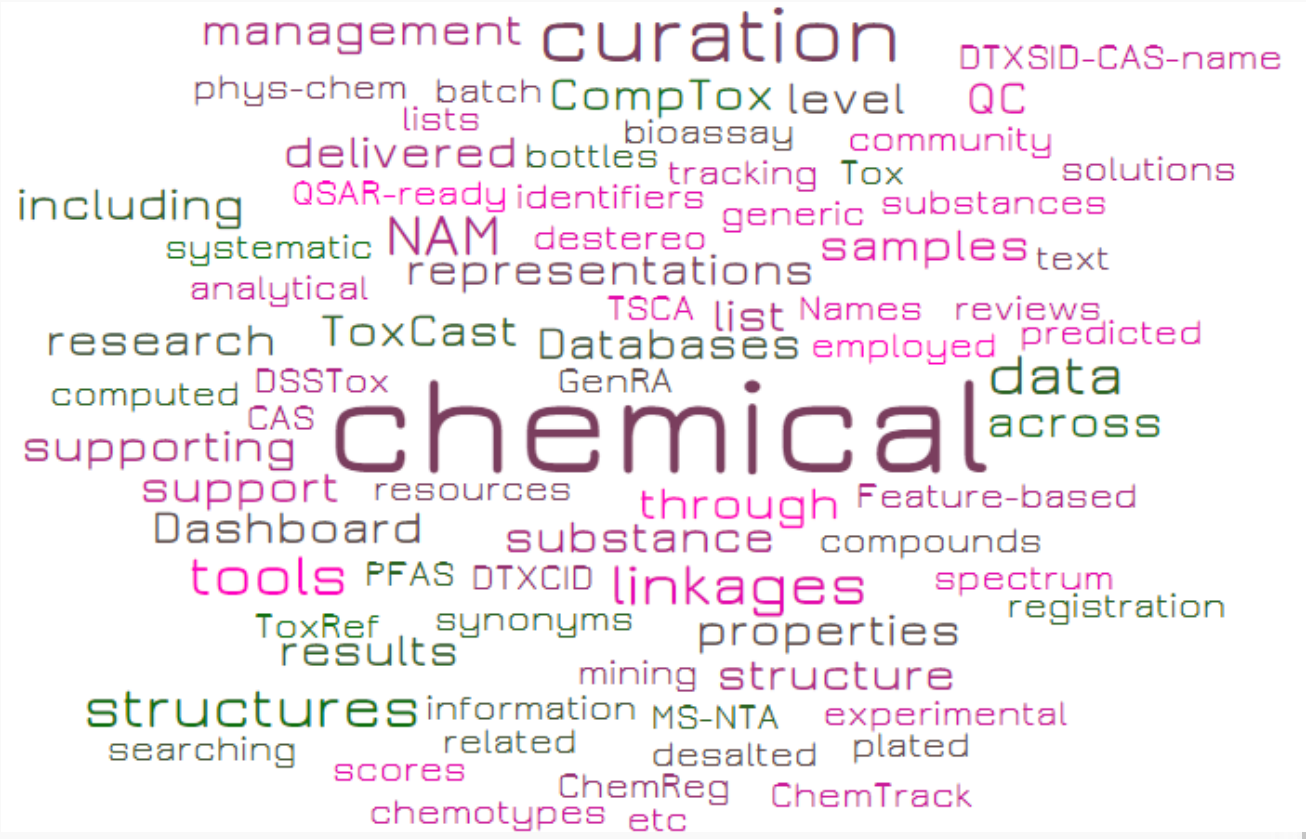
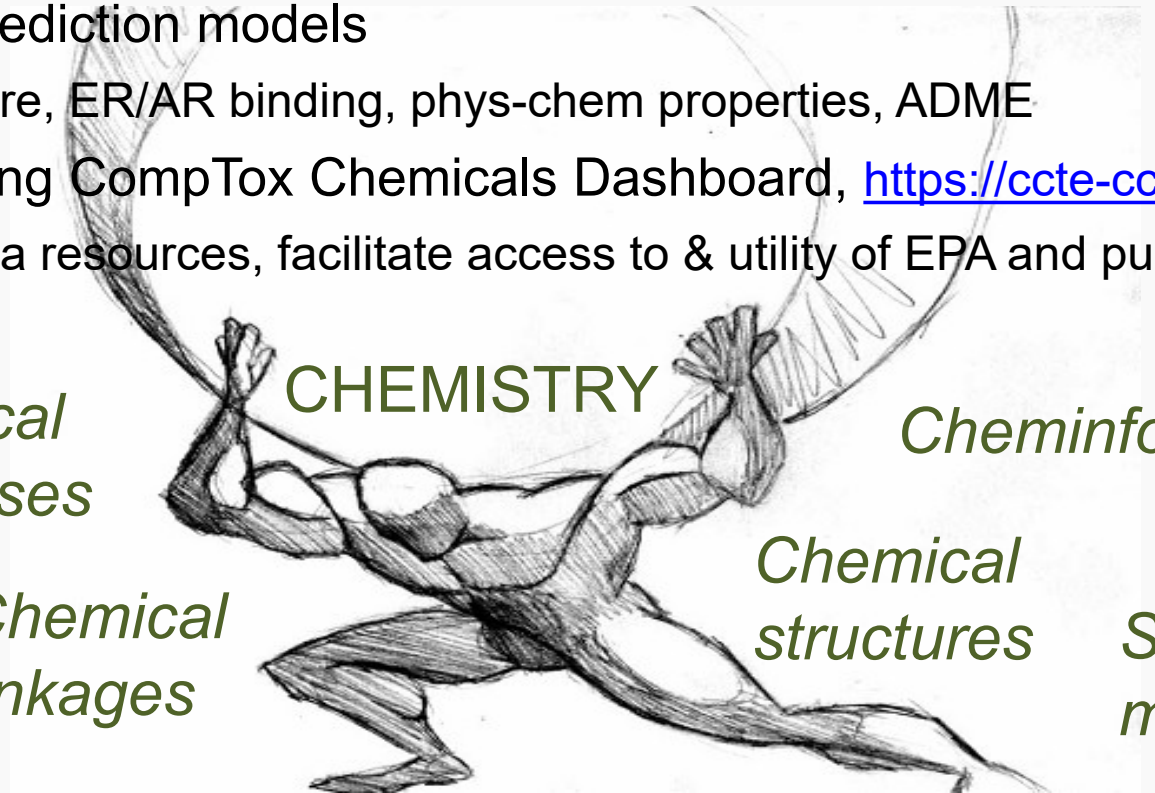
EPA's DSSTox Database: The strategic role and requirements of chemical curation



Ann M. Richard
Center for Computational Toxicology & Exposure
Office of Research & Development
US Environmental Protection Agency

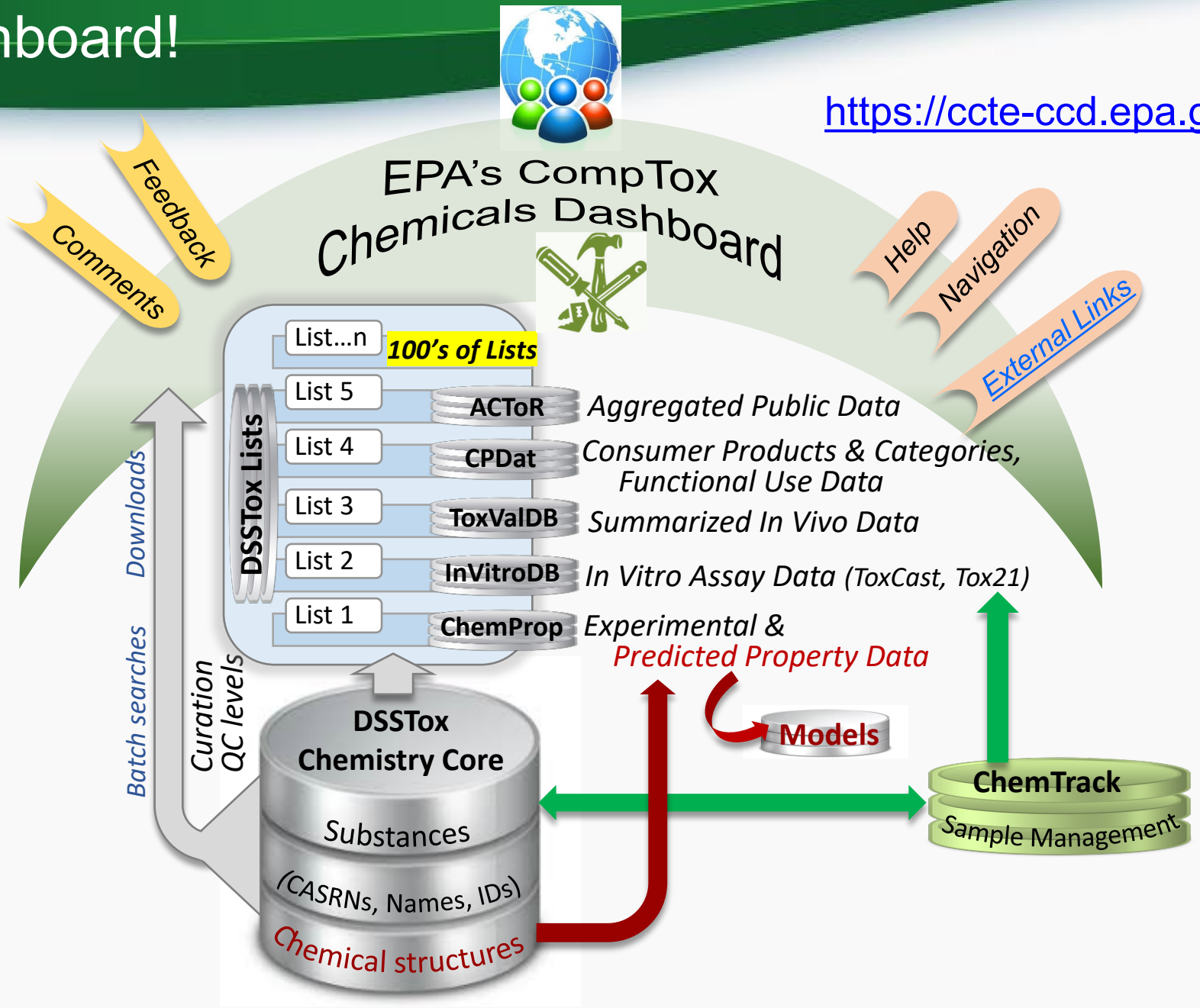
Linking data resources to support EPA Programs

- ToxCast (EPA) & Tox21 (Multi-Agency)
  - High-throughput screening >4000 (ToxCast) to >10K (Tox21) environmentally relevant chemicals across 10's to 100's of assays
- ACToR, ExpoCast, CPDat, ToxRef DB, TSCA, PFAS, EcoTox …. Lots of lists!!
  - meshed CAS lists, product-use database, *in vivo* reference data, etc.
- *In Silico* prediction models
  - exposure, ER/AR binding, phys-chem properties, ADME
- Public-facing CompTox Chemicals Dashboard, https://ccte-ccd.epa.gov/dashboard/
  - link data resources, facilitate access to & utility of EPA and public data



The Chemistry beast feeding the CompTox Chemicals Dashboard!

https://ccte-ccd.epa.gov/dashboard/

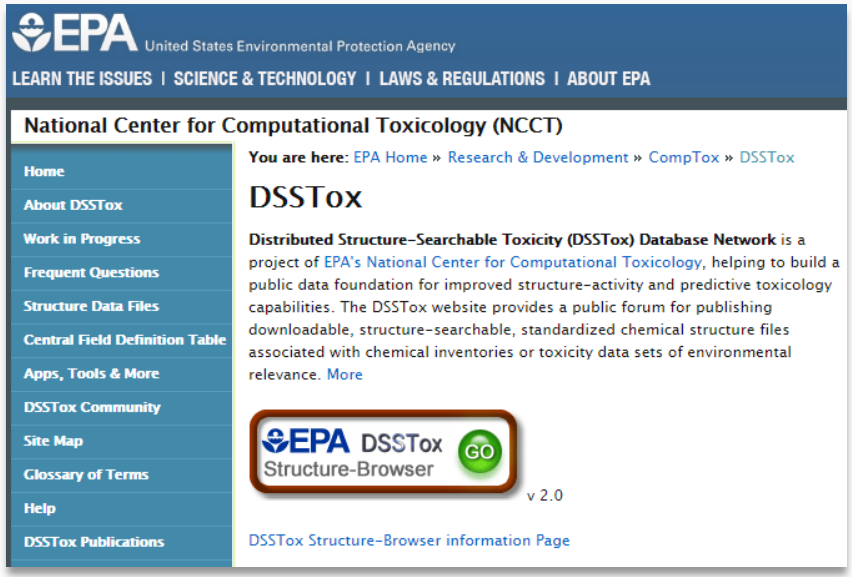


Why build yet another public chemistry database and web-interface?

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

DSSTox Update

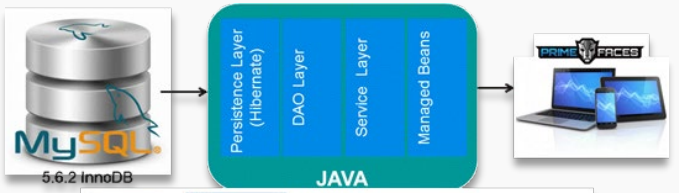
DSSTox_v1

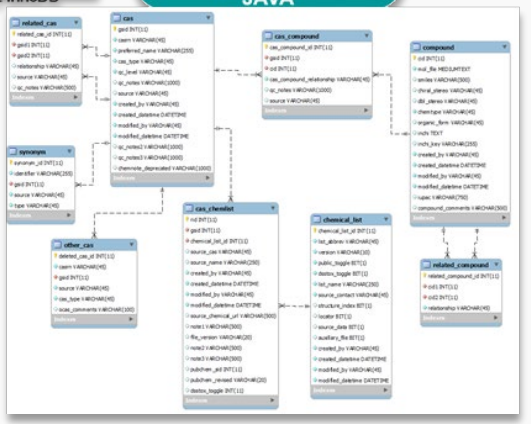


- Manually curated 25K substance records
- EPA-focus, environmental tox datasets
- Accurate CAS-name-structure annotations
- Public resource for high-quality SDF files

DSSTox_v2

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

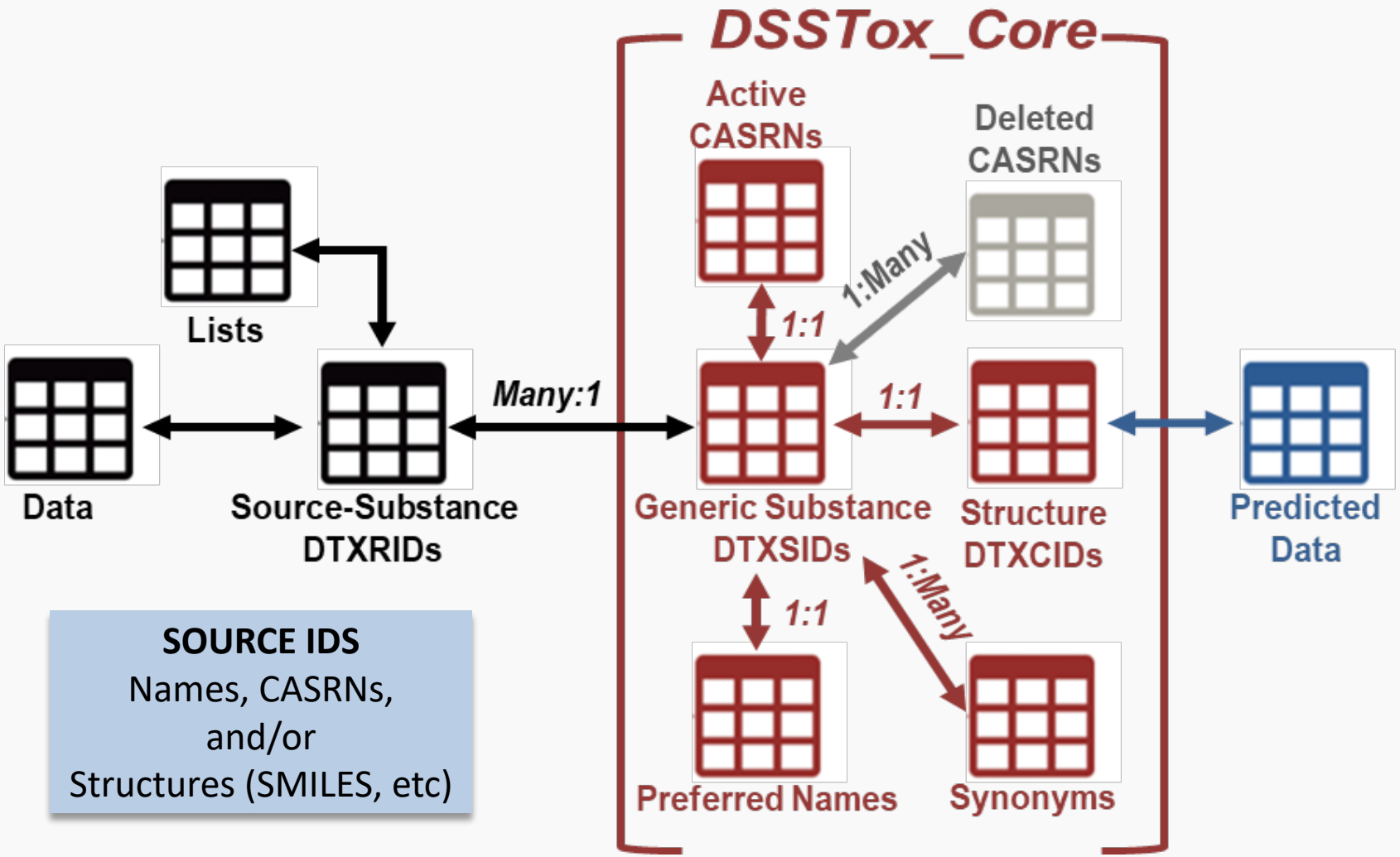




Grulke, et al., *Comput Toxicol*, 12:100096, 2019.

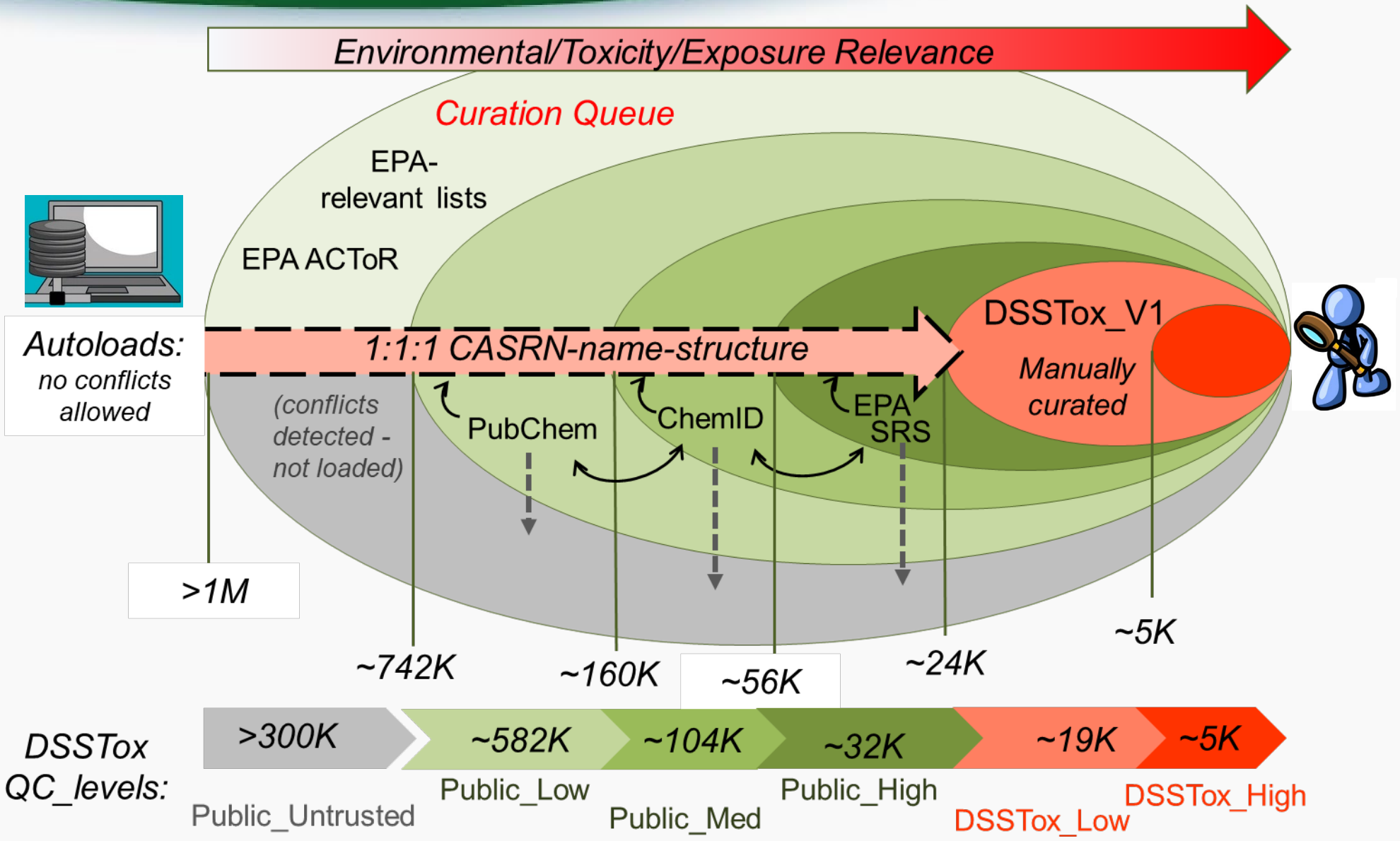
2005 → *2012* *2014* → *present*

DSSTox Data Model



How did we go from 25K to ~1M chemicals while addressing EPA's needs & quality concerns?

Building DSSTox_v2 (*circa 2015*)



DSSTox_v2 Construction (*circa 2015*)

Data source auto-load order:

1) DSSTox_v1 (~22K)
   - ✓ 1:1 CAS-structure mappings

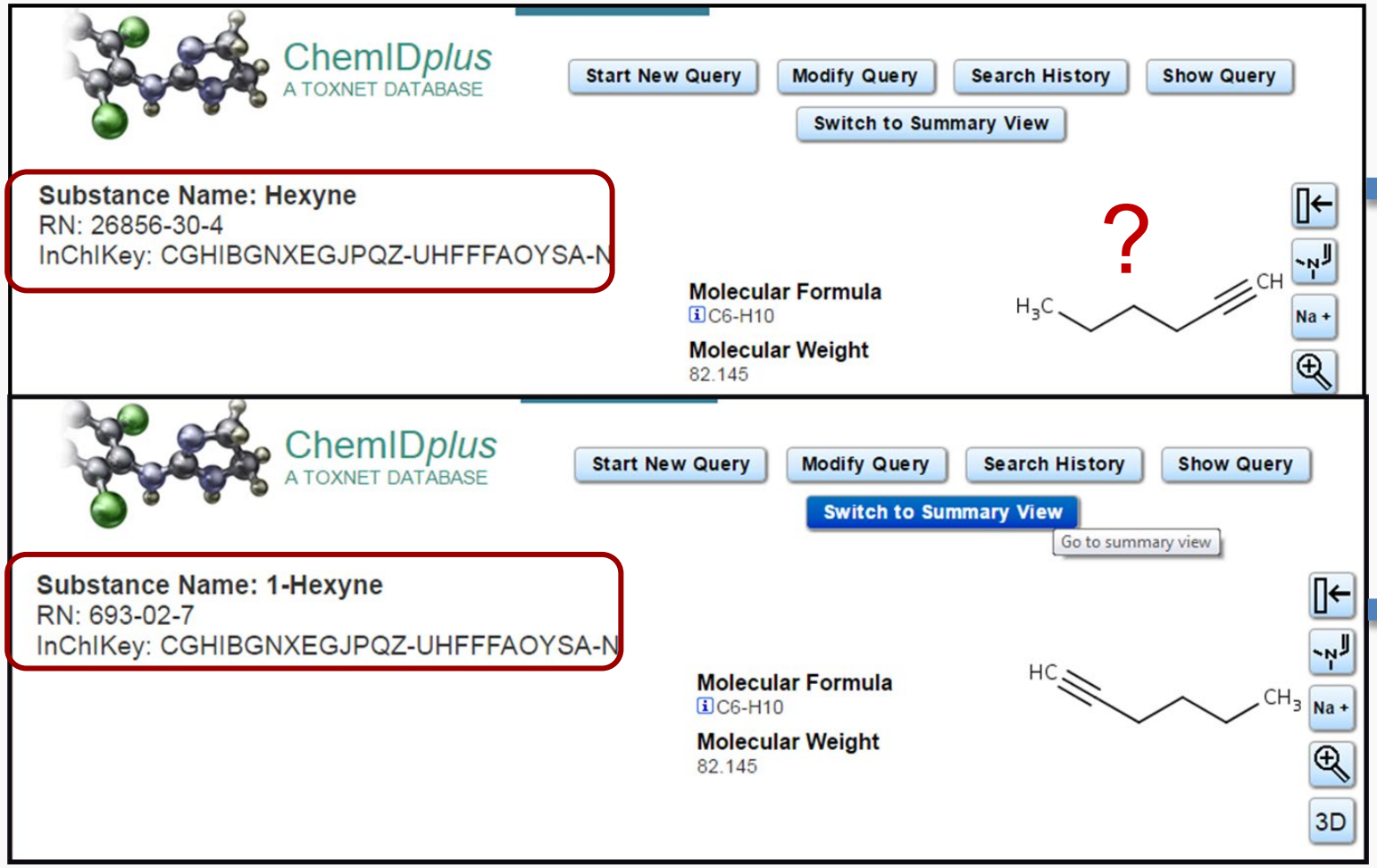
2) EPA SRS (~77K)
   - ✓ *systematic name → structure conversion*
   - ✓ *internal CAS-structure conflicts (12.5%)*
   - ✓ *ChemID conflicts (24% of 30K overlaps)*
   - ✓ *DSSTox conflicts (8% of 6200 overlaps) → queue for curation*

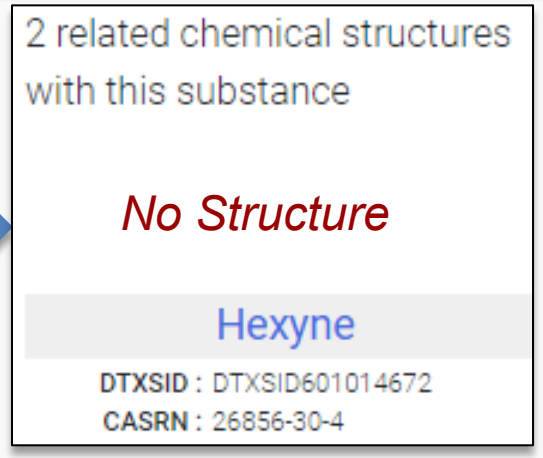
3) ChemID (~400K)
   - ✓ *internal CAS-structure conflicts (4.5%)*
   - ✓ *PubChem conflicts (45% of 225K overlaps) … OUCH!!*
   - ✓ *DSSTox conflicts (11% of 2300 overlaps) → queue for curation*

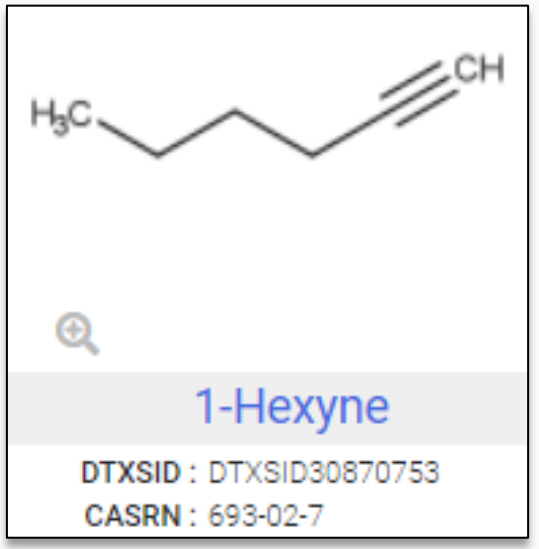
4) And so on …

Substance-structure ambiguity

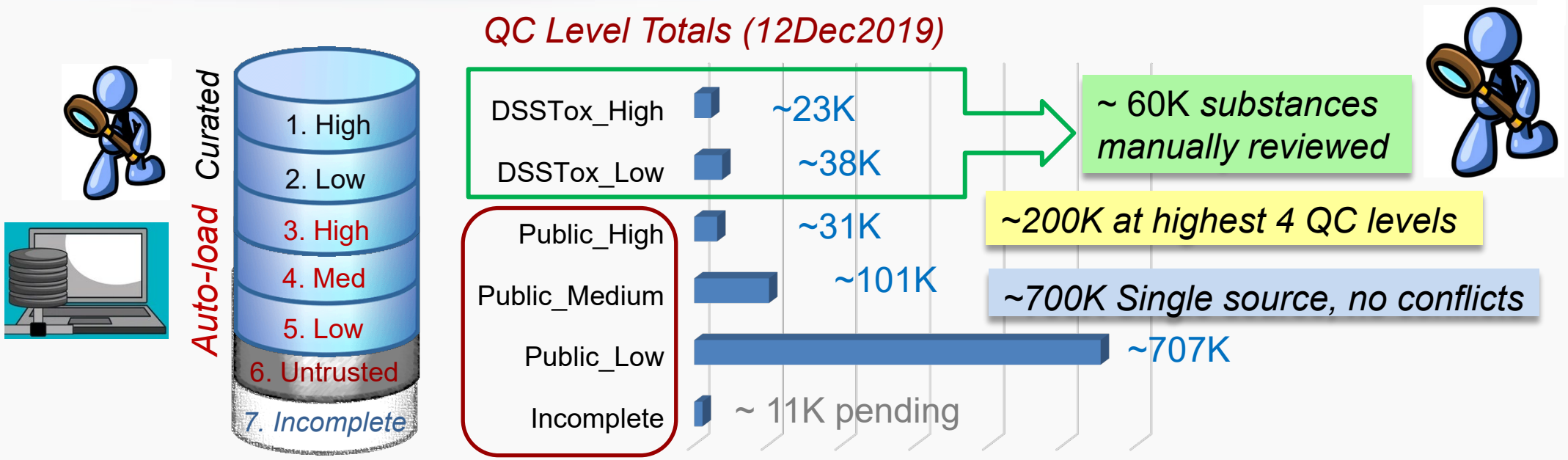
DSSTox Curation
1:1:1 CAS:Name:Structure







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

So, how and when do we manually curate DSSTox content?

Curate list of “Flame Retardants”

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

Functional Use DB:

List of 176 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

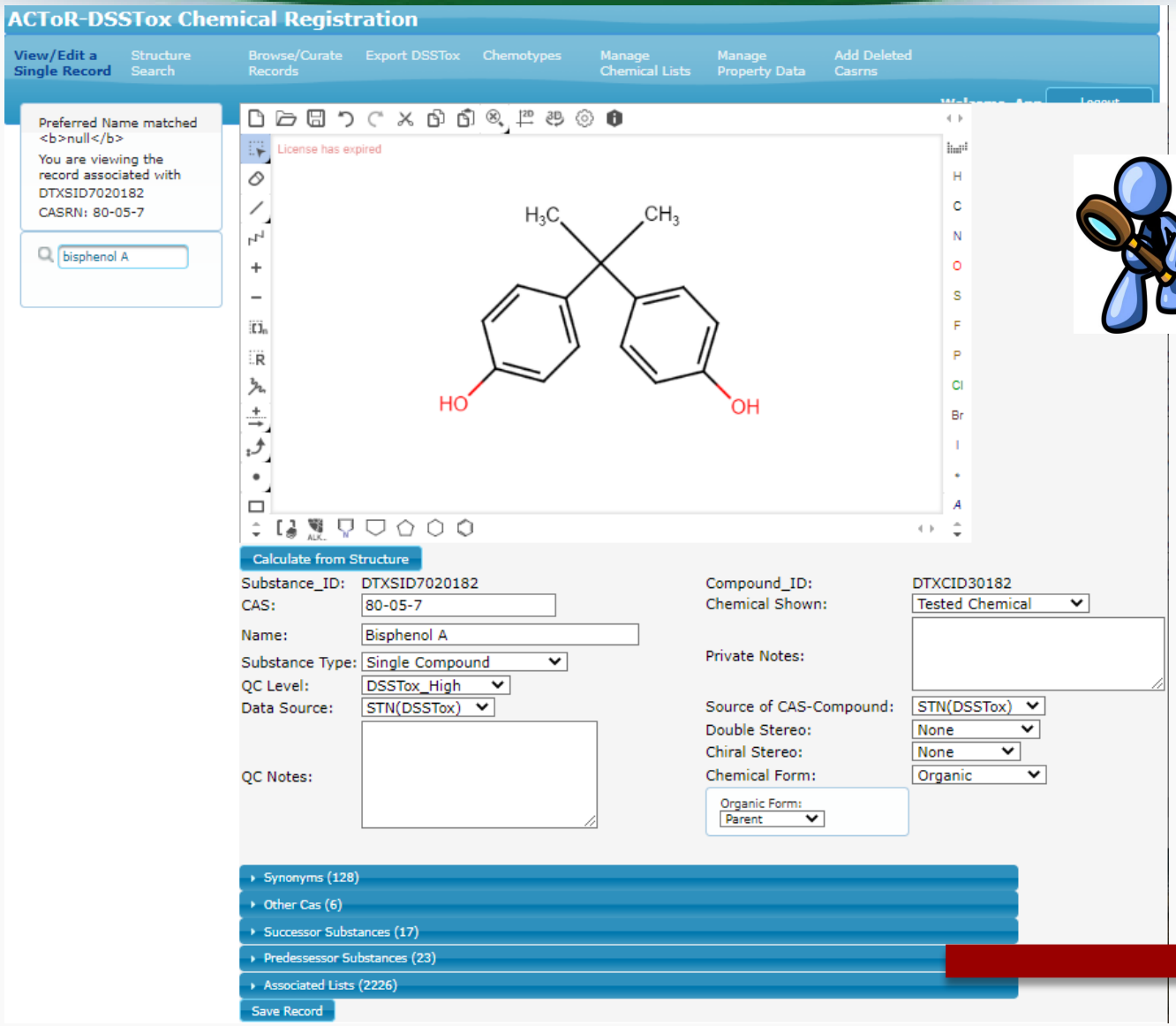
153 cleaned list, no duplicates

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 content
32 curated as new chemical registrations

DSSTox Chemical Registration/Curation Tool



DSSTox Chemical Registration/Curation Tool

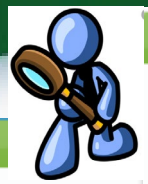
EPA United States Environmental Protection Agency

Synonyms (128)

Other CAS (6)

Successor Substances (17)

Predecessor Substances (23)



Associated Lists (2226)

Relationship	DTXSID	CAS-RN	Sou
Predecessor: Component	DTXSID70872791	26265-08-7	STN(DSS
Predecessor: Component	DTXSID201015347	26402-79-9	STN(DSS
Predecessor: Component	DTXSID40105886	106906-26-7	STN(DSS
Predecessor: Component	DTXSID4097128	68152-46-5	STN(DSS
Predecessor: Component	DTXSID6027840	25037-45-0	STN(DSS
Predecessor: Component	DTXSID601037135	202483-49-6	STN(DSS
Predecessor: Component	DTXSID001037149	235420-85-6	Public
Predecessor: Component	DTXSID701037164	235420-83-4	Public
Polymer	DTXSID3049627	25085-75-0	STN(DSS
Polymer	DTXSID0050479	25068-38-6	STN(DSS
Polymer	DTXSID9050480	28906-96-9	STN(DSS

DTXRID	Source Identifier	Inventory
DTXRID7020182	Bisphenol A	CPDBAS
DTXRID4022363	bisphenol A	NCTRER
DTXRID3023922	Bisphenol A.	IRISTR
DTXRID6024624	Bisphenol A	NTPGTZ
DTXRID2026492	Phenol, 4,4'-(1-methylethylidene)bis-	HPVCSI
DTXRID7030852	Bisphenol A	NTPBSI
DTXRID0033257	Bisphenol A	NTPHTS
DTXRID5033258	Bisphenol A	NTPHTS
DTXRID3034119	Bisphenol A	ICCVAM
DTXRID6036675	Bisphenol A	NCTRAR
DTXRID4037748	4,4'-Propane-2,2-diyldiphenol (bisphenol A)	KIERBL
DTXRID903978693	80-05-7	IRIS
DTXRID004834374		WIKIDATA
DTXRID204891415	80-05-7	COASummaries020920
DTXRID104924744	0000080-05-7	CPDAT
DTXRID804978661	80-05-7	toxval2
DTXRID004994736	80-05-7	CHEMINV
DTXRID805065186	80057	ECOTOX
DTXRID602677009	80-05-7	NCCTCPP_BCF
DTXRID505135671	80-05-7	EDSPuPDF
DTXRID305455617	80-05-7	DNTREF
DTXRID205459230	80-05-7	NEMILIST
DTXRID005493723	80-05-7	ARinvitro2016
DTXRID705494253	80-05-7	CTORDER1
DTXRID505494388	80-05-7	ARAntagonistRL2016d

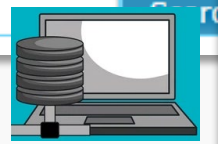
DSSTox List Registration/Curation Tool

Create a new chemical list **Create List**

Select a chemical list EPASPECIATE

Edit	Add/Edit Chemicals
Edit List	Add/Edit Chemicals

Search for a list



Source CASRN&Names auto-mapped by:

- *Preferred name*
- *CASRN (other CASRN)*
- *Synonym (valid, exact, unique, ambiguous, Source IDs)*
- *Name-to-Structure*

2814 Total records

- *67 Conflict bins*
- *757 No Hits*

ACToR-DSSTox Chemical Registration

Export DSSTox | Chemotypes | Manage Chemical Lists | Manage Property Data | Add Deleted Casrns | Welcome, Ann | Logout

Identifier conflicts binned to facilitate curation

Editing Listname: EPASPECIATE

Duplicates:

External Check Results

Description	Records
CAS Unique Synonym matched other record: **NAME1**	4
Mapped Identifier matched **NAME1**	8
Preferred Name matched **NAME1** CAS-RN matched other record: **CAS**	10
CAS-RN matched **CAS** Valid Synonym matched other record: **NAME1**	6
CAS-R **CAS** Valid matc Valid matc recor	

Substance Mapping

(1 of 1) 1 25

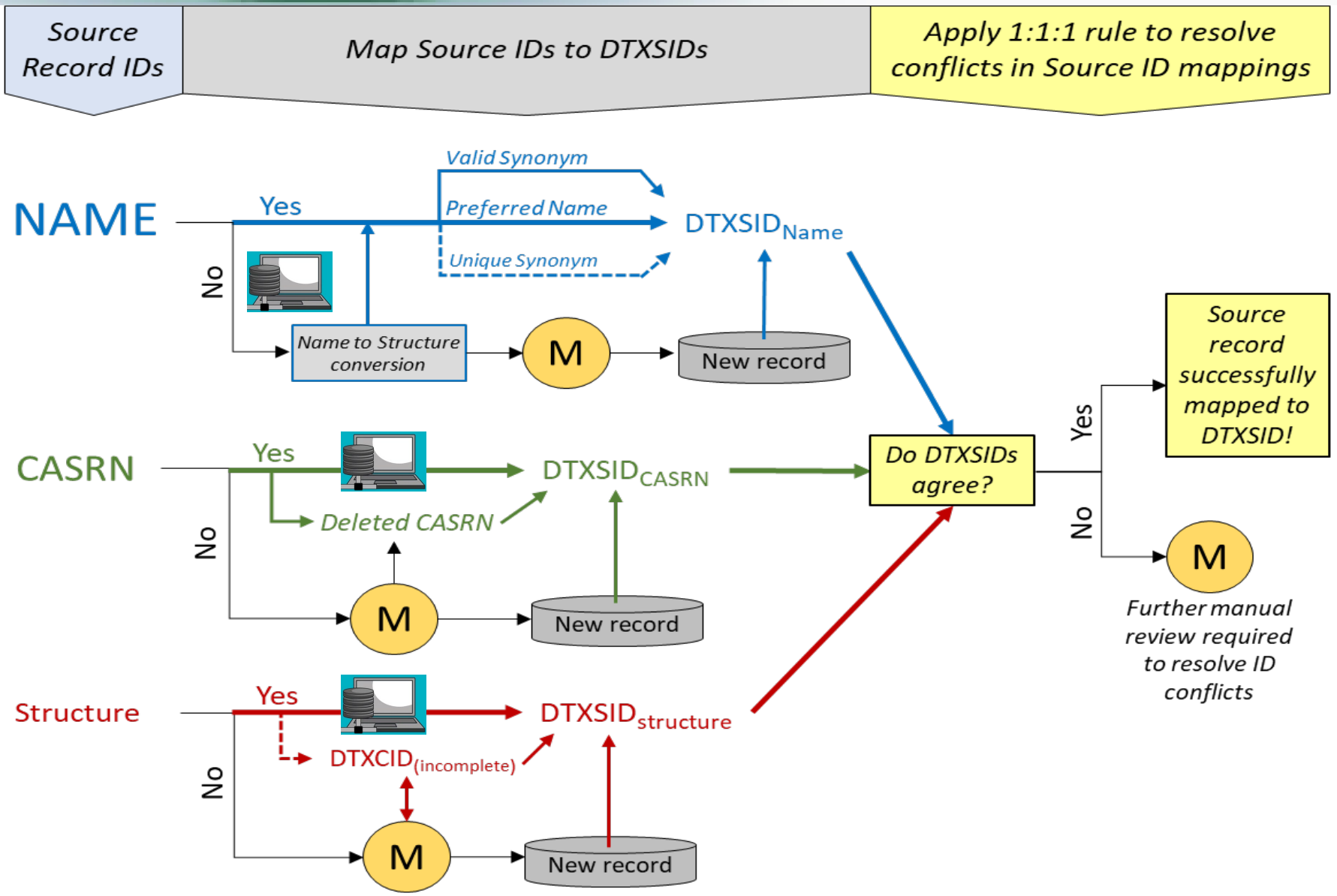
	Source Casrn	Source Name	Hit Substance_ID	Hit Casrn	Hit Name	
●	68917-57-7	Terpene	DTXSID0029501	68917-57-7	Terpenes and Terpenoids, mixed sour and sweet Orange-oil	Other Hits
●	27323-28-0	1-Methylindole	DTXSID50950041	27323-28-0	2-Methyl-1H-indole--5-methyl-1H-indole (1/1)	Other Hits
●	7782-41-4	Fluoride ion	DTXSID3024106	7782-41-4	Fluorine	Other Hits
●	156-59-2	1,2-Dichloroethene	DTXSID2024030	156-59-2	(Z)-1,2-Dichlor ene	Other Hits
●	27813-02-1	2-Hydroxypropyl methacrylate	DTXSID5027936	27813-02-1	Hydrox opyl methac e	Other Hits

Hits

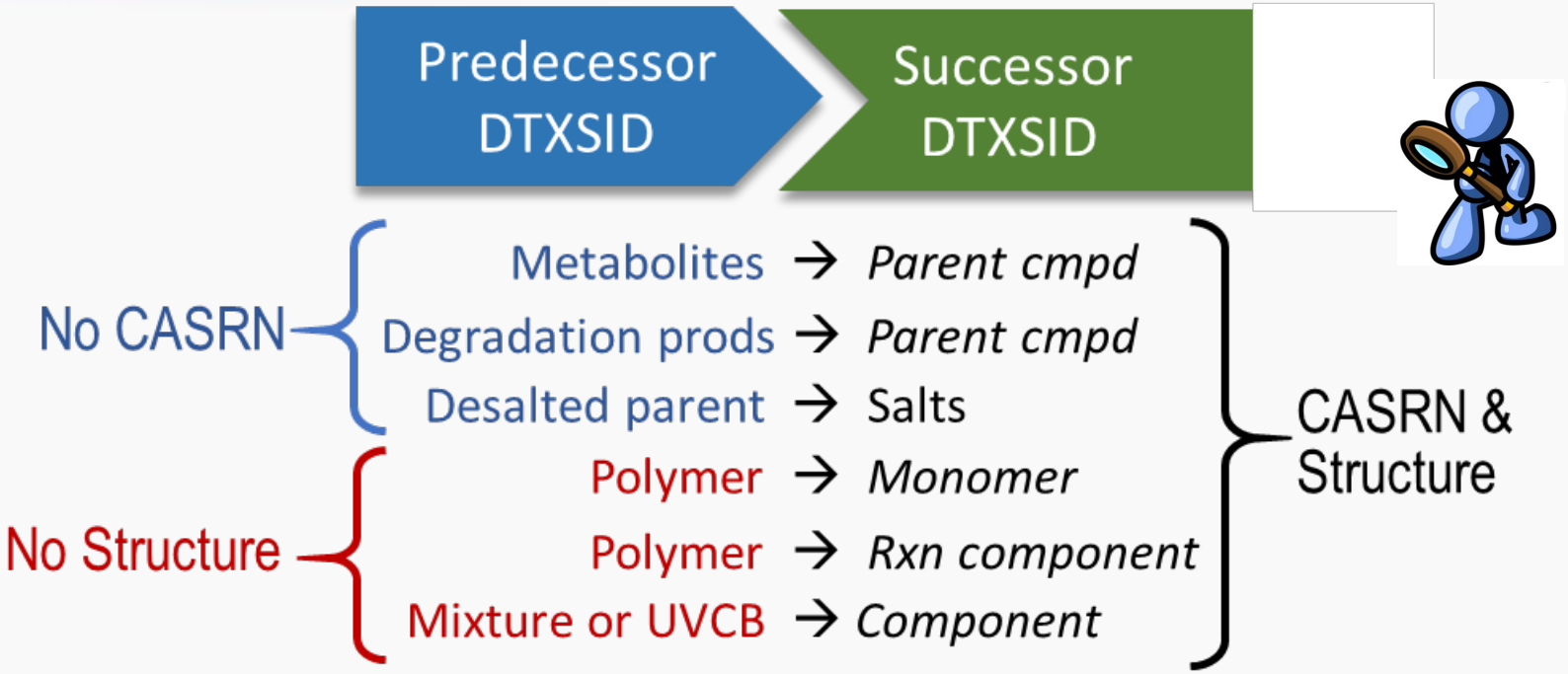
	ssCAS-RN	ssName	Hit Desc	Hit Substance_ID	Hit Casrn	Hit Name
●	156-59-2	1,2-Dichloroethene	CAS-RN matched **CAS**	DTXSID2024030	156-59-2	(Z)-1,2-Dichloroethylene
●	156-59-2	1,2-Dichloroethene	Valid Synonym matched **NAME1**	DTXSID8024991	540-59-0	1,2-Dichloroethylene

Map hit | Cancel

Chemical Curation Workflow



Substance Relationship Mapping



- Manually added relationship tags
- Establish linkages of No CASRN → CASRN records
- Establish linkages of No Structure (e.g., UVCBs) → Structure records

No representative structures violating 1:1:1 rule

Chemical Families, e.g. PCBs

Successor Substances (209)

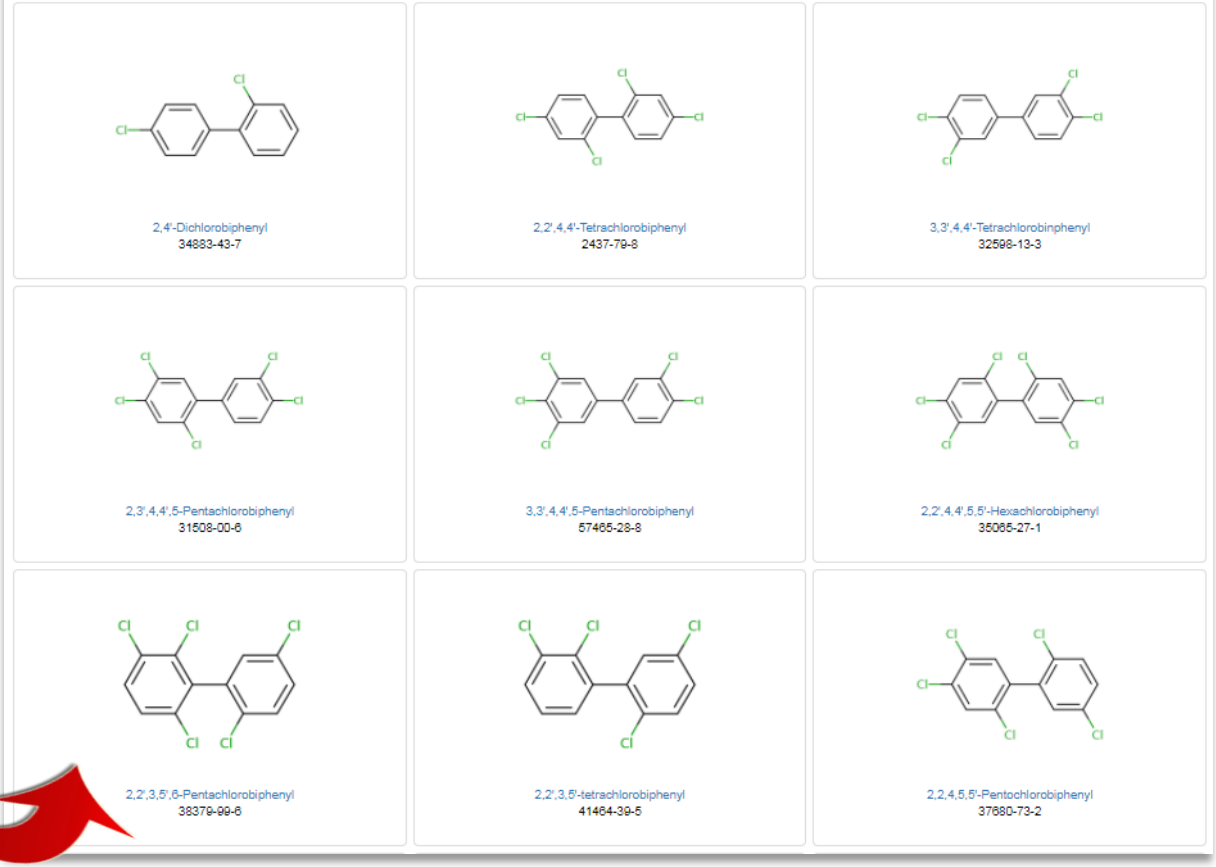
	CAS-RN	Relationship	Source
	32774-16-6	is a Representative Isomer of this	STN(DSSTox)
	2051-60-7	is a Representative Isomer of this	Public
	2051-61-8	is a Representative Isomer of this	Public
	2051-62-9	is a Representative Isomer of this	Public
	13029-08-8	is a Representative Isomer of this	
	16605-91-7	is a Representative Isomer of this	
	25569-80-6	is a Representative Isomer of this	
	33284-50-3	is a Representative Isomer of this	Public
	34883-43-7	is a Representative Isomer of this	Public
	34883-39-1	is a Representative Isomer of this	Public
	33146-45-1	is a Representative Isomer of this	Public
	2050-67-1	is a Representative Isomer of this	Public
	2974-92-7	is a Representative Isomer of this	Public
	2974-90-5	is a Representative Isomer of this	Public
	34883-41-5	is a Representative Isomer of this	Public
	2050-68-2	is a Representative Isomer of this	Public

https://ccte-ccd.epa.gov/dashboard/

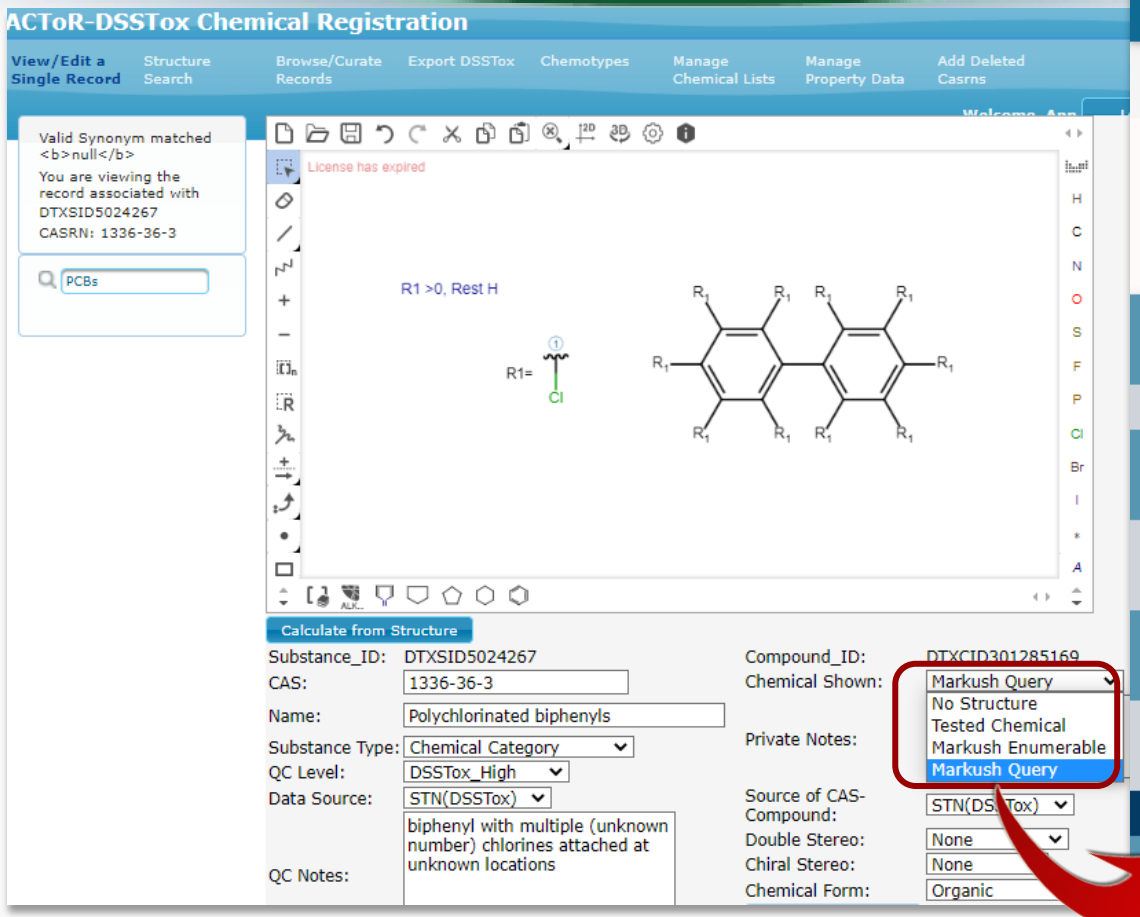
Related Chemicals

Found 209 chemicals

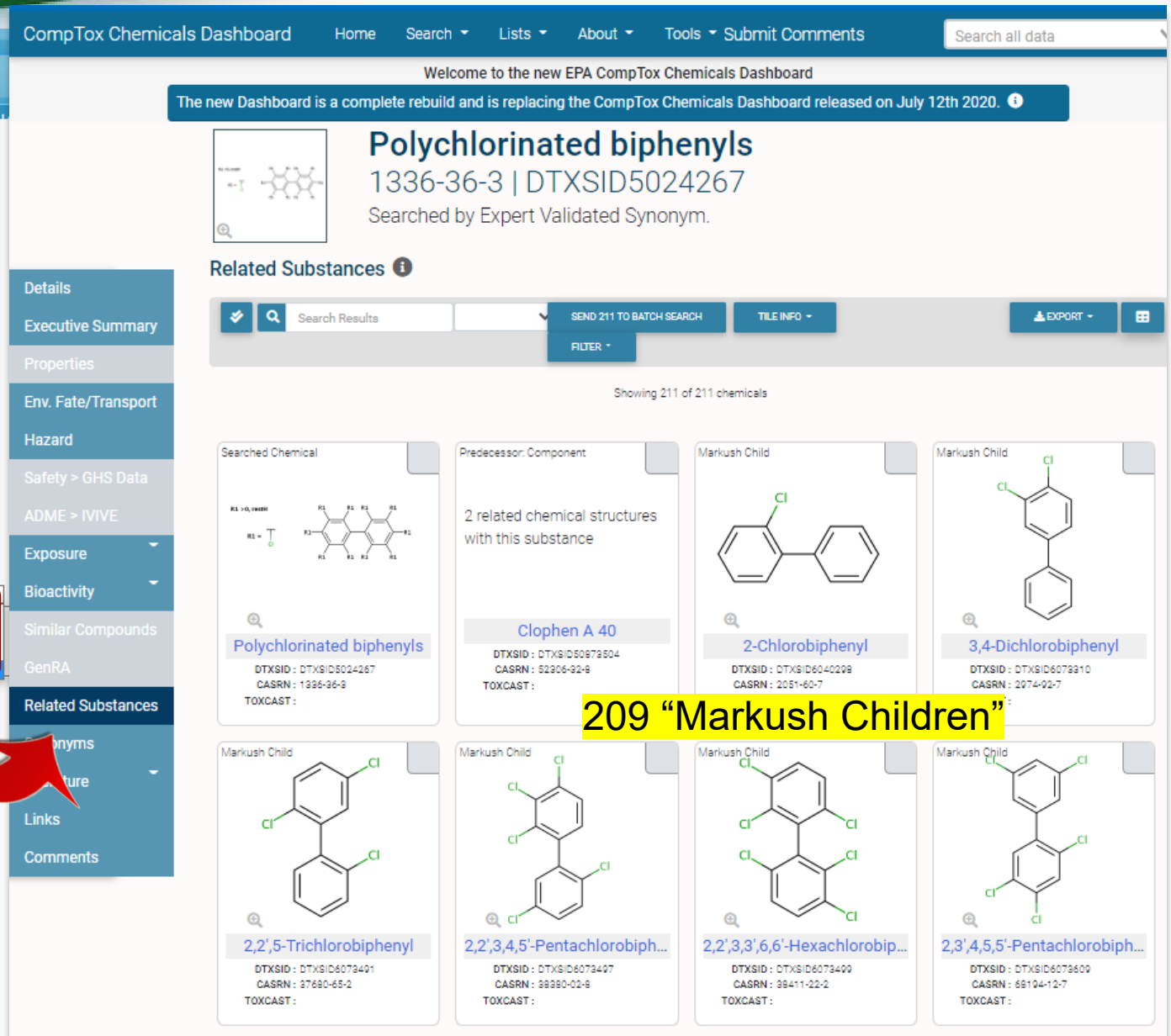
Download as: TSV Excel SDF



Markush Representations, e.g PCBs

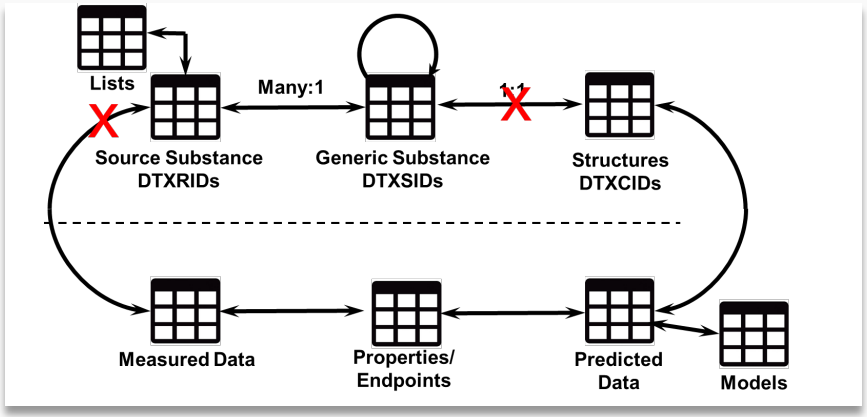


ChemAxon Markush Tools

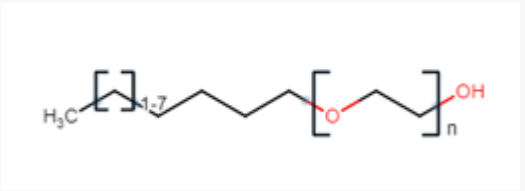


Representing UVCBs with Markush

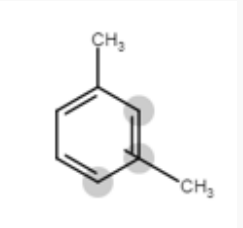
- For most UVCBs, measured data not available
- A single structure cannot fully represent the substance



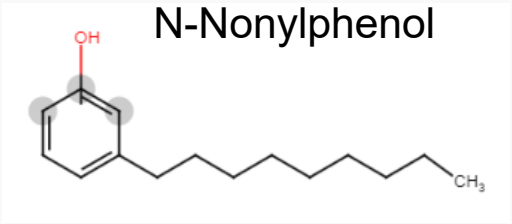
Alcohols, C6-12, ethoxylated



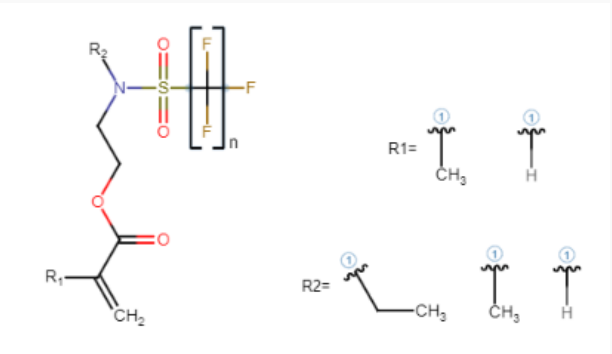
Xylenes



N-Nonylphenol



(N-Alkylperfluoroalkanesulfonamido)ethyl acrylate



- ~1300 total Markush registered
- ~330 PFAS Markush registered

Impact of Expert Chemical Curation, e.g., PFAS

EPA's PFAS Action Plan – *Released February 14, 2019*

2001: first scient)S and
PFOA in the glob
2000-2002: volu

Science Invent

You are here: EPA Home » Science Inver

DEVELOPMENT

Citation:

LAU, C. S. DEVELOPMENTAL TOXI
8th Annual National Forum on Co
Septemb

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Toxicol Sci. 2007 Feb;9

Development
mouse after c

Wolf CJ[1], Fenton SE,
Lau CS, Abbott BD.

Author informa

Abstract
Perfluorooctanoic a
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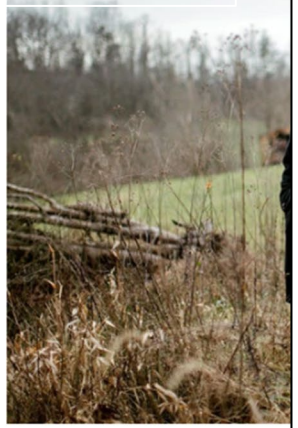
commercial produc
and in mice affects

The New York Times Magazine

The Story Behind the E.P.A's Contaminated Water Revelation

https://www.nytimes

May 27, 2016



Rob Bilott near Parkersburg, W.Va., in D

By Nathaniel Rich

May 27, 2016

Last week 5.2 million American
contaminated with man-made c
Environmental Protection Ager
compounds: perfluorooctanoic
manufacture of Teflon and othe
perfluorooctane sulfonic acid (PFOS). An E.P.A. health advisory is not

ENVIRONMENTAL Science & Technology LETTERS

Nov, 2016

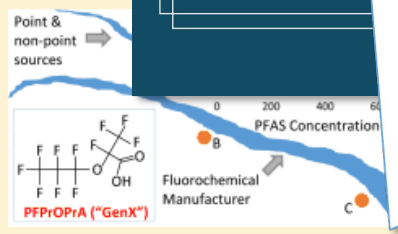
Legacy and Emerging Perfluoroalkyl Substa
Drinking Water Contaminants in the Cape F
North Carolina

Mei Sun,[*,†,‡] Elisa Arevalo,[‡] Mark Strynar,[§] Andrew Lindstrom,[§]
Adam Pickett,[⊥] Chris Smith,[#] and Detlef R. U. Knappe[‡]

[†]Department of Civil and Environmental Engineering, University of North Carolina
United States
[‡]Department of Civil, Construction, and Environmental Engineering, North Carolin
27695, United States
[§]National Exposure Research Laboratory, U.S. Environmental Protection Agency Re
United States
[∥]Cape Fear Public Utility Authority, Wilmington, North Carolina 28403, United St
[⊥]Town of Pittsboro, Pittsboro, North Carolina 27312, United States
[#]Fayetteville Public Works Commission, Fayetteville, North Carolina 28301, United

Supporting Information

ABSTRACT: Long-chain per- and polyfluoroalkyl substances (PFASs) are being replaced by short-chain PFASs and fluorinated alternatives. For ten legacy PFASs and seven recently discovered perfluoroalkyl ether carboxylic acids (PFECAs), we report (1) their occurrence in the Cape Fear River (CFR) watershed, (2) their fate in water treatment processes, and (3) their adsorbability on powdered activated carbon (PAC). In the headwater region of the CFR basin, PFECAs were not detected in raw water of a drinking water treatment plant (DWTP), but concentrations of legacy PFASs were high. The U.S. Environmental Protection Agency's



Feb 14, 2019

EPA Takes Aim at PFAS

PFAS, or poly- and perf
range of pr
perfluorooc
action plan

s drinking water contaminants. They are used in a wide
routes. The two most commong forms of PFAS are
S). DEQ will work with our water systems once the EPA
hat are affecting drinking water sources in the Utah.

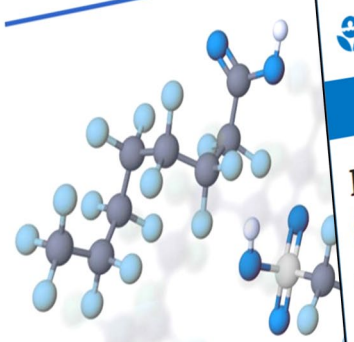
Health Effects
Exposure to these compounds has been linked to a number of health concerns including cancer, hormone disruption, liver and kidney toxicity, harm to immune system, and reproductive and development toxicity.

4yea
It can take up to
for the level of PF
body to go down

4,00
PFAS is a group of
than 4,000 very sta
synthetic chemicals.

EPA United States Environmental Protection Agency
EPA B23R18004 | February 2019 | www.epa.gov/pfas

EPA's Per- and Polyfluoroalkyl Substances (PFAS) Action Plan



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Per- and Polyfluoroalkyl Substances (PFAS)

EPA's PFAS Action Plan

February 14, 2019 - EPA's PFAS Action Plan responds to extensive public interest and input the agency has received over the past year and represents the first time EPA has built a multi-media, multi-program, national communication and research plan to address an emerging environmental challenge like PFAS. Read more.

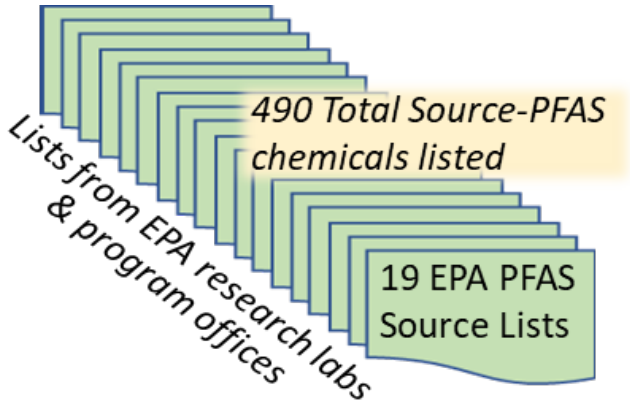
"We are moving forward with several important actions, including the maximum contaminant level process, that will help affected communities better monitor, detect, and address PFAS."

-- EPA Administrator, Andrew Wheeler

https://www.epa.gov/pfas/epas-pfas-action-plan

PFAS: EPA Cross-Agency Research List

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



Curation

- ✓ *Correct misspelled names*
- ✓ *Correct CASRN*
- ✓ *Fix errors in mappings of anions, salts, parents*
- ✓ *Create unique acronym*
- ✓ *Map to unique DTXSID*

EPAPFASRL

19 lists collapsed to single list of 194 unique DTXSID substances

DTXSID	Substance_Name	Substance_CASRN	Source_Name (incorrect or ambiguous)	Source_CASRN (incorrect or invalid)	Source_Acronym (incorrect or ambiguous)	Unique_Acronym
DTXSID20874028	2H,2H,3H,3H-Perfluorooctanoic acid	914637-49-3	5:3 Polyfluorinated acid	914637-49-3	5:3 acid	5:3 PFOA
DTXSID7027831	N-Methyl-N-(2-hydroxyethyl)perfluorooctanesulfonamide	24448-09-7	N-Methyl perfluorooctanesulfonam		NMeFOSE, MeFOSE	NMeFOSE
DTXSID10892352	Perfluoro-2-{[perfluoro-3-(perfluoroethoxy)-2-p	749836-20-2	Ethanesulfonic acid, 2-[1-[tetrafluroroethoxy)methyl]-1,2,2,2-tetrafluoroethoxy]-1,1,2,2-tetrafluoro	2	PFESA Byproduct 2	PFESA Byproduct 2
DTXSID70892479	Pe	375-05-36-9	Pe	2706-91-4	PFPeS	PFPeS_ion
[illegible]1354	Ammonium perfluoropentanesulfonate	68259-09-6	Am te	68259-09-6		APFPeS
[illegible]381350	4,8-Dioxa-3H-perfluorononanoic acid	919005-14-4	2,2,3-Trifluoro-3-(1,1,2,2,3,3-hexafluoro-3-(trifluoromethoxy)propoxy)propanoic acid	919005-14-4	ADONA	ADONA parent acid
DTXSID00874026	Ammonium 4,8-dioxa-3H-perfluorononanoate	958445-44-8	Ammonium 4,8-dioxa-3H- pe	958445-44-8	ADONA	ADONA
DTXSID3037707	Potassium perfluorobutanesulfonate	29420-49-3	Po ate		PFBS	PFBS-K
DTXSID5030030	Perfluorobutanesulfonic acid	375-73-5	Pe	375-73-5	PFBS	PFBS
DTXSID60873015	Perfluorobutanesulfonate	45187-15-3	Perfluorobutanesulfonate	375-73-5	PFBS	PFBS_ion
DTXSID3040148	Perfluorodecanesulfonic acid	335-77-3	Perfluorodecanesulfonic acid		PFDS	PFDS

"5:3 acid"

Mispelled names

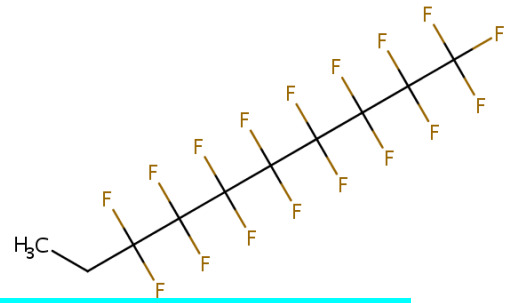
Incorrect CAS

Anions

Ambiguous acronyms

PFAS Name-Structure Curation Challenges

- Name too short – what the heck is it??
  - Surflon S 382, 5:3 Acid, ? (Fluowet® PL 80B)



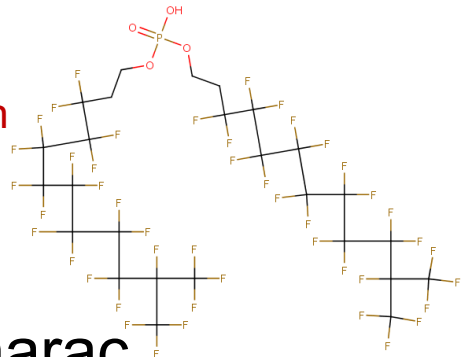
- Long systematic names obscure perfluoro aspect

  1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-Heptadecafluorodecane → (Perfluoro-n-octyl)ethane

- Long names difficult to use or decipher to structures

  1-Dodecanol, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,12,12,12-eicosafluoro-11-(trifluoromethyl)-, hydrogen phosphate

  → Bis((perfluoro-9-methyldecyl)ethyl) phosphate



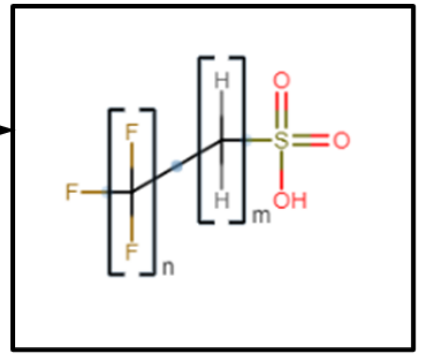
- Names so long (>256 charac) they truncated on import, incl. funky charac

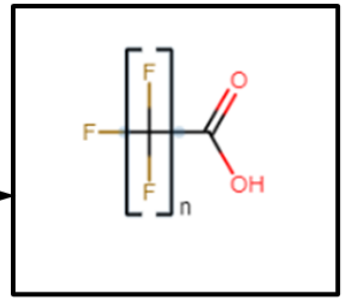
  2-Propenoic acid, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-heneicosafluorododecyl ester, polymer with 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl 2-propenoate, [illegible]-(2-methyl-1-oxo-2-propenyl)-¤ë-(2-methyl-1-oxo-2-propenyl)oxypoly(oxy-1,2-ethanediyl), 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,15,15,16,16,16-nonacosafluorohexadecyl 2-propenoate, octadecyl 2-propenoate and 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-pentacosafluorotetradecyl 2-propenoate

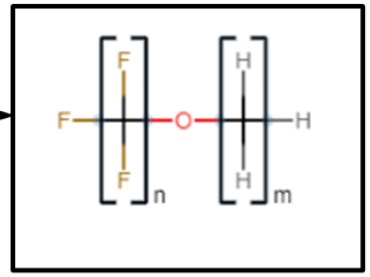
  → DTXSID40882569, 119973-84-1 (name too long)

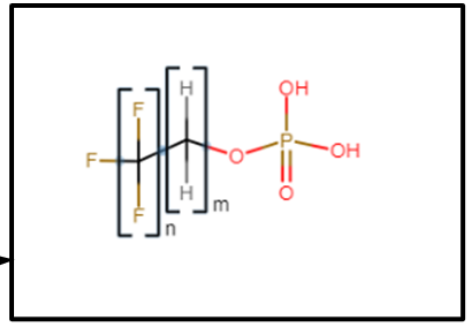
Translating Expert Categories to Markush

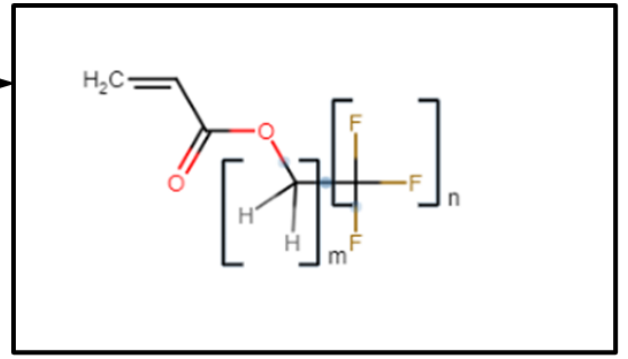
Expert category
Fluorotelomer acrylates
Fluorotelomer alcohols
Polyfluorinated alcohols
Fluorotelomer sulfonates
N-alkyl perfluoroalkyl sulfonamidoacetic acids
N-alkyl perfluoroalkyl sulfonamidoethanols
Perfluoroalkyl aldehydes
Perfluoroalkyl amides
Perfluoroalkyl carboxylates
Perfluoroalkyl acyl fluorides
Perfluoro vinyl esters
Perfluoroalkyl ketones
Semi-fluorinated alkenes
Perfluoroalkyl vinyl ethers
Perfluoroalkyl alkyl ethers
Fluorotelomer amines
Perfluoroalkyl sulfonamides
Semi-fluorinated alkanes
Perfluoroalkyl sulfonates
Perfluoroalkyl sulfonamido amines
Polyfluoroalkyl carboxylates
Perfluoroalkyl ethers
Fluorotelomer phosphates

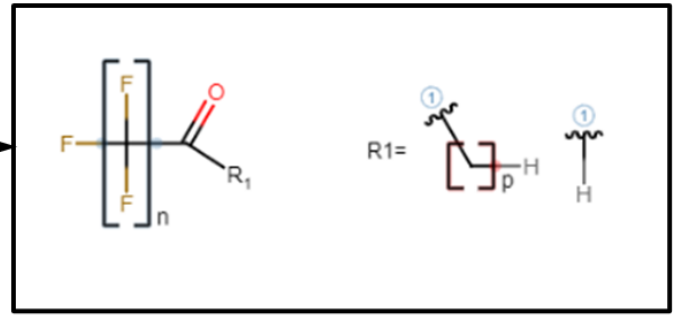


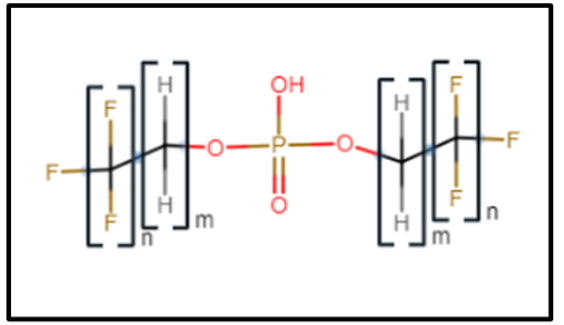






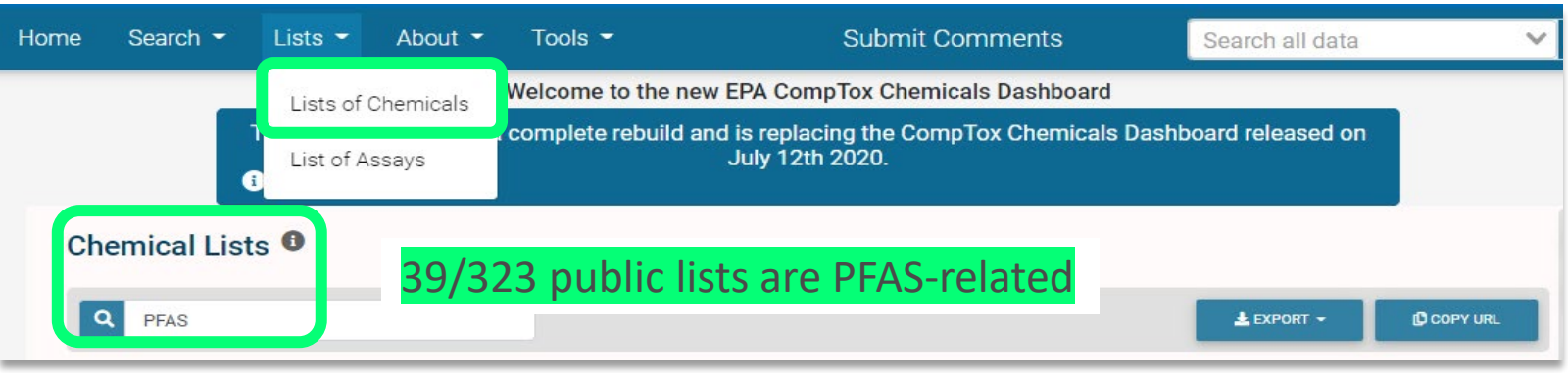






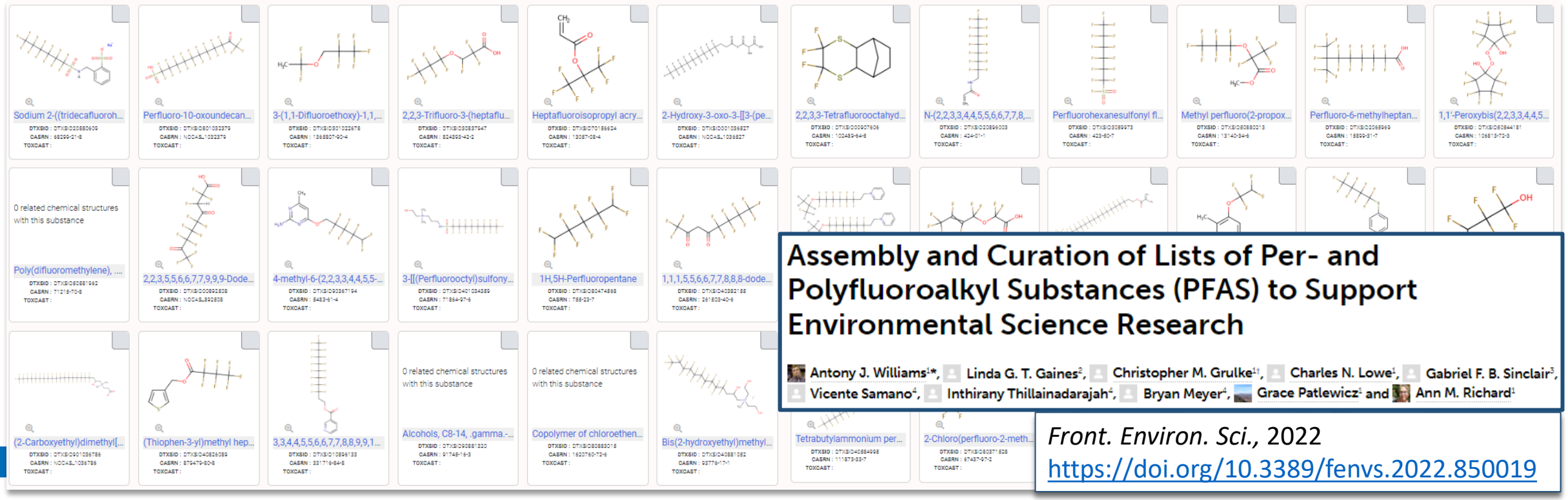
PFAS Lists on the Dashboard

https://comptox.epa.gov/dashboard/chemical_lists/?search=PFAS



PFASMASTER (12034) list includes:

- 10776 structures (PFASSTRUCT)
- 1258 Non-structurables *(UVCBs, polymers, mixtures, etc.)*
- Covers all PFAS lists (e.g., PFASOECD)



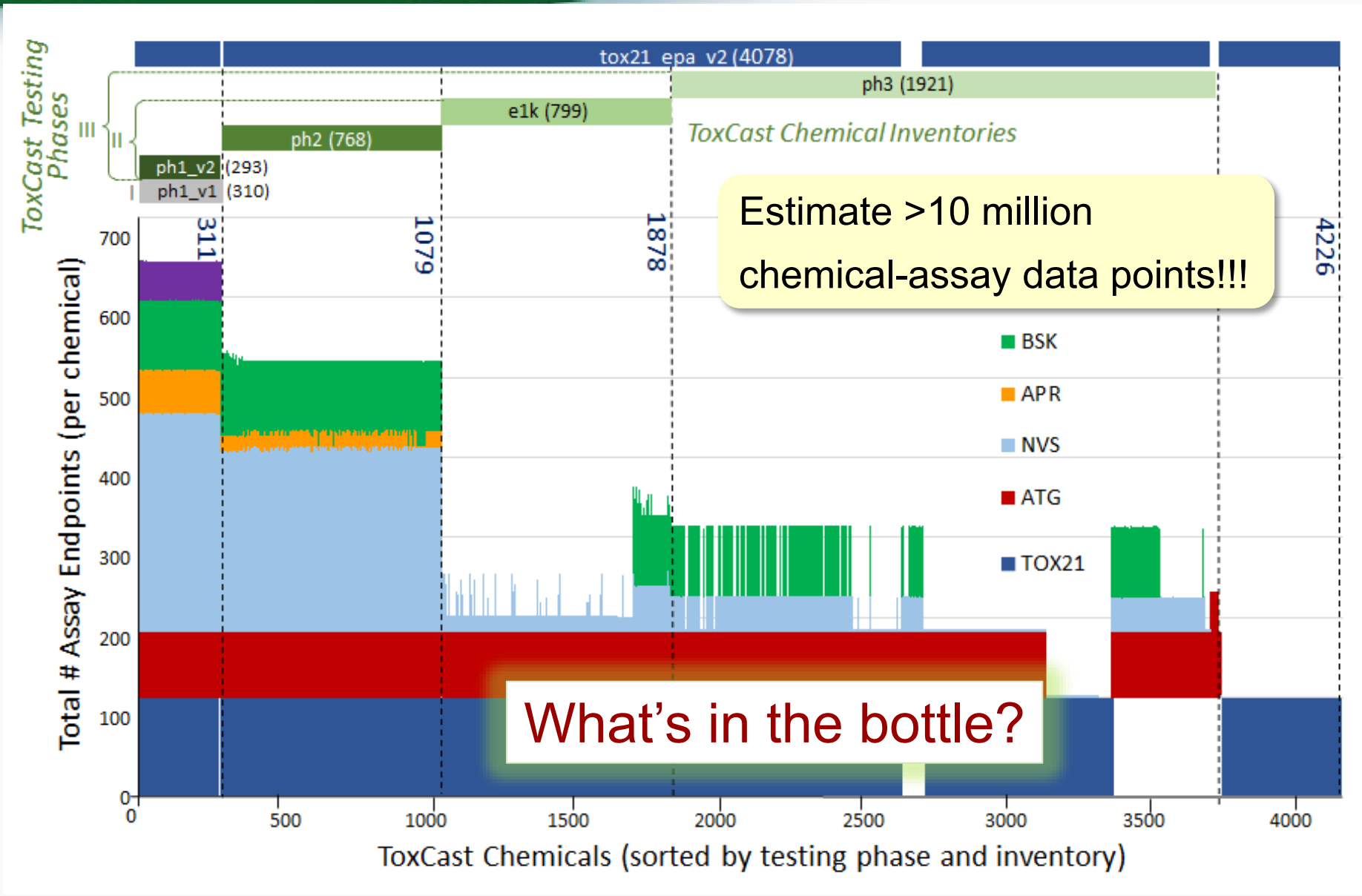
Assembly and Curation of Lists of Per- and Polyfluoroalkyl Substances (PFAS) to Support Environmental Science Research

Antony J. Williams[1]*, Linda G. T. Gaines[2], Christopher M. Grulke[1†], Charles N. Lowe[1], Gabriel F. B. Sinclair[3], Vicente Samano[4], Inthirany Thillainadarajah[4], Bryan Meyer[4], Grace Patlewicz[1] and Ann M. Richard[1]

Front. Environ. Sci., 2022
https://doi.org/10.3389/fenvs.2022.850019

Impact of Expert Chemical Curation, cont.

ToxCast/Tox21 High-throughput Screening



ChemTrack:
Chemical Sample Management

chemtrack | Inventory | Partnerships | Ordering | Data | Single Chemical Search | Ann

Bottle Inventory

Add New M

Uploaded MOSAIC Files 48 | Curated Bottles 53607 | Uncurated Bottles 3360

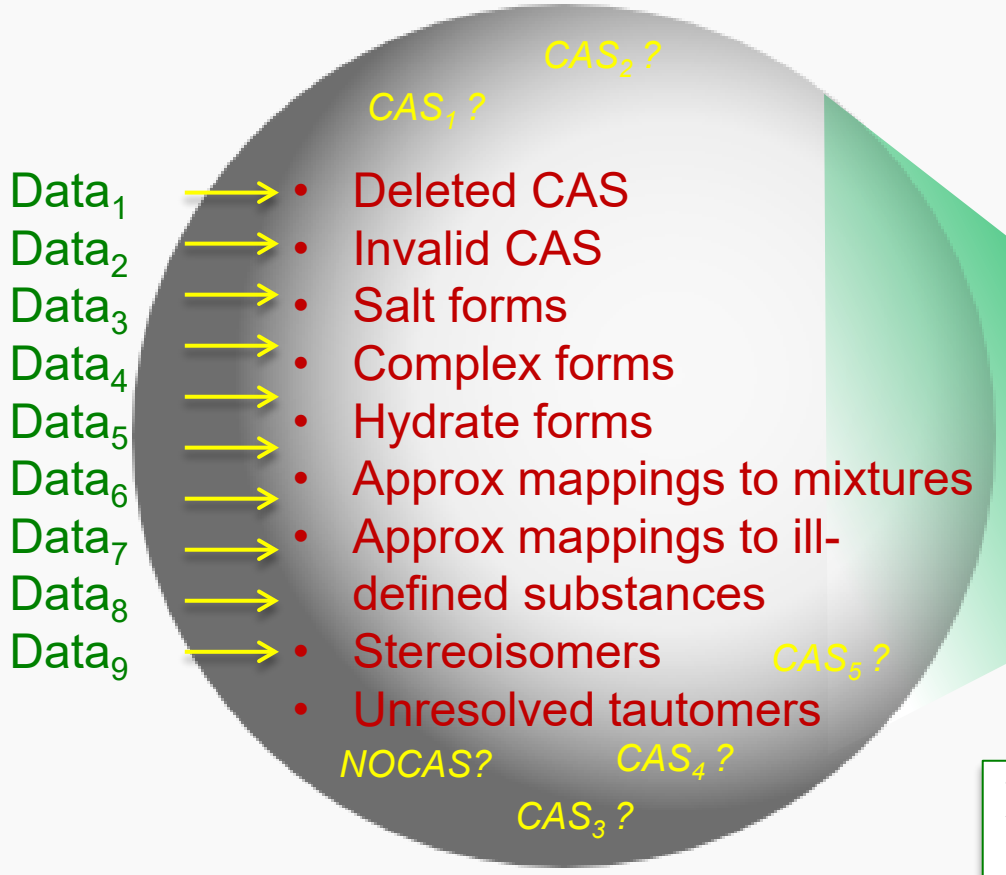
Columns | 10

Barcode	CoA Summary Id	Barcode type	DTXSID	Compound name	Casrn	Qty available	Concentration (mM)	Vendor
Filter by Barc	Filter b	Filter by Barcode ty	Filter by DTXSI	Filter by Compou	Filte	Filter	Filter by Co	Filter
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

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

Non-targeted MS screening of environmental samples

CAS-Name-Structure "Sphere of Confusion"



many:1

Monoisotopic Mass

↓

Formula

↓

Parent structure
(no stereo, desalted)

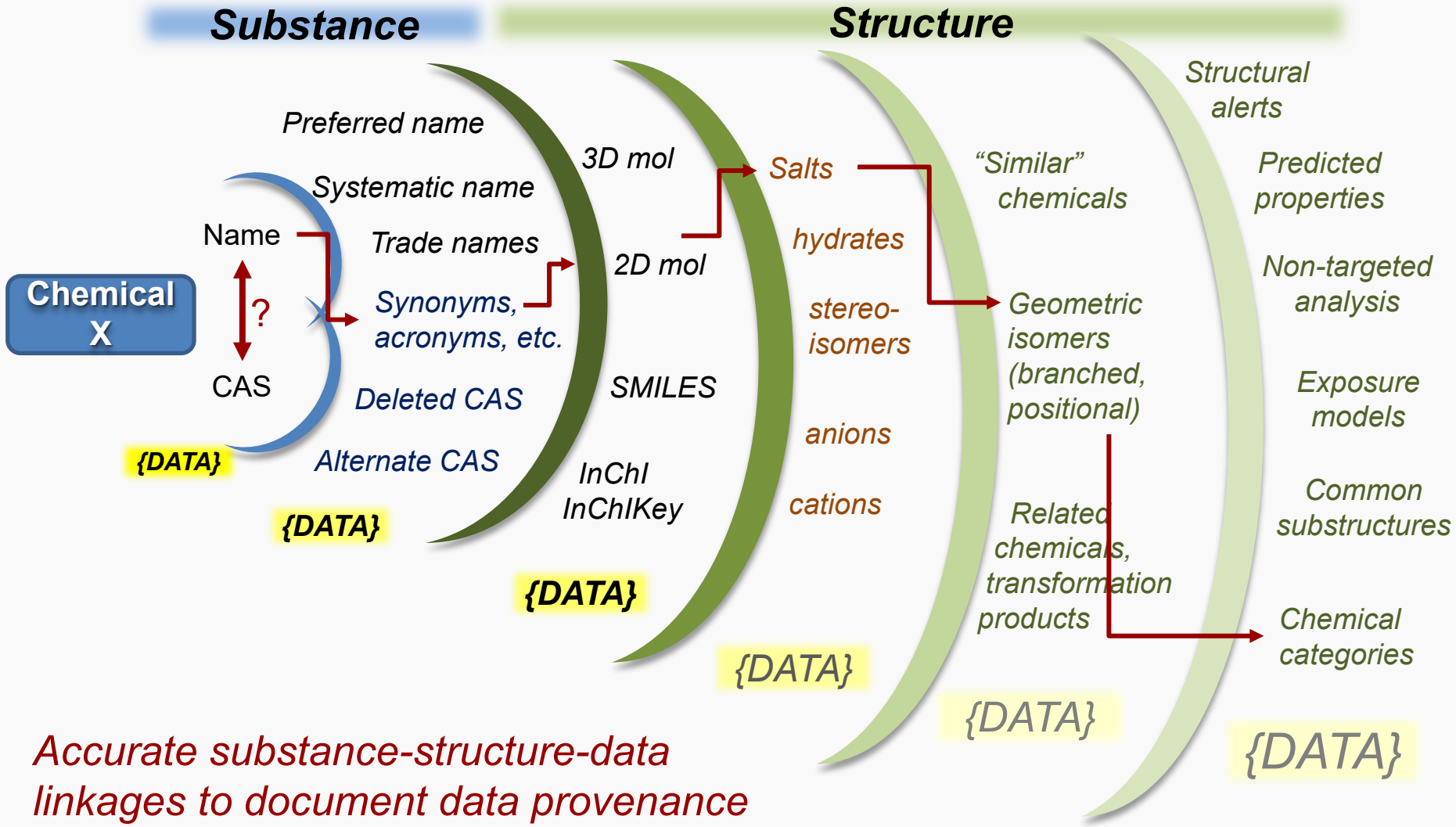
↓

Valid CAS-substance?

DSSTox_v2 Database & Cheminformatics Layer

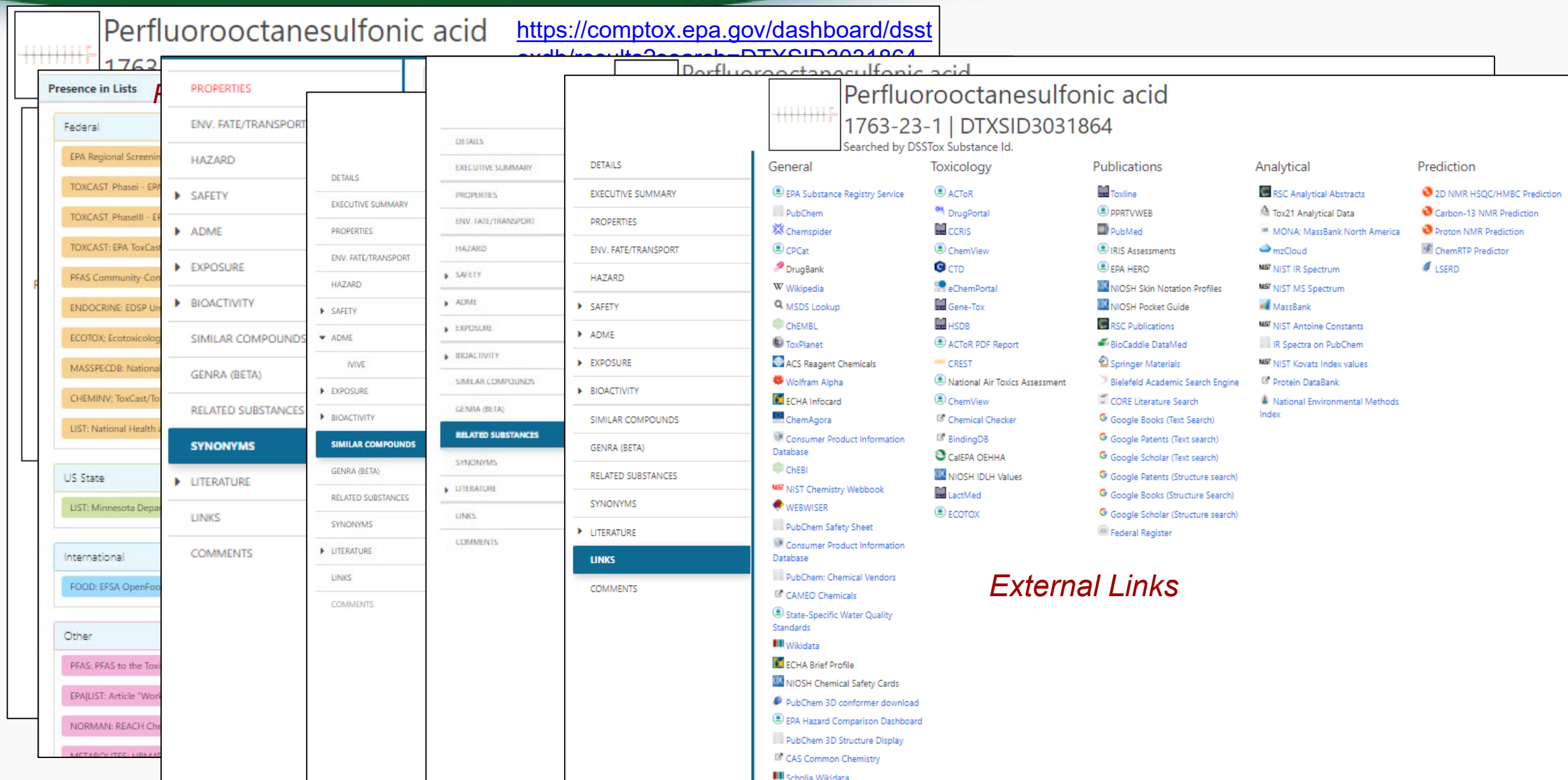
- Resolve CAS-structure mappings for accurate data mapping
- Collapse sphere to collect all data at parent structure-formula level

Chemical-data gathering for systematic reviews

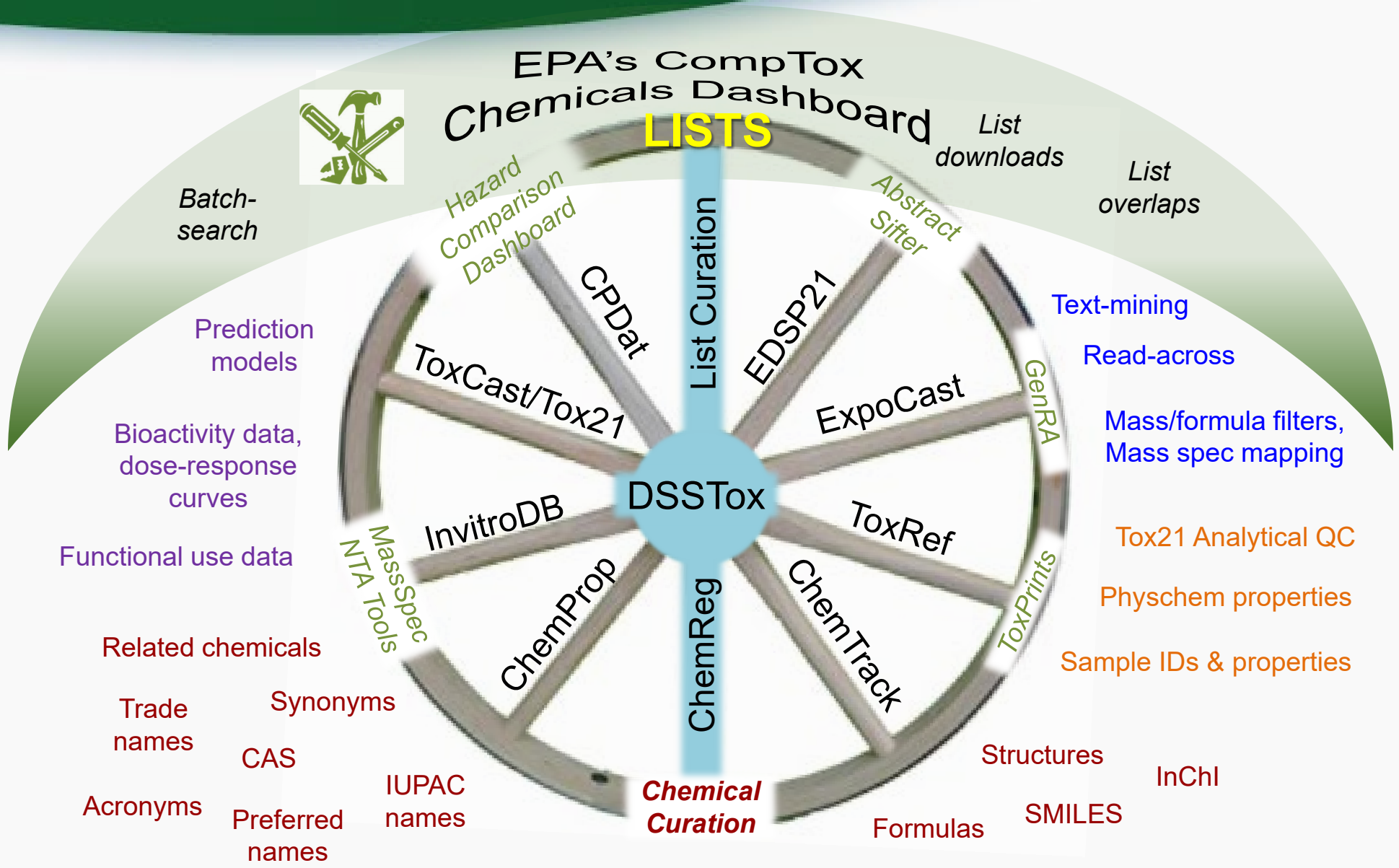


Accurate substance-structure-data linkages to document data provenance

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

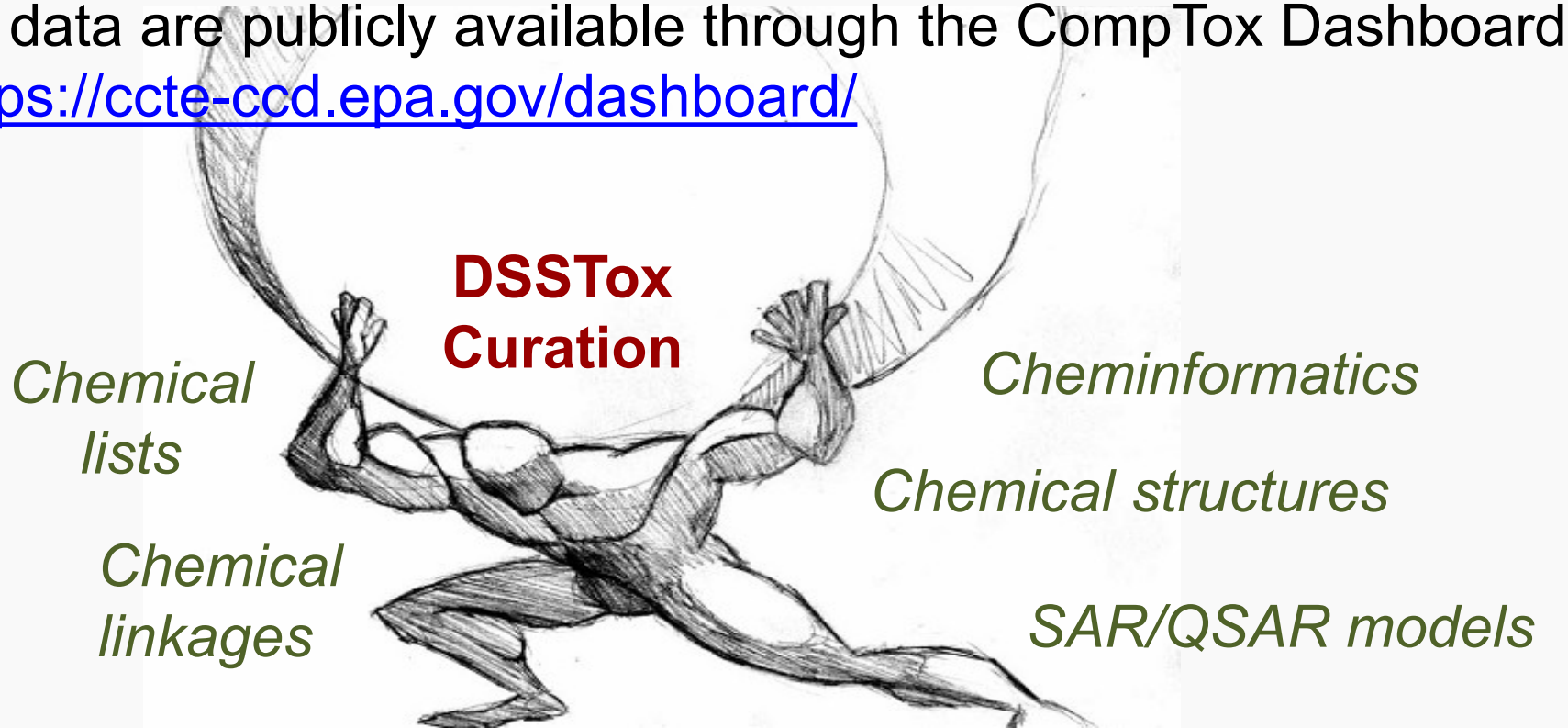


DSSTox Chemical Hub



Conclusions

- DSSTox has gained a reputation for quality chemical substance-structure content supporting a wide range of EPA programs
- Strict data model constraints (1:1:1) and expert manual curation are critical components
- All data are publicly available through the CompTox Dashboard https://ccte-ccd.epa.gov/dashboard/



Chemical Curation Team

EPA's Senior Environmental Employment (SEE) Program

DSSTOX-884

Register No Hits in SWGDRUGv2 (228 NOHITS) - Batch 4

Opioids, Cannabin...

DSSTOX-877

Register No Hits in SWGDRUGv2 (1342 NOHITS) - Batch 2

Opioids, Cannabin...

DSSTOX-885

Register No Hits in SWGDRUGv2 (182 NOHITS) - Batch 5

Opioids, Cannabin...

DSSTOX-888

Curate 10 NOHITS for the MTox700 metabolic

Metabolites and M...

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BA/MS Chemistry,
>15 yrs EPA laboratory & DSSTox curation experience

Brian Meyer
PhD Medicinal & Pharmacognosy Chemistry (Bayer Crop Sciences, retired)

Vicente Samano
PhD Organic Chemistry (GlaxoSmithKline, retired)

Sakuntala (Saku) Sivasupramaniam
PhD Entomology & Plant Sciences (Monsanto, retired)

Acknowledgements:

EPA's Incredible DSSTox Chemistry Team

Chris Grulke (formerly EPA- we miss him terribly!)
Current position - Assoc. Dir. Cheminformatics, Wave Life Sciences

Antony Williams, EPA's Chemistry & Cheminformatics Branch

Gabriel Sinclair, ORAU Student Services Contractor to US EPA

Indira Thillainadarajah
Brian Meyer
Saku Sivasupramaniam
Vicente Samano

} EPA's Senior Environmental Employment (SEE) Program

This work was reviewed by EPA and approved for publication but does not necessarily reflect official Agency policy. Mention of trade names or commercial products does not constitute endorsement.