# Synonym Sourcing & Chemical Name Searching



- Entering high-low quality chemical name synonyms for DSSTox (**NO COLLISIONS ALLOWED!**)
- 500,000 “synonyms” (names + IDs) loaded and growing
  - DSSTox historical resources (Done)
  - ChemID-Plus (Done)
  - CAS Common Chemistry (Done)
  - *ChEBI (to come)*
  - *ChemSpider Validated Synonyms (to come)*
- “Caffeine Fix” (used by ChemSpider & others) for partial & fuzzy name searching



# Where are we now?

- Public iCSS Chemistry Dashboard to be released April 2016
- DSSTox External IDs created for RDF linkages wherever DSSTox content is used publicly
  - e.g. Atrazine:
    - DTXSID9020112 (DTXSID.cksum.0.GSID)
- Curation continues...
  - *Prioritized EPA and ACToR lists*
- Coming over next year:
  - *Structure/substructure/similarity searching*
  - *List searching, structure downloads*
  - *Expanded webservices, open data & APIs*

- ▼ Curation Queue
  - ACToR
  - › ADME Database
    - AOP ADME/Exposure data
  - CERAPP
  - CTD (Comparative Toxicogenomics Database)
  - Curation Task Template
  - DrugBank
  - DSSTox\_v2 clean-up
  - ECHA skin sensitization
  - EcoTox Database
  - EPA Mechanism of Action
  - FDA Drugs (Leadscope)
  - FooDB
  - IRIS Dataset
  - LOPAC
  - Mass Spec Library Consolidation
  - NERL Scraped Names
  - NERL Scraped Names Part 2
  - NTPGTZ - NTP Zeiger GeneTox
  - OPP Inerts
  - OSWER Chemicals of Interest
  - PBPK Chemical Lists
  - PPRTV
  - Stereo Error Correction
  - Synonym addition
  - Tox21 Curation
  - ToxCast Curation
  - TSCA Work Plan 2014 Update
  - VTM Chemicals

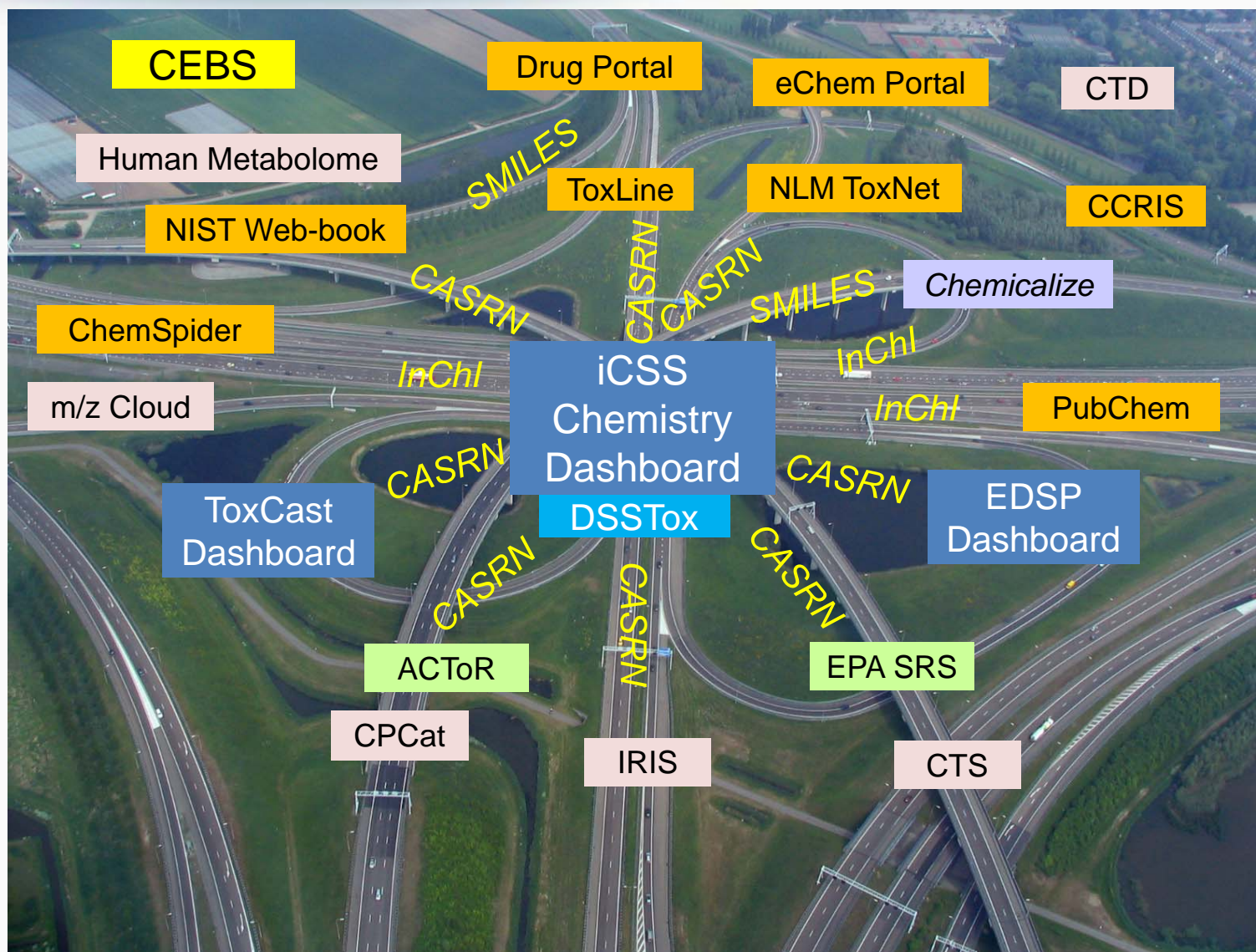
# How can others contribute & benefit?



- Chemically indexed content is crucial!
- Encourage use of DSSTox content, chemical list registration tool, and use of quality metrics for chemical annotations of data
- Greater linkages, use of web-services, standardized chemistry resources, cheminformatics
- But chemical indexing, linkages, and annotations are NOT enough

*→ Quality of chemical-data annotations needs to be improved!!!*

# A possible future for EPA ...





# Acknowledgements



## NCCT Contributors to DSSTox & Chemistry Dashboard

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