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EPA United States Environmental Protection Agency

Introduction to Cheminformatics: Accessing data through the CompTox Dashboard

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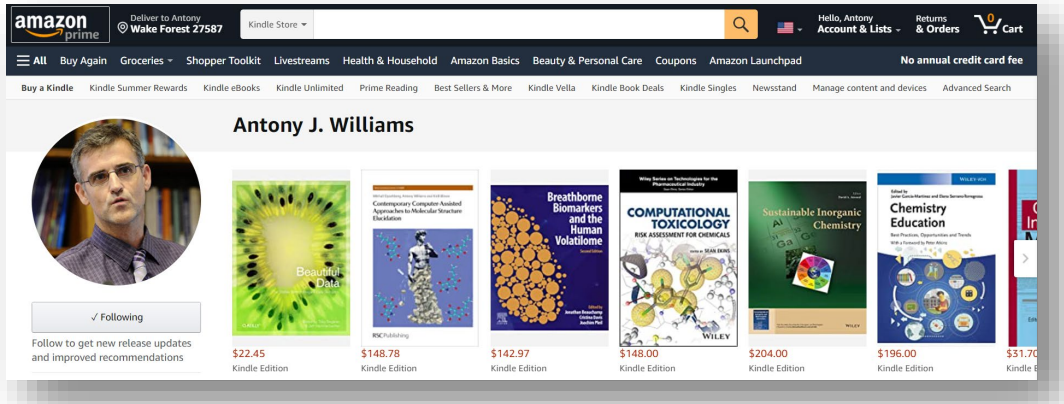
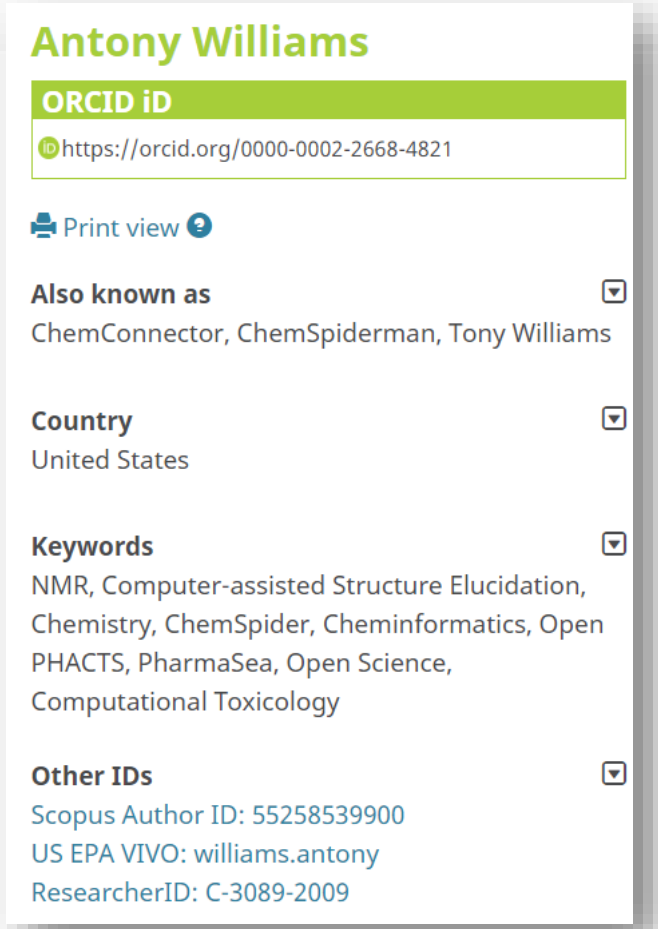
UNC Chapel Hill: September 20th 2021

Who am I?
https://orcid.org/0000-0002-2668-4821

United States Environmental Protection Agency

- Computational chemist at the US-EPA – **scientist**
- Responsibility for cheminformatics projects, internal & external collaborations, "product marketing"– **cheminformatician**
- Work with a team of people developing software solutions – "**product & project manager**"
- Scientific publications, books, blogger – **author;** I am @ChemConnector – **social networker**





Learning Objectives

- A *very short* overview of cheminformatics focused on
  - Chemical identifiers and some associated challenges
  - Molecular fingerprints
  - Molecular similarity
  - Structure-based modeling (QSAR/QSPR/QSUR)

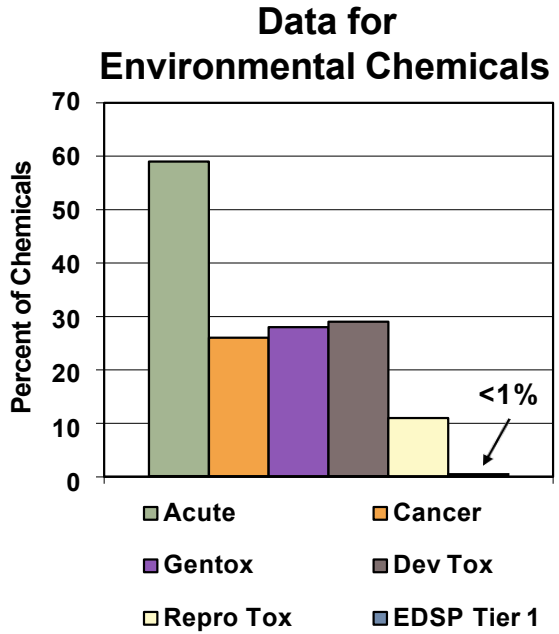
- An overview of the CompTox Chemicals Dashboard and how it can help to:
  - Search, source, visualize and download data for singleton or thousands of chemicals
  - Perform real-time prediction calculations and read-across
  - Navigate into dozens of other online resources that contain additional data

Problem: Too Many Chemicals and Too Few Resources

- Fast characterization of human and ecological risk posed by existing and emerging chemicals is a critical challenge
- Chemistry never stops. But there is sparse and distributed data…

CAS
A DIVISION OF THE
AMERICAN CHEMICAL SOCIETY

CAS REGISTRY® contains more than **171 million unique organic and inorganic chemical substances**, such as alloys, coordination compounds, minerals, mixtures, polymers and salts, and more than 68 million protein and DNA sequences



Modified from Judson *et al.*, EHP 2010

Solution

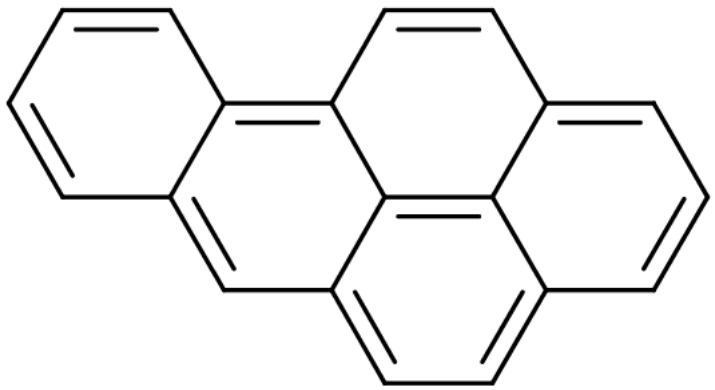
- Develop a “first-stop-shop” for environmental chemical data to support EPA and partner decision making:
  - **Centralized location** for relevant chemical data
  - Chemistry, exposure, hazard and dosimetry
  - Combination of existing data and predictive models
  - Publicly accessible, periodically updated, curated
- Easy access to data improves efficiency and ultimately accelerates chemical risk assessment

Cheminformatics and the Dashboard

- Cheminformatics is the application of computer science and informatics-based approaches to:
  - Represent chemical structures, substances and reactions
  - Store chemistry-related data
  - Search for chemistry related data
  - Model data sets to provide predictive capabilities
  - Visualize and analyse chemistry related data

- The US-EPA uses cheminformatics (and bioinformatics) to manipulate, integrate, store, model and deliver access to our data. The CompTox Chemicals Dashboard is built on a solid cheminformatics foundation

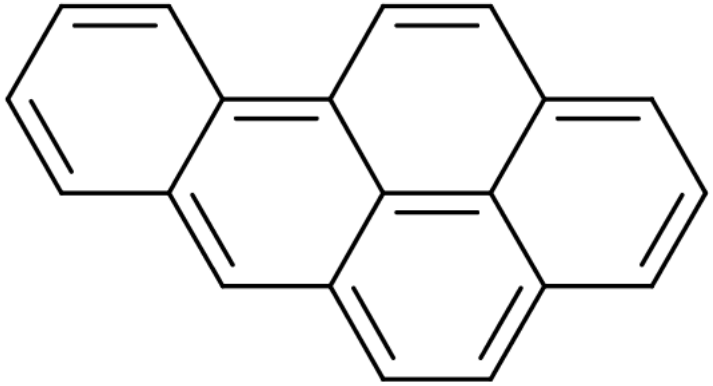
Types of Chemical Identifiers



- Structural Identifiers
- The visual depiction
- Multiple electronic formats
- InChI (Key): FMMWHPNWAFZXNH-UHFFFAOYSA-N

- Common Name: Benzo(a)pyrene
- Systematic Name: Benzo[pqr]tetraphene
- CAS Registry Number(s) : 50-32-8
- Lots of other “common names and trade names”

Information Associated with a Chemical Structure?



INTRINSIC PROPERTIES

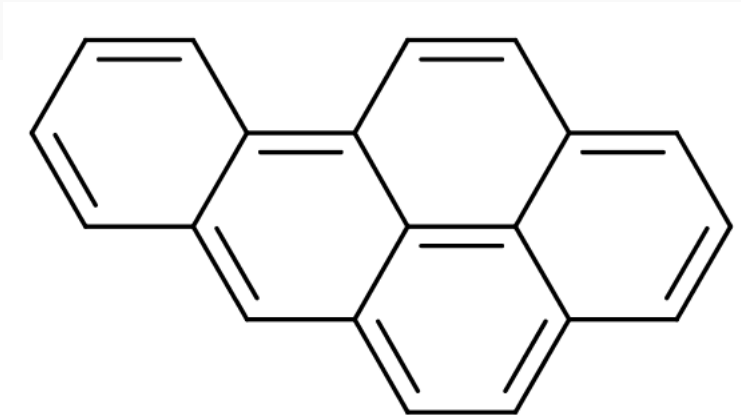
- Formula : $C_{20}H_{12}$
- Molecular weight: 252.316 g/mol
- Monoisotopic Mass: 252.093900 g/mol

MEASURED PROPERTIES

- LogKow 6.13
- Melting Pt177°C
- Boiling Pt 485°C
- ….and many more

How to Store a Chemical Structure

- Multiple approaches:
  - Names and identifiers
  - 2D or 3D structure “molfile”



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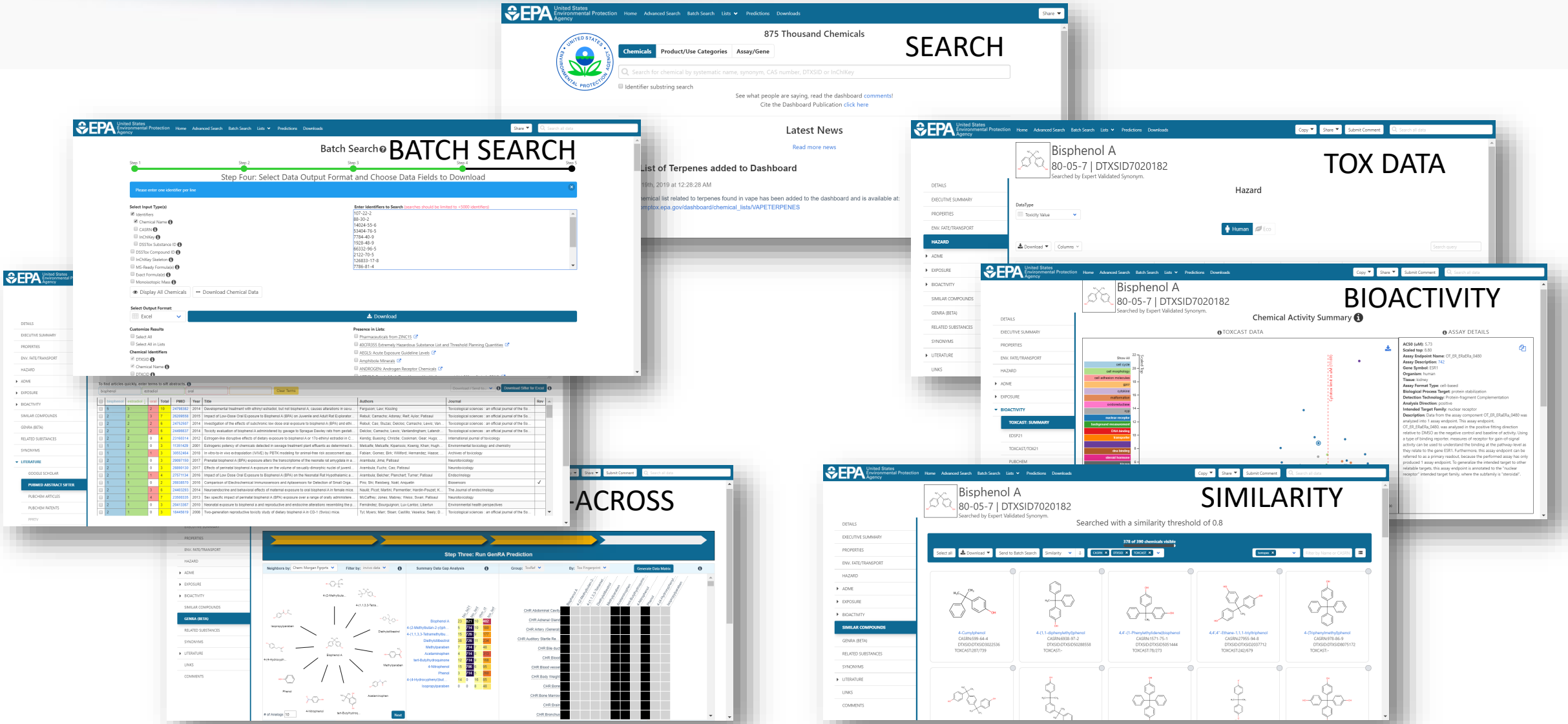
  0  0  0     0  0            999 V3000
M  V30 BEGIN CTAB
M  V30 COUNTS 20 24 0 0 0
M  V30 BEGIN ATOM
M  V30 1 C 5.3801 0 0 0
M  V30 2 C 6.9201 0 0 0
M  V30 3 C 7.6901 -1.33 0 0
M  V30 4 C 9.2302 -1.33 0 0
M  V30 5 C 10.0003 -2.67 0 0
M  V30 6 C 9.2302 -4.0001 0 0
M  V30 7 C 7.6901 -4.0001 0 0
M  V30 8 C 6.9201 -5.3301 0 0
M  V30 9 C 5.3801 -5.3301 0 0
M  V30 10 C 4.6201 -4.0001 0 0
M  V30 11 C 5.3801 -2.67 0 0
M  V30 12 C 6.9201 -2.67 0 0
M  V30 13 C 4.6201 -1.33 0 0
M  V30 14 C 3.0801 -1.33 0 0
M  V30 15 C 2.31 -2.67 0 0
M  V30 16 C 3.0801 -4.0001 0 0
M  V30 17 C 0.77 -2.67 0 0
M  V30 18 C 0 -1.33 0 0
M  V30 19 C 0.77 0 0 0
M  V30 20 C 2.31 0 0 0
M  V30 END ATOM
M  V30 BEGIN BOND
M  V30 1 2 1 2
M  V30 2 1 1 13
M  V30 3 1 2 3
M  V30 4 2 3 4
M  V30 5 1 3 12
M  V30 6 1 4
```

- SMILES:
  - c1cc2c3ccc4cccc5ccc(cc2cc1)c3c45
  - C1=CC2=CC3=CC=C4C=CC=C5C=CC(=C2C=C1)C3=C45
  - and many other variants….
- InChI=1S/C20H12/c1-2-7-17-15(4-1)12-16-9-8-13-5-3-6-14-10-11-18(17)20(16)19(13)14/h1-12H
- InChIKey: FMMWHPNWAFZXNH-UHFFFAOYSA-N

If We Database Chemical Structures…

- …then we can search the dataset by inherent **structural** properties
  - Formula
  - Mass
  - Substructure
  - Structural similarity
- …we can **integrate** other info into the database for retrieval
- …available data, both experimental and predicted, is a click away
- …data can be downloaded, distributed and shared
- …linking out to other resources enabled by adopting specific standards
- …structure collections, with associated data, are available for modeling

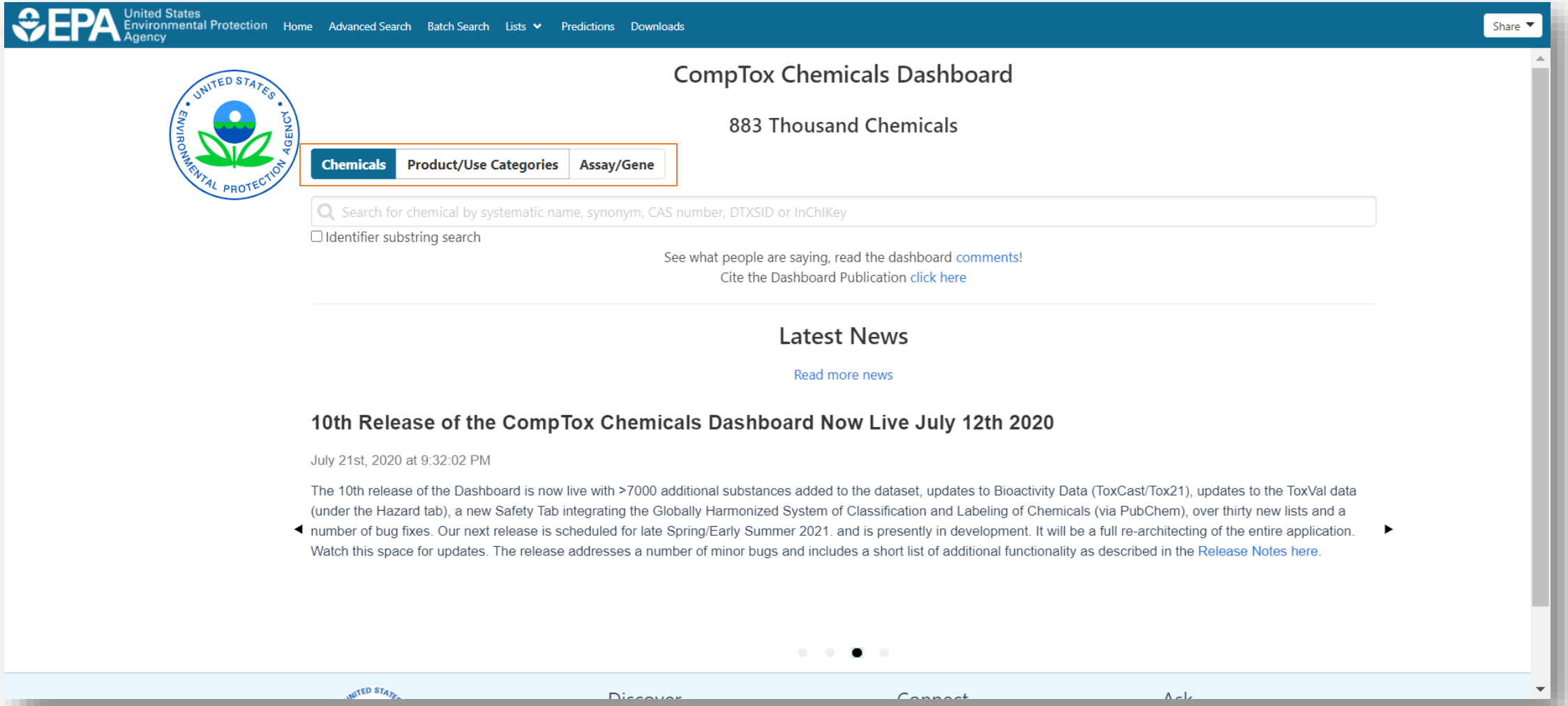
CompTox Chemicals Dashboard
https://comptox.epa.gov/dashboard



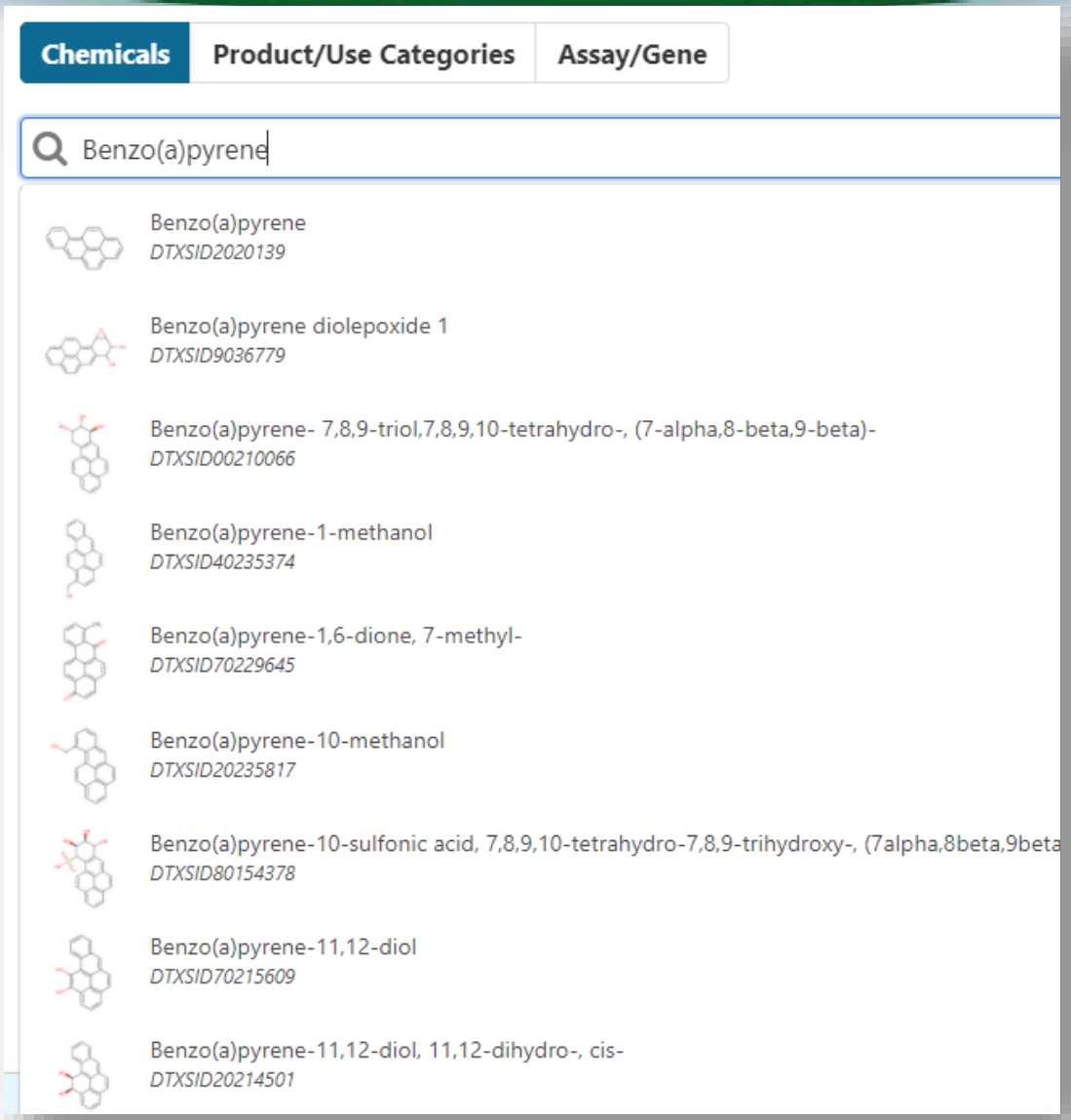
CompTox Chemicals Dashboard

EPA United States Environmental Protection Agency

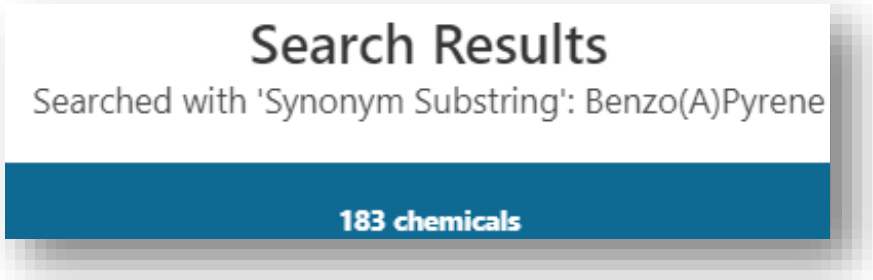
883k Chemical Substances



BASIC Search

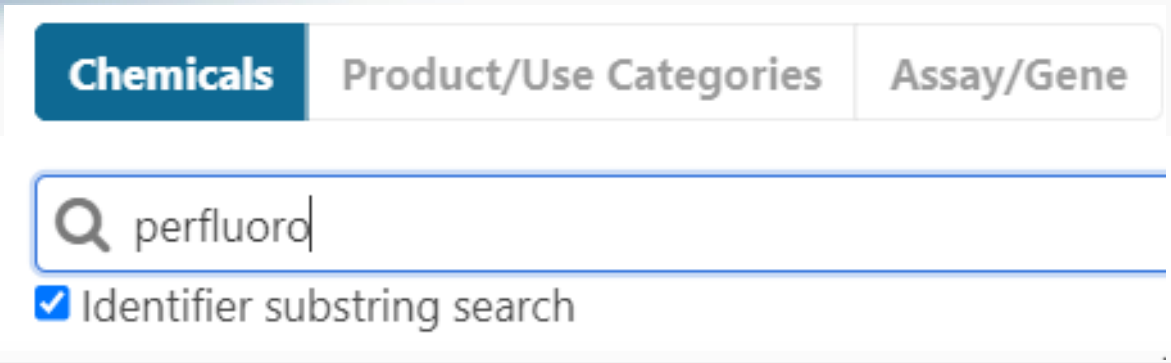


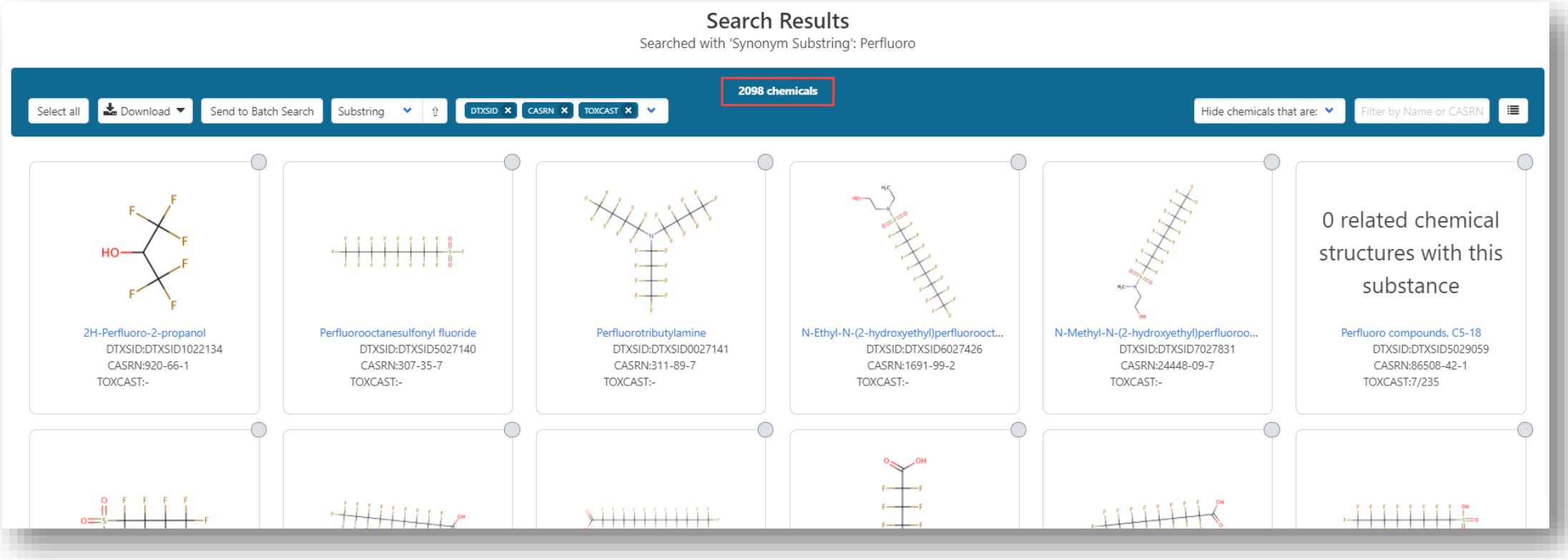
- Type ahead search using Names, synonyms and CASRNs
- Millions of identifiers
- Substring search



Search for classes of chemicals

- Examples: “perfluoro”





Challenges with Nomenclature

- Be CAREFUL with names! There is a LOT of confusion in the public domain. CHOOSE sources wisely!
- There are MANY public databases but not many are curated
- All public databases have value but not many curate data

- Example: METHANE on PubChem https://pubchem.ncbi.nlm.nih.gov/compound/297

CAS Registry Numbers on PubChem

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2.3.1 CAS

74-82-8

- CAMEO Chemicals; CAS Common Chemistry; ChemIDplus; DrugBank; EPA Chemicals under the TSCA; EPA DSSTox; European Chemicals Agency (ECH...

8006-14-2

- CAMEO Chemicals; EPA Chemicals under the TSCA; EPA DSSTox; European Chemicals Agency (ECHA)

7440-44-0

- ChemIDplus

7782-40-3

- ChemIDplus

7782-42-5

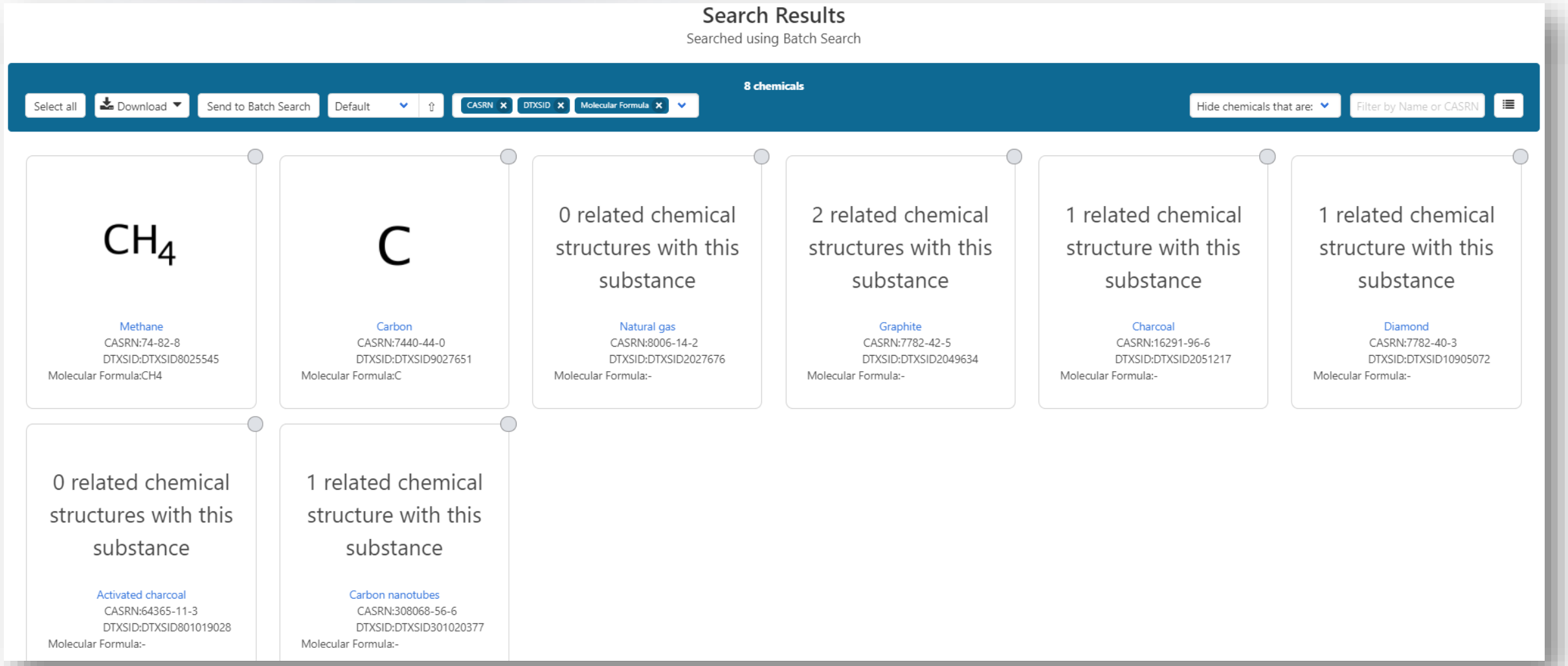
- ChemIDplus

16291-96-6

- ChemIDplus

64365-11-3

CASRN lookup on the dashboard



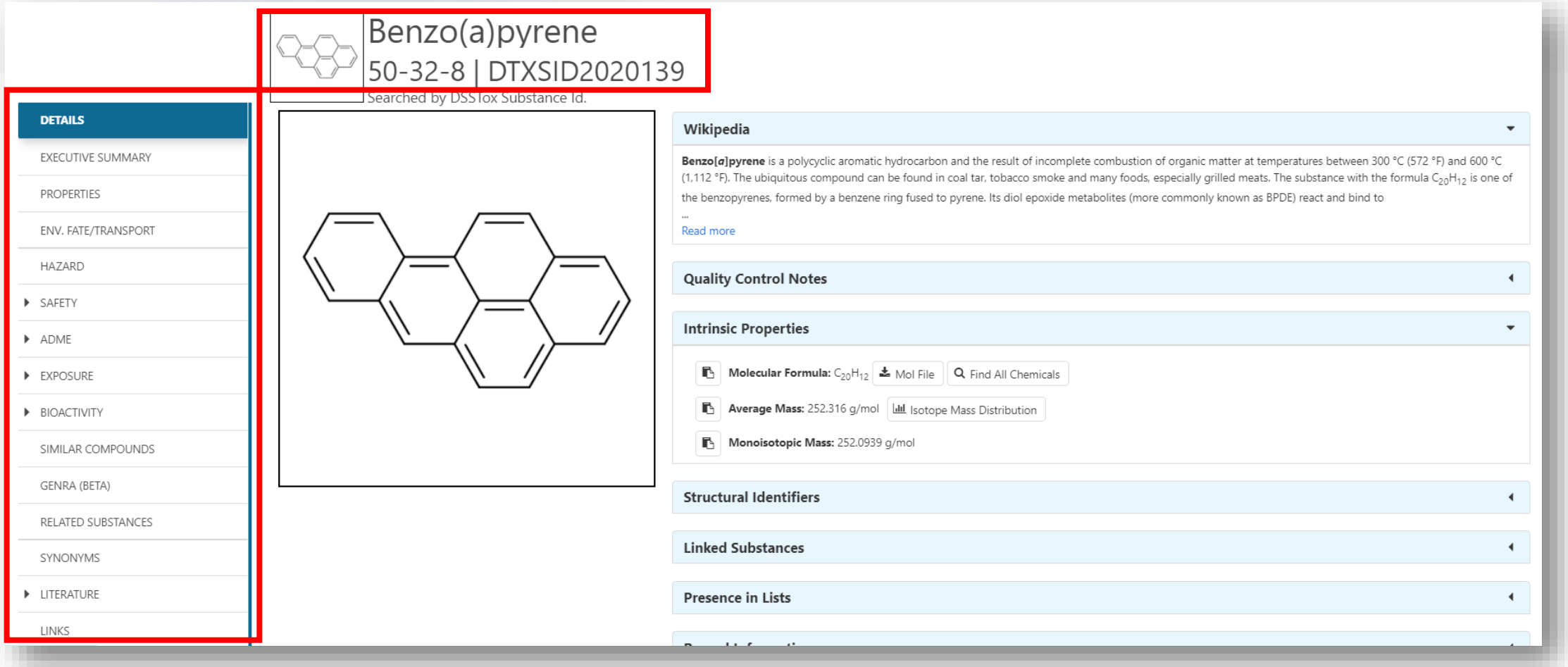
Methane is Diamond and Nanotubes?

- These are all Depositor Names for Methane ☹

2.4.2 Depositor-Supplied Synonyms

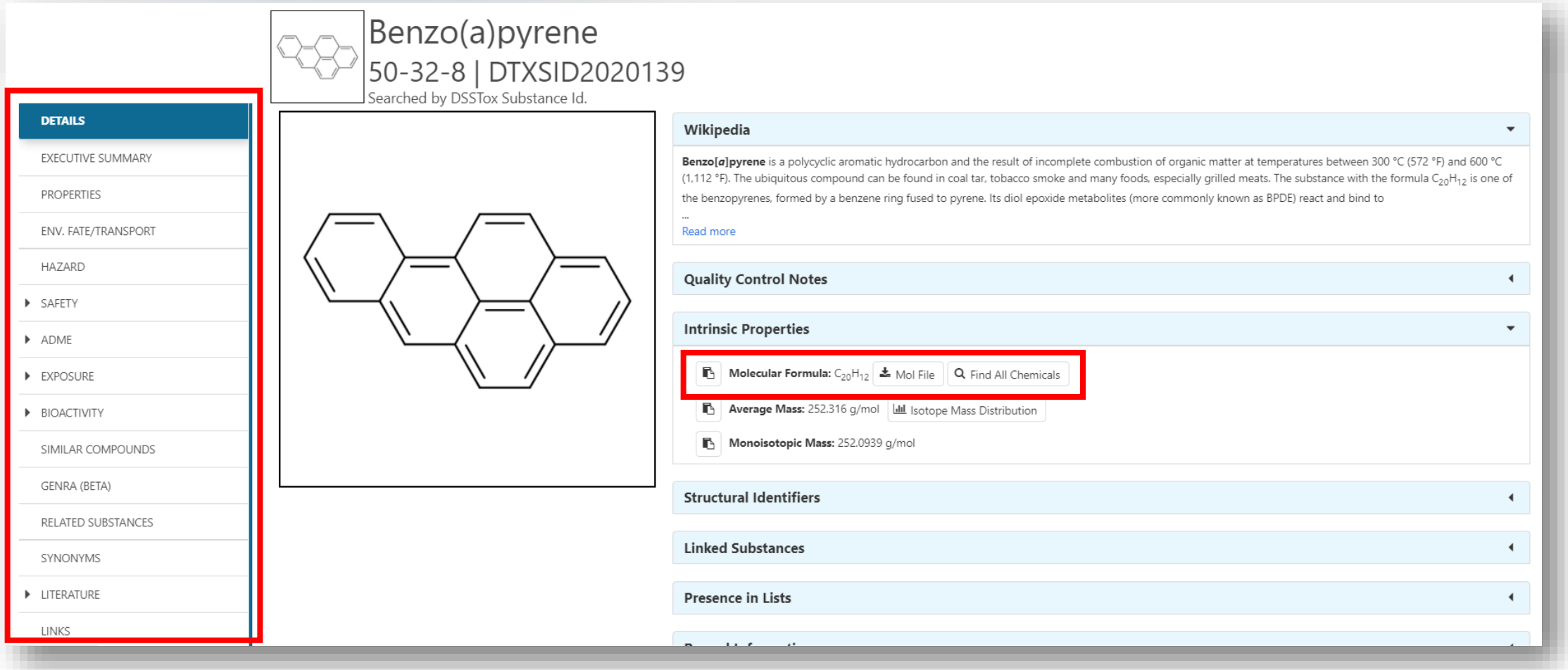
UN 1971 (Salt/Mix)	Fullerene soot, (as produced)	Carbon Nanotube sponges XFCN01	DTXSID9027651
UN 1972 (Salt/Mix)	MWNTs Butyl acetate suspension	Carbon Nanotube sponges XFCN07	Graphite electrode, rotrode disc
Activated carbon, pellets 3mm	QuadraPure C, 0.3-0.8mm	Carbon Nanotube sponges XFCN08	Carbon conductive cement adhesive
Graphene quantum dots(Powder)	6GRV67N0U2	Carbon, activated, -4+8 mesh	Conductive Flexible TPU Filament
Multiwall Nanotubes 5-15 nm	GO quantum dots yellow(Powder)	Carbon, activated, 2mm & down	GO quantum dots yellow(1mg/ml)
GO quantum dots(C: 1mg/ml)	Graphene electric aqueous slurry	CHEMBL2106049	Graphite powder, -20+84 mesh
MWNTs ethyl acetate suspension	Graphene powder Physical methods	Diamond Synthesized, 95% Nano	Carbon black, Super P Conductive
Reduced Graphene Oxide@ SnO2	Reduced Graphene Oxide@ Co3O4	Diethyl Cyanomethyl Phosphonate	DTXSID50179391
Carbon nanotubes aqueous slurry	Carbon Conductive Adhesive Tapes	DTXSID8025545	NanoIntegris metallic SWCNTs70%

Detailed Chemical Pages
One more identifier – the DTXSID



- Chemical page: Wikipedia snippet when available, intrinsic properties, structural identifiers, linked substances

Detailed Chemical Pages
Easy Navigation



- Chemical page: Wikipedia snippet when available, intrinsic properties, structural identifiers, linked substances

From the Chemical Details Page… all chemicals with same FORMULA

EPA United States Environmental Protection Agency

Intrinsic Properties

Molecular Formula: $C_{20}H_{12}$ | Mol File | Find All Chemicals

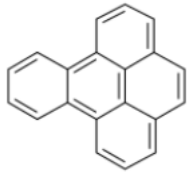
Search Results

Searched by Exact Molecular Formula: C20H12.

27 chemicals

Download | Send to Batch Search | Default | CASRN | DTXSID | Hide chemicals that are: | Filter by Name or C

Benzo(a)pyrene
CASRN:50-32-8
DTXSID:DTXSID2020139



Benzo(e)pyrene
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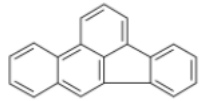
DTXSID:DTXSID3023764



Benzo(b)fluoranthene
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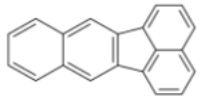
DTXSID:DTXSID0023907



Benzo(k)fluoranthene
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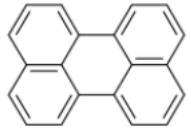
DTXSID:DTXSID0023909



Perylene
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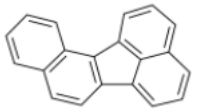

Benzo(j)fluoranthene
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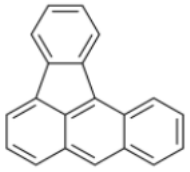

Benzo[a]fluoranthene
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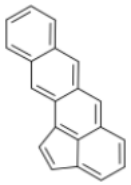
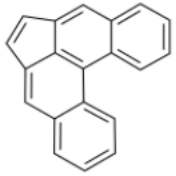
DTXSID:DTXSID4059756



Cyclopenta(de)naphthacene
CASRN:16683-64-0
DTXSID:DTXSID80168197



Benz(a)acephenanthrylene
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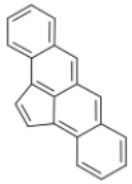

Cyclopenta(fg)naphthacene
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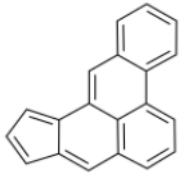

Benzo(de)cyclopent(a)anthracene
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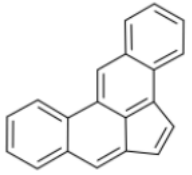
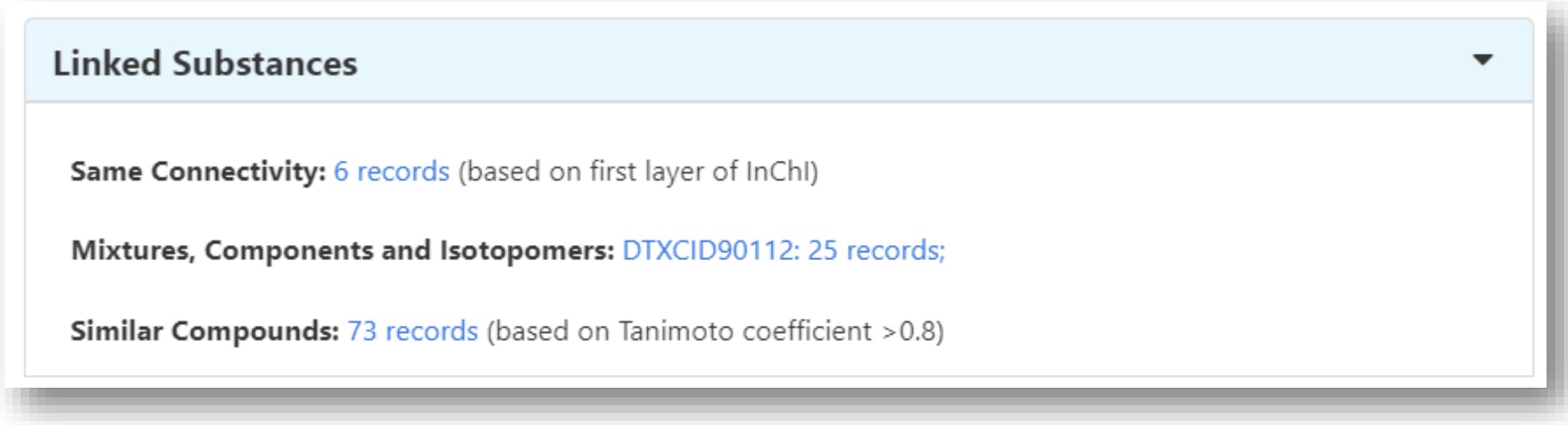


Benz(e)aceanthrylene
CASRN:199-54-2
DTXSID:DTXSID30173675

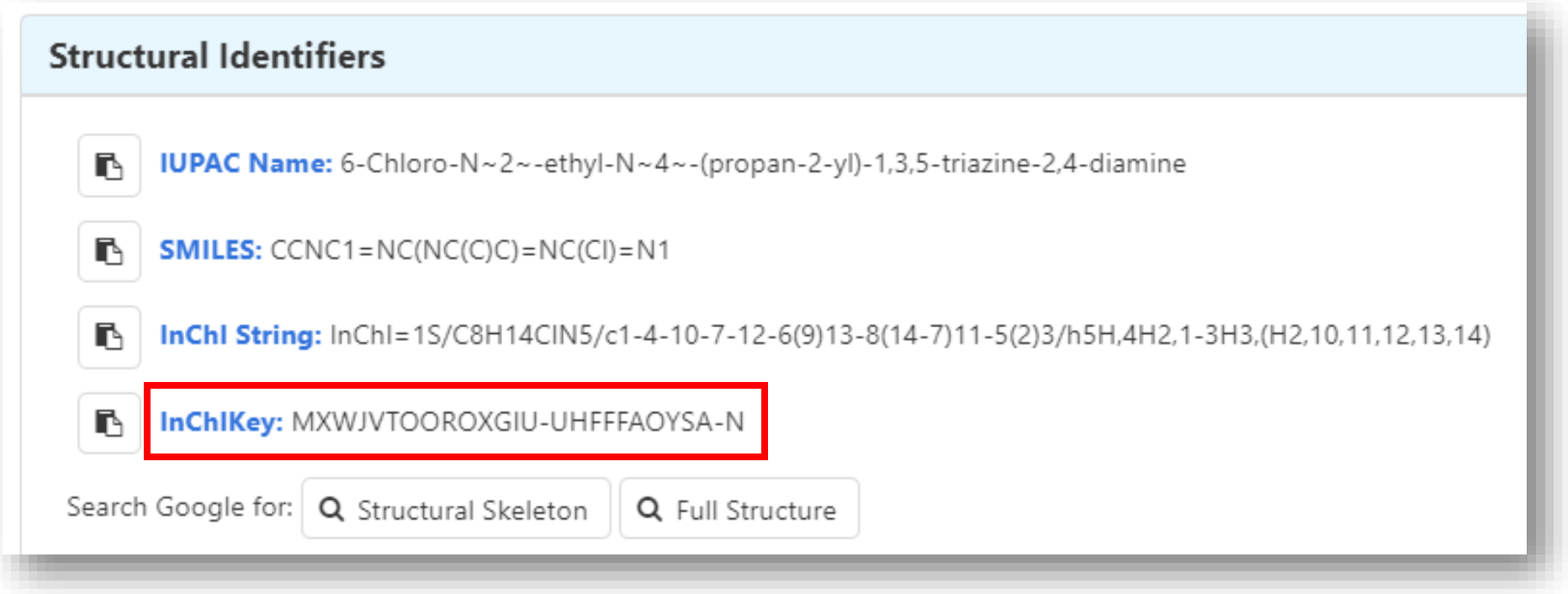
How many chemicals are associated through LINKED SUBSTANCES?

- Atrazine, is a herbicide – in MANY commercial products
- The dashboard has salt forms, isotopically labelled forms, multicomponent forms
- How do we identify what they are???



A little more about the InChI

- An InChIKey is made up of two blocks…
  - Block 1 – “the connectivity” of atoms and bonds
  - Block 2 – isotopes, charge, stereo



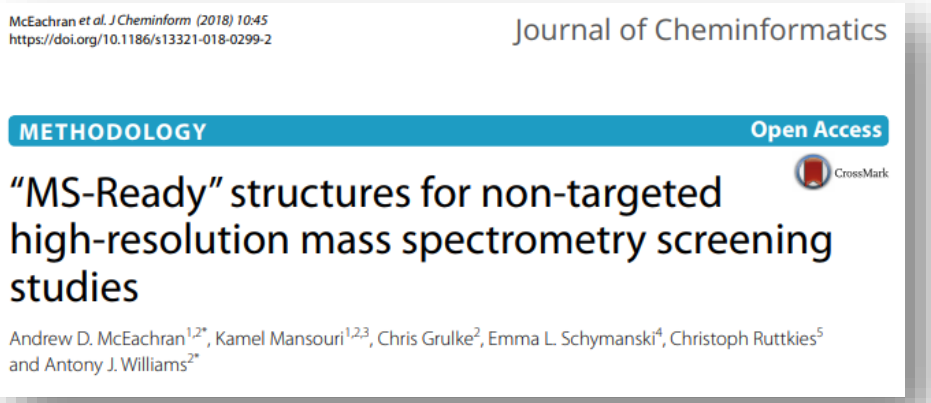
- The InChIKey is VERY USEFUL

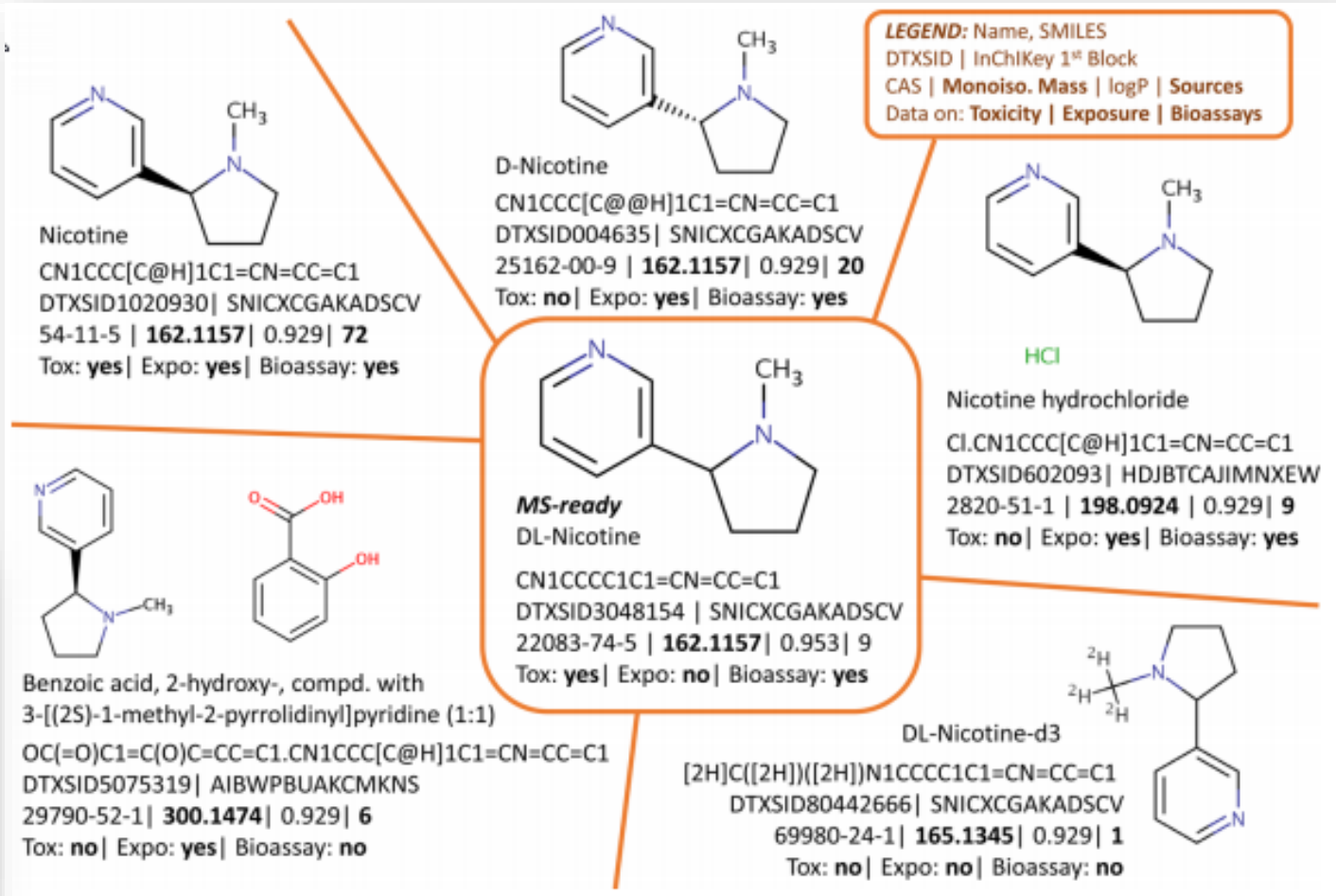
Searching using InChI

- Demo an internet search using InChIs – Cholesterol has the InChIKey: HVYWMOMLDIMFJA-DPAQBDIFSA-N
- Demo Atrazine – Linked Substances – Skeleton
- More about Linked Substances….

Linked Substances – more interesting

- We map chemicals together using cheminformatics approaches
- Use desalting, destereo, split multicomponents etc to map chemicals together





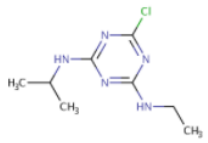
Atrazine Linked Substances

EPA United States Environmental Protection Agency

MS-Ready Mappings of Atrazine (Isotopes pre-filtered)

20 of 25 chemicals visible

Select all | Download | Send to Batch Search | Default | DTXSID | CASRN | TOXCAST | Isotopes | Filter by Name or CASRN



Atrazine
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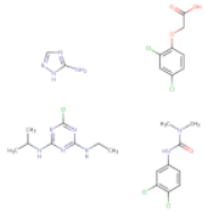
CASRN:1912-24-9
TOXCAST:62/1024



Anox M
DTXSID:DTXSID50156021
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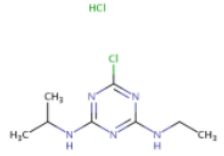
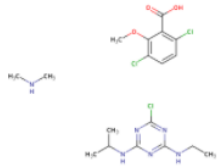
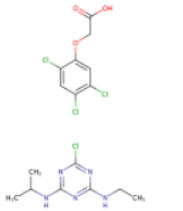
TOXCAST:-



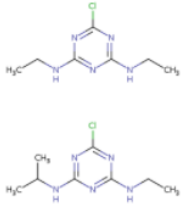
s-Triazine, 2-chloro-4-(ethylamino)-6-(is...
DTXSID:DTXSID30165459
CASRN:15386-47-7
TOXCAST:-



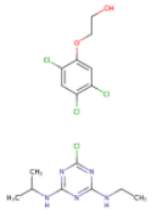
Marksman
DTXSID:DTXSID80166936
CASRN:160544-50-3
TOXCAST:-



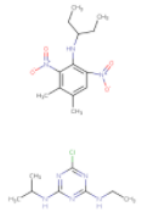
Acetic acid, (2,4,5-trichlorophenoxy)-, mi...
DTXSID:DTXSID70192527
CASRN:39283-62-0
TOXCAST:-



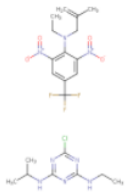
1,3,5-Triazine-2,4-diamine, 6-chloro-N,N...
DTXSID:DTXSID60192556
CASRN:39331-45-8
TOXCAST:-



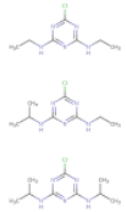
Buvinol
DTXSID:DTXSID10199555
CASRN:51602-05-2
TOXCAST:-



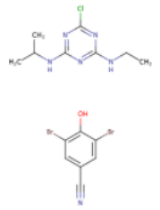
Atrazine mixture with pendimethalin
DTXSID:DTXSID10209527
CASRN:60704-01-0
TOXCAST:-



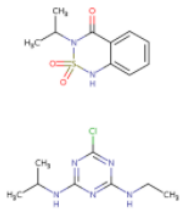
Maizor
DTXSID:DTXSID20215154
CASRN:64867-15-8
TOXCAST:-



Polytriazine
DTXSID:DTXSID00222508
CASRN:72172-70-4
TOXCAST:-



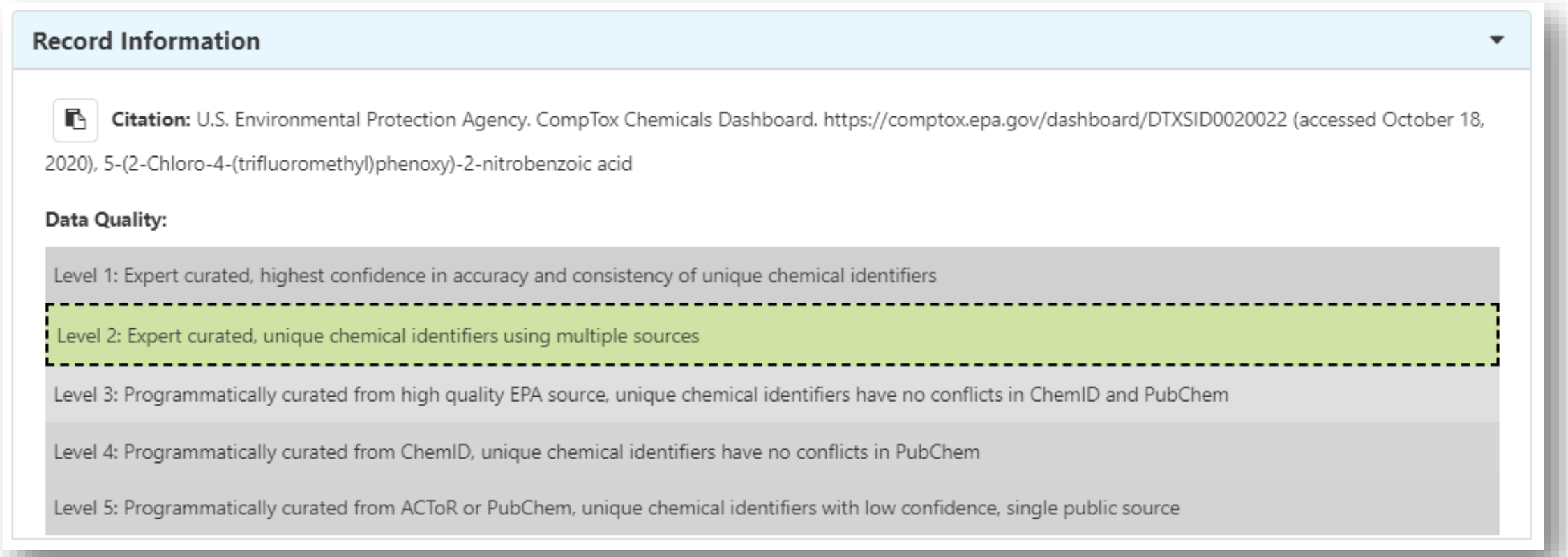
Benzonitrile, 3,5-dibromo-4-hydroxy-, m...
DTXSID:DTXSID20226063
CASRN:75084-56-9
TOXCAST:-



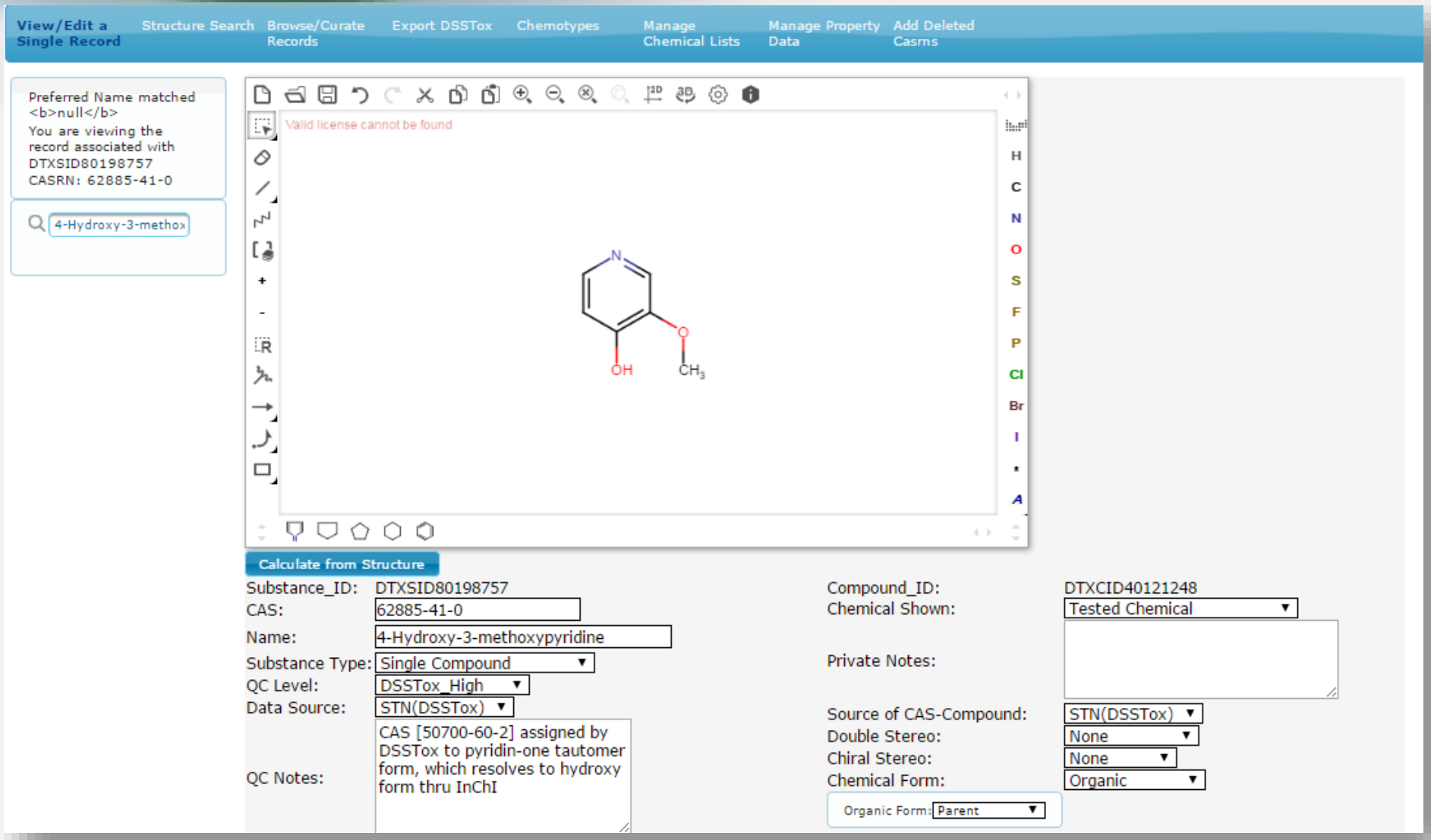
Bentazon / atrazine
DTXSID:DTXSID80226064
CASRN:75084-57-0
TOXCAST:-

A little more about our data quality

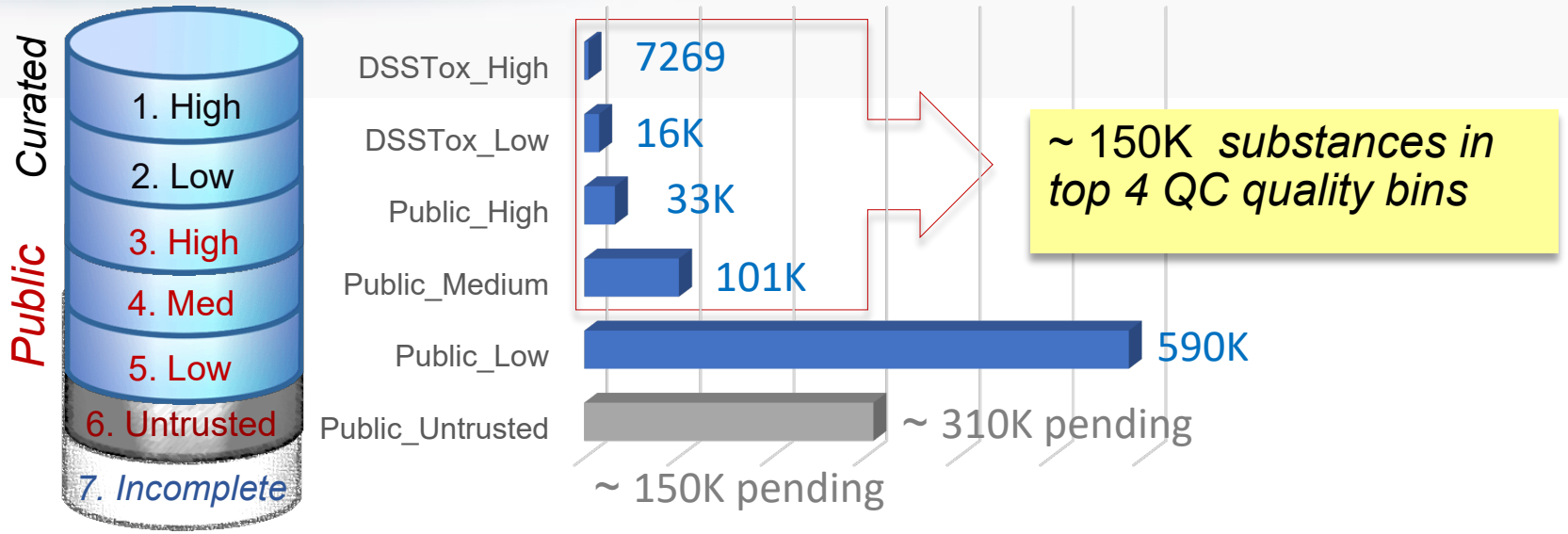
- Five full time curators register and curate data to elevate quality



Underneath the Dashboard



Distribution of curated data
Now at >1.2 MILLION substances



QC Levels	
DSSTox_High:	Hand curated and validated
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
Public_Untrusted:	Postulated, but found to have conflicts in public sources

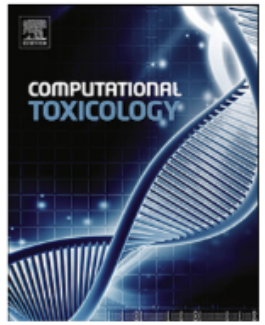
A little more about our data quality

Computational Toxicology 12 (2019) 100096

Contents lists available at ScienceDirect

Computational Toxicology

journal homepage: www.elsevier.com/locate/comtox



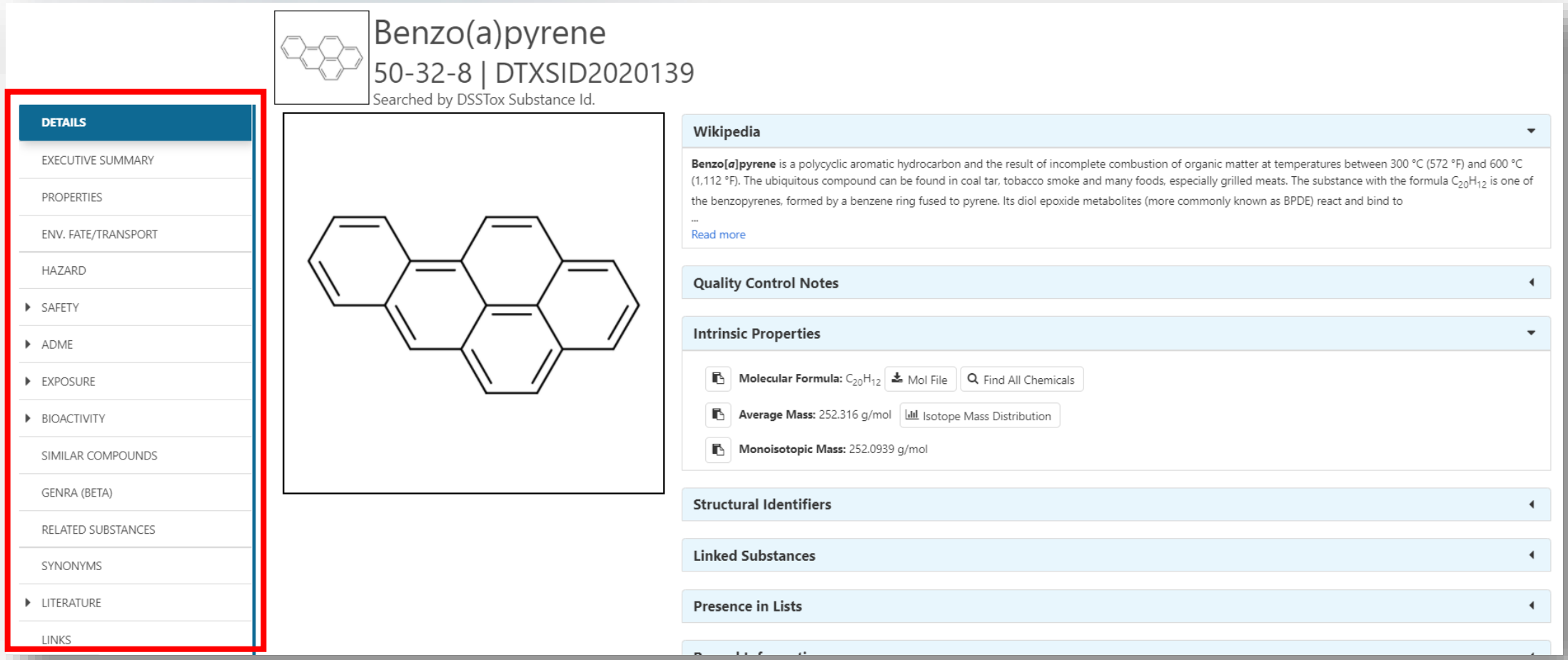
EPA's DSSTox database: History of development of a curated chemistry resource supporting computational toxicology research

Christopher M. Grulke[a], Antony J. Williams[a], Inthirany Thillanadarajah[b], Ann M. Richard[a,*]

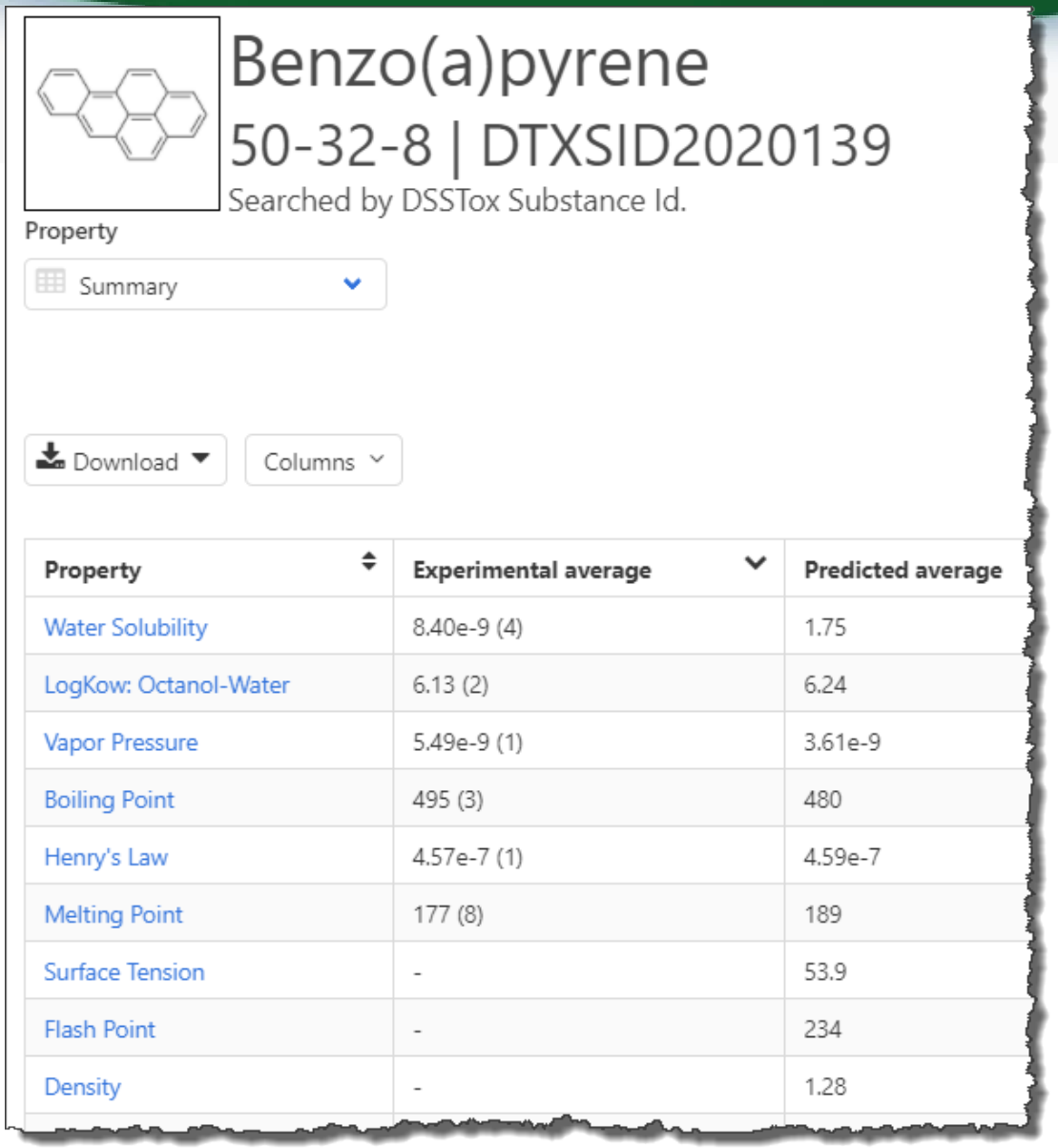
[a] National Center for Computational Toxicology, Office of Research & Development, US Environmental Protection Agency, Mail Drop D143-02, Research Triangle Park, NC 27711, USA

[b] Senior Environmental Employment Program, US Environmental Protection Agency, Research Triangle Park, NC 27711, USA

Navigating data via the Left Hand Tabs



Experimental and Predicted Data



Benzo(a)pyrene

50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

Property

Summary

Download Columns

Property	Experimental average	Predicted average
Water Solubility	8.40e-9 (4)	1.75
LogKow: Octanol-Water	6.13 (2)	6.24
Vapor Pressure	5.49e-9 (1)	3.61e-9
Boiling Point	495 (3)	480
Henry's Law	4.57e-7 (1)	4.59e-7
Melting Point	177 (8)	189
Surface Tension	-	53.9
Flash Point	-	234
Density	-	1.28

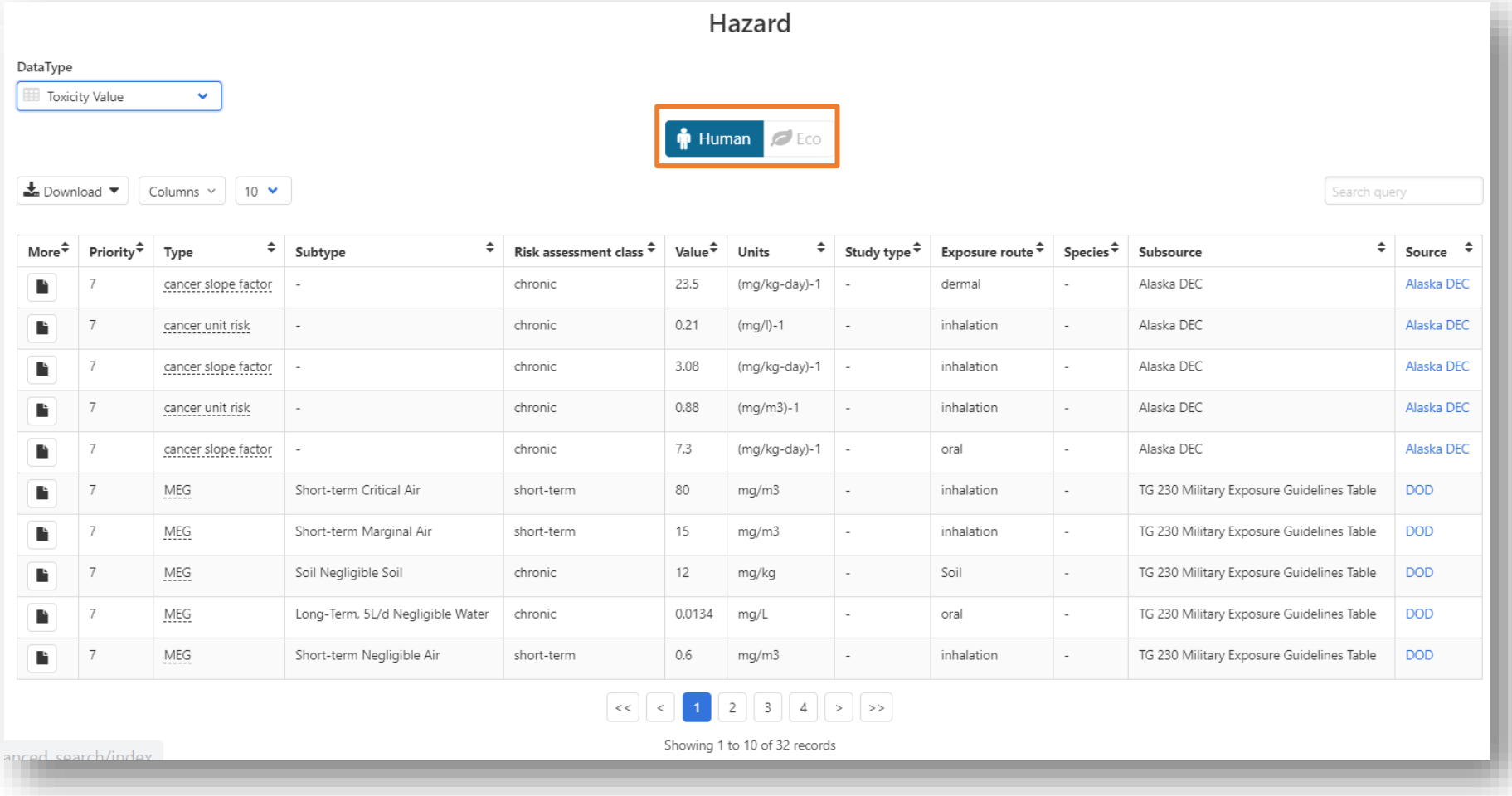
- Physchem and Fate & Transport experimental and predicted data
- Data can be downloaded as Excel, TSV and CSV files
- Predictions: multiple algorithms
  - EPI Suite: Estimation Program Interface
  - ACD/Labs (commercial)
  - TEST: **T**oxicity **E**stimation **S**oftware **T**ool
  - OPERA: **OPE**n structure–activity/ property **R**elationship **A**pp

Chemical Hazard Data

EPA United States Environmental Protection Agency

ToxVal Database

- >50k chemicals
- >770k tox. values
- >30 sources of data
- ~5k journals cited
- ~70k citations



More	Priority	Type	Subtype	Risk assessment class	Value	Units	Study type	Exposure route	Species	Subsource	Source
	7	cancer slope factor	-	chronic	23.5	(mg/kg-day)-1	-	dermal	-	Alaska DEC	Alaska DEC
	7	cancer unit risk	-	chronic	0.21	(mg/l)-1	-	inhalation	-	Alaska DEC	Alaska DEC
	7	cancer slope factor	-	chronic	3.08	(mg/kg-day)-1	-	inhalation	-	Alaska DEC	Alaska DEC
	7	cancer unit risk	-	chronic	0.88	(mg/m3)-1	-	inhalation	-	Alaska DEC	Alaska DEC
	7	cancer slope factor	-	chronic	7.3	(mg/kg-day)-1	-	oral	-	Alaska DEC	Alaska DEC
	7	MEG	Short-term Critical Air	short-term	80	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Short-term Marginal Air	short-term	15	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Soil Negligible Soil	chronic	12	mg/kg	-	Soil	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Long-Term, 5L/d Negligible Water	chronic	0.0134	mg/L	-	oral	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Short-term Negligible Air	short-term	0.6	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD

Safety Data

GHS Data

Print Page

PUBCHEM > BENZO[A]PYRENE > LABORATORY CHEMICAL SAFETY SUMMARY (LCSS) > GHS CLASSIFICATION

CID 2336

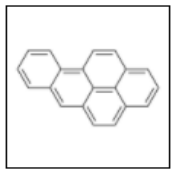
Benzo[a]pyrene

GHS Classification

Showing 6 of 6

Pictogram(s)	 Irritant, Health Hazard, Environmental Hazard
Signal	Danger
GHS Hazard Statements	H317: May cause an allergic skin reaction [Warning Sensitization, Skin] H340: May cause genetic defects [Danger Germ cell mutagenicity] H350: May cause cancer [Danger Carcinogenicity] H360FD: May damage fertility; May damage the unborn child [Danger Reproductive toxicity] H400: Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard] H410: Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard]
Precautionary Statement Codes	P201, P202, P261, P272, P273, P280, P281, P302+P352, P308+P313, P321, P333+P313, P363, P391, P405, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)

Identifiers Support Searches in other systems



Benzo(a)pyrene

50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

Synonyms

Download 25 Search query

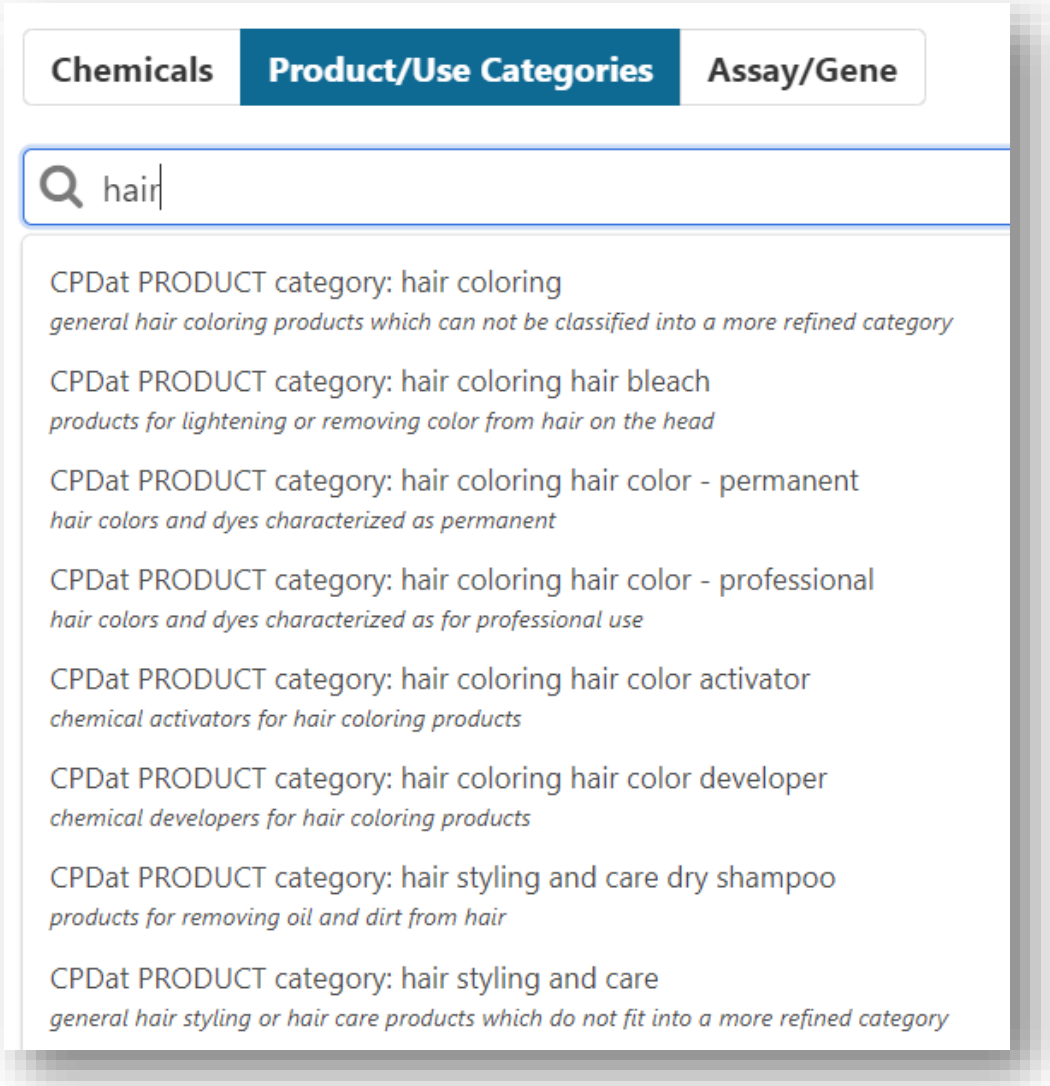
Synonym	Quality
Benzo(a)pyrene	**Valid**
Benzo[pqr]tetraphene	**Valid**
Benzo[a]pyrene	**Valid**
50-32-8 Active CAS-RN	**Valid**
BaP	**Valid**
Benzo[a]pyrene	*Good*
3,4-Benz[a]pyrene	*Good*
3,4-Benzopyrene	*Good*
3,4-Benzpyrene	*Good*
6,7-Benzopyrene	*Good*
BENZ(A)PYREN	*Good*
Benz(a)pyrene	*Good*
Benz[a]pyrene	*Good*

More About CASRNs

- CASRNs are very useful, and still limited
- Not every chemical has a STRUCTURE…substances vs structures
- “Chemical Abstracts Service” – numbers don’t exist until they abstracted and indexed
- Not every chemical on the dashboard necessarily has a CASRN – how would you find those that didn’t??? Hint: Search NOCAS_
- There are ~6000 chemicals without CASRN on the dashboard
- A chemical can also have many deleted CASRNs

Products Searching

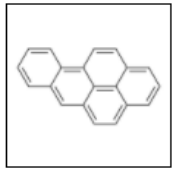
What chemicals are in hair care products?



Let’s Talk Exposure

- Types of Exposure Data on the Dashboard
  - Consumer product categories and uses
  - Products containing the chemical
  - Predicted exposure levels from modeling (more in next session)

Sources of Exposure to Chemicals



Benzo(a)pyrene

50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

Chemical Weight Fractions

Download | Columns | 10 | Search query

Product Name	Product Use Category	Minimum Weight Fraction	Maximum Weight Fraction	Data Type	Source
m-525-1-5x pah mixtures 0.5 mg/ml for method 525	Not Yet Categorized:			MSDS	SIRI
mm6125 surface conditioner	Not Yet Categorized:			Health Product Declaration	Health Product Declaration Collaborative
monolithic membrane 6125 (mm6125) / monolithic membrane	Not Yet Categorized:			Health Product Declaration	Health Product Declaration Collaborative
organic potablewatr pw 32_component h:reg semi-volatile 690	Not Yet Categorized:	0.00	1.00e-3	MSDS	SIRI
polynuclear aromatic hydrocarbon mixture_ ep84627	Not Yet Categorized:			MSDS	SIRI
prestone(r) power steering fluid	engine maintenance: auto fluids and additives			MSDS	CPCPdb
r-12 shield tite wet surface coating	Not Yet Categorized:	0.00	0.500	MSDS	SIRI
sea tar 1010_ 0028	Not Yet Categorized:			MSDS	SIRI
supelpreme-hc kit pah mix_ 48909	Not Yet Categorized:			MSDS	SIRI
supelpreme-hc pah mix 1ml_ 48905	Not Yet Categorized:			MSDS	SIRI

<< < 1 2 3 > >>

Showing 11 to 20 of 21 records

QSAR modeling

- What do you trust more? Experimental or predicted data?
- Do you trust individual models or consensus models
- What if there are no experimental data, how good are predictions?

Data Curation Pipelines plus Manual Curation Processes

EPA United States Environmental Protection Agency

SAR QSAR Environ Res. 2016 Nov;27(11):939-965. doi: 10.1080/1062936X.2016.1253611.

An automated curation procedure for addressing chemical errors and inconsistencies in public datasets used in QSAR modelling

K Mansouri [1] [2], C M Grulke [2], A M Richard [2], R S Judson [2], A J Williams [2]

Research article | Open Access | Published: 08 March 2018

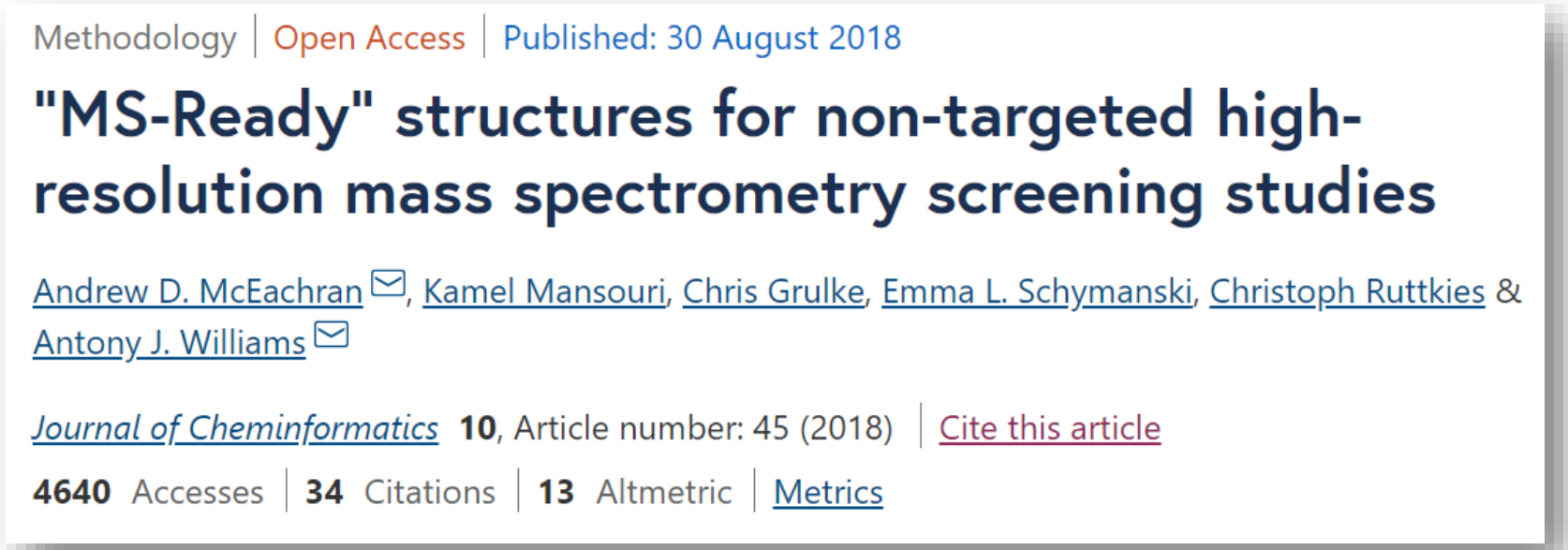
OPERA models for predicting physicochemical properties and environmental fate endpoints

Kamel Mansouri, Chris M. Grulke, Richard S. Judson & Antony J. Williams

Journal of Cheminformatics **10**, Article number: 10 (2018) | Cite this article

Property and Fate and Transport Data
~25 MILLION pre-predicted values

- We have built QSPR models based on tens of thousands of property data points curated over the past decade
- We push our “QSAR-Ready” chemical structures through predictions to produce property predictions



Methodology | Open Access | Published: 30 August 2018

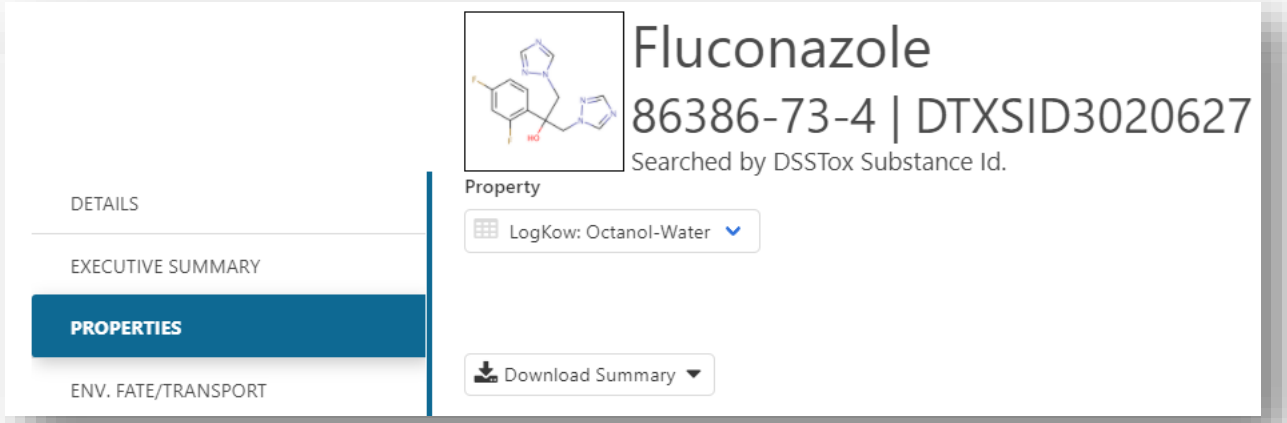
"MS-Ready" structures for non-targeted high-resolution mass spectrometry screening studies

Andrew D. McEachran, Kamel Mansouri, Chris Grulke, Emma L. Schymanski, Christoph Ruttkies & Antony J. Williams

Journal of Cheminformatics **10**, Article number: 45 (2018) | Cite this article

4640 Accesses | **34** Citations | **13** Altmetric | Metrics

Access to Predictions



Predicted

Download Predicted Data

Source	Result	Calculation Details	QMRF
EPISUITE	0.250	Not Available	Not Available
ACD/Labs Consensus	0.698	Not Available	Not Available
ACD/Labs	0.500	Not Available	Not Available
OPERA	0.501	OPERA Model Report [Inside AD]	Available

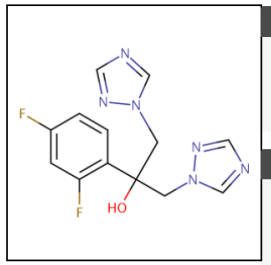
OPERA Reports

OPERA Models: LogKow: Octanol-Water

Fluconazole

86386-73-4 | DTXSID3020627

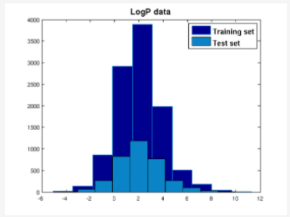
Print PDF

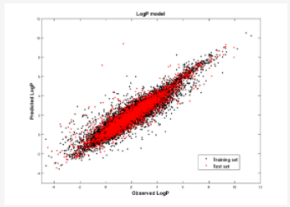


Model Results

Predicted value: 0.501
Global applicability domain: Inside
Local applicability domain index: 0.998
Confidence level: 0.732

Model Performance





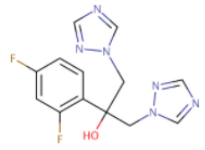
QMRF

Weighted KNN model

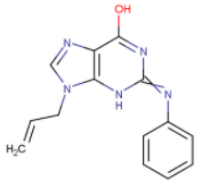
Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.850	0.690	0.860	0.670	0.860	0.780

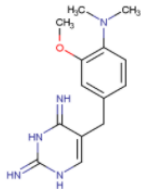
Nearest Neighbors from the Training Set



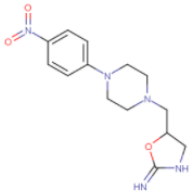
Fluconazole
Measured:0.5
Predicted: 0.50



GUANINEN2PHENYL9ALLYL
Measured:1.75
Predicted: 1.75



2,4-PYRIMIDINEDIAMINE, 5-[[4-(DIMETHYLAMINO)-3-M
Measured:1.87
Predicted: 1.87



5-(1-P-NITROPHENYL-4-PIPERAZINYL)METHYL-2-AMINO-
Measured:1.23
Predicted: 1.23

Similar reports for TEST predictions

EPA United States Environmental Protection Agency

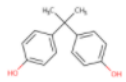
Predicted Normal boiling point for 80-05-7 from Consensus method

Prediction results

Endpoint	Experimental value	Predicted value
Normal boiling point Â°C	N/A	359.93

Individual Predictions

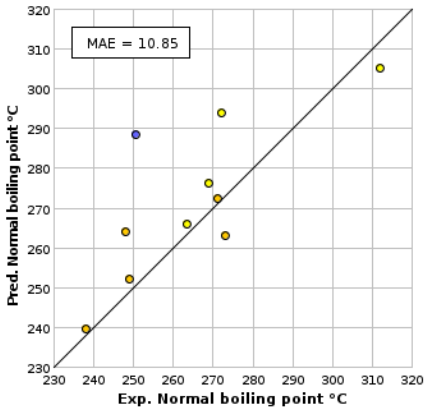
Method	Predicted value Â°C
Hierarchical clustering	372.06
Group contribution	377.41
Nearest neighbor	330.33



Predictions for the test chemical and for the most similar chemicals in the external test set

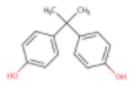
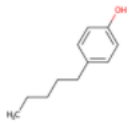
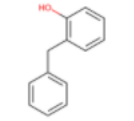
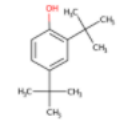
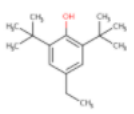
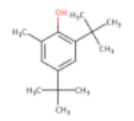
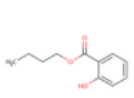
If the predicted value matches the experimental values for similar chemicals in the test set (and the similar chemicals

Prediction results (colors defined in table below)

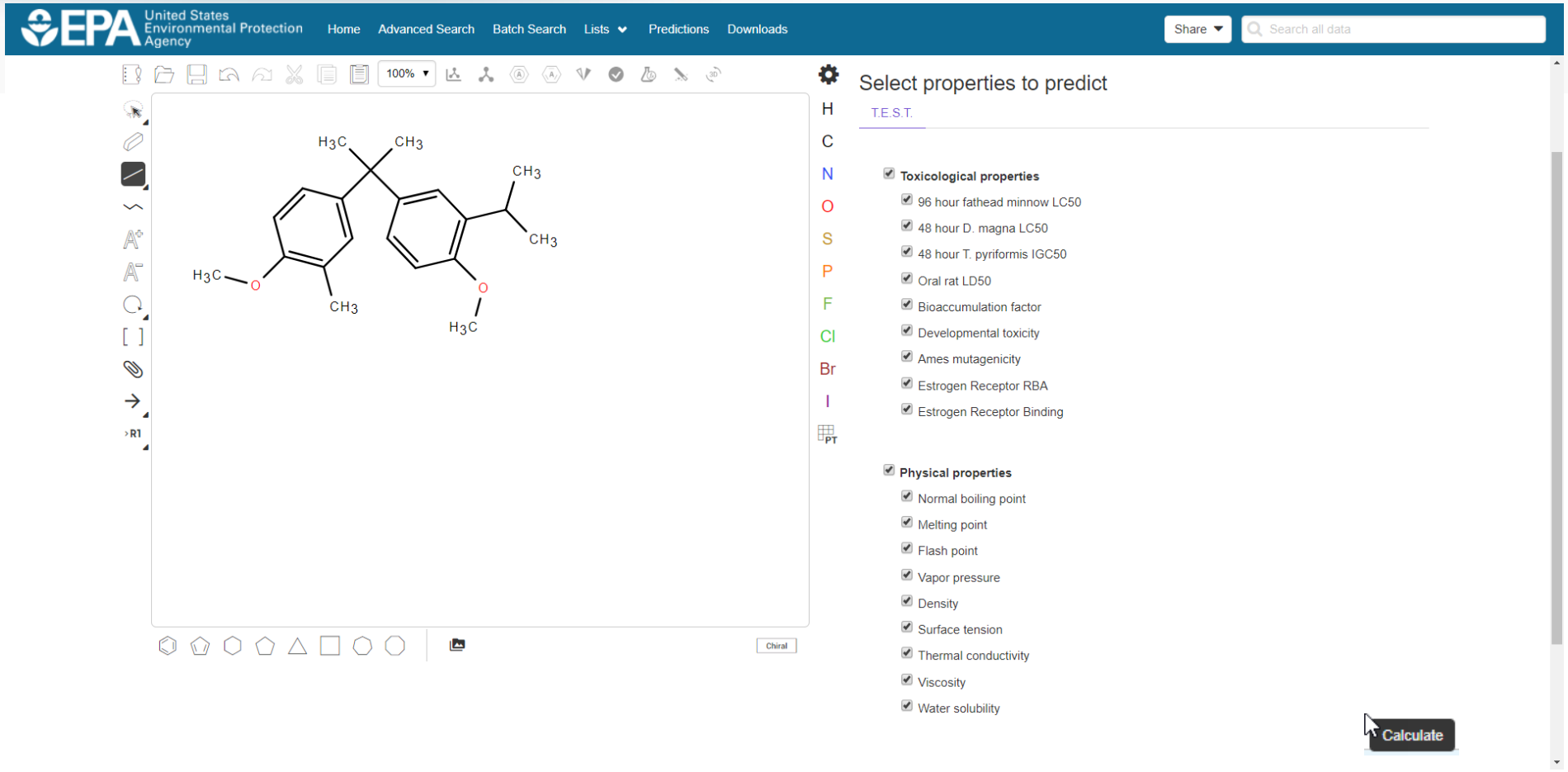


Chemicals	MAE*
Entire set	11.46
Similarity coefficient ≥ 0.5	10.85

*Mean absolute error in Â°C

CAS	Structure	Similarity Coefficient	Experimental value Â°C	Predicted value Â°C
80-05-7 (test chemical)			N/A	359.93
14938-35-3		0.81	250.50	288.54
28994-41-4		0.75	312.00	305.28
96-76-4		0.71	263.50	265.93
4130-42-1		0.70	272.00	293.96
616-55-7		0.70	269.00	276.42
2052-14-4		0.69	271.00	272.30

Real-Time Predictions

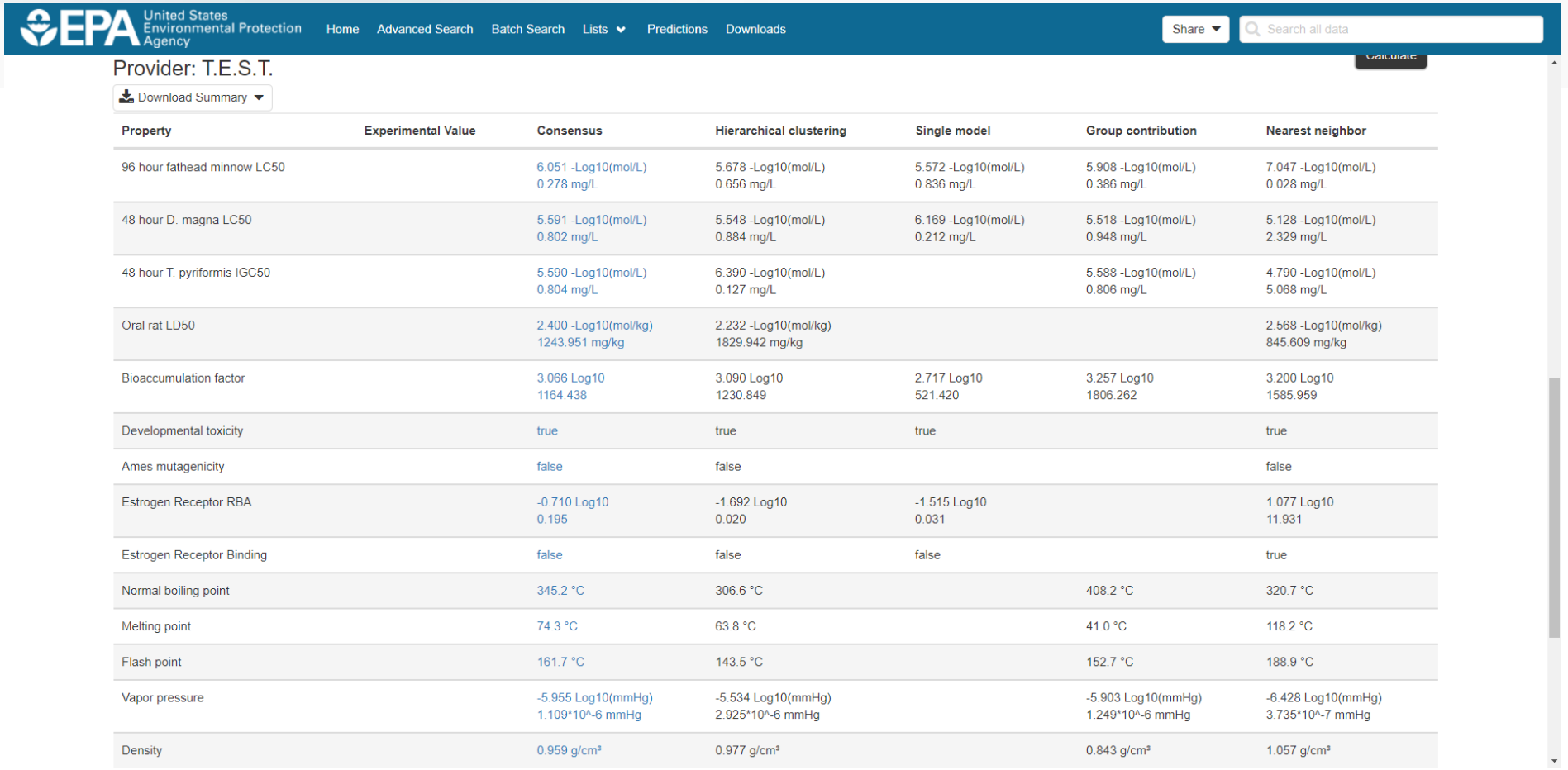


Toxicity and Properties

- Toxicological properties
  - 96 hour fathead minnow LC50
  - 48 hour D. magna LC50
  - 48 hour T. pyriformis IGC50
  - Oral rat LD50
  - Bioconcentration factor
  - Developmental toxicity
  - Ames mutagenicity
  - Estrogen Receptor RBA
  - Estrogen Receptor Binding

- Physical properties
  - Normal boiling point
  - Melting point
  - Flash point
  - Vapor pressure
  - Density
  - Surface tension
  - Thermal conductivity
  - Viscosity
  - Water solubility

Real-Time Predictions



Property	Experimental Value	Consensus	Hierarchical clustering	Single model	Group contribution	Nearest neighbor
96 hour fathead minnow LC50		6.051 -Log10(mol/L) 0.278 mg/L	5.678 -Log10(mol/L) 0.656 mg/L	5.572 -Log10(mol/L) 0.836 mg/L	5.908 -Log10(mol/L) 0.386 mg/L	7.047 -Log10(mol/L) 0.028 mg/L
48 hour D. magna LC50		5.591 -Log10(mol/L) 0.802 mg/L	5.548 -Log10(mol/L) 0.884 mg/L	6.169 -Log10(mol/L) 0.212 mg/L	5.518 -Log10(mol/L) 0.948 mg/L	5.128 -Log10(mol/L) 2.329 mg/L
48 hour T. pyriformis IGC50		5.590 -Log10(mol/L) 0.804 mg/L	6.390 -Log10(mol/L) 0.127 mg/L		5.588 -Log10(mol/L) 0.806 mg/L	4.790 -Log10(mol/L) 5.068 mg/L
Oral rat LD50		2.400 -Log10(mol/kg) 1243.951 mg/kg	2.232 -Log10(mol/kg) 1829.942 mg/kg			2.568 -Log10(mol/kg) 845.609 mg/kg
Bioaccumulation factor		3.066 Log10 1164.438	3.090 Log10 1230.849	2.717 Log10 521.420	3.257 Log10 1806.262	3.200 Log10 1585.959
Developmental toxicity		true	true	true		true
Ames mutagenicity		false	false			false
Estrogen Receptor RBA		-0.710 Log10 0.195	-1.692 Log10 0.020	-1.515 Log10 0.031		1.077 Log10 11.931
Estrogen Receptor Binding		false	false	false		true
Normal boiling point		345.2 °C	306.6 °C		408.2 °C	320.7 °C
Melting point		74.3 °C	63.8 °C		41.0 °C	118.2 °C
Flash point		161.7 °C	143.5 °C		152.7 °C	188.9 °C
Vapor pressure		-5.955 Log10(mmHg) 1.109*10^-6 mmHg	-5.534 Log10(mmHg) 2.925*10^-6 mmHg		-5.903 Log10(mmHg) 1.249*10^-6 mmHg	-6.428 Log10(mmHg) 3.735*10^-7 mmHg
Density		0.959 g/cm³	0.977 g/cm³		0.843 g/cm³	1.057 g/cm³

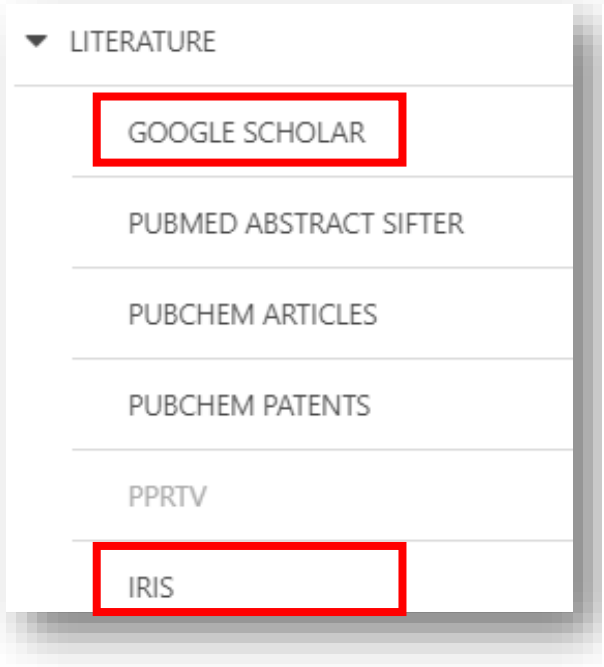
What's the best way to search the internet for chemical data?

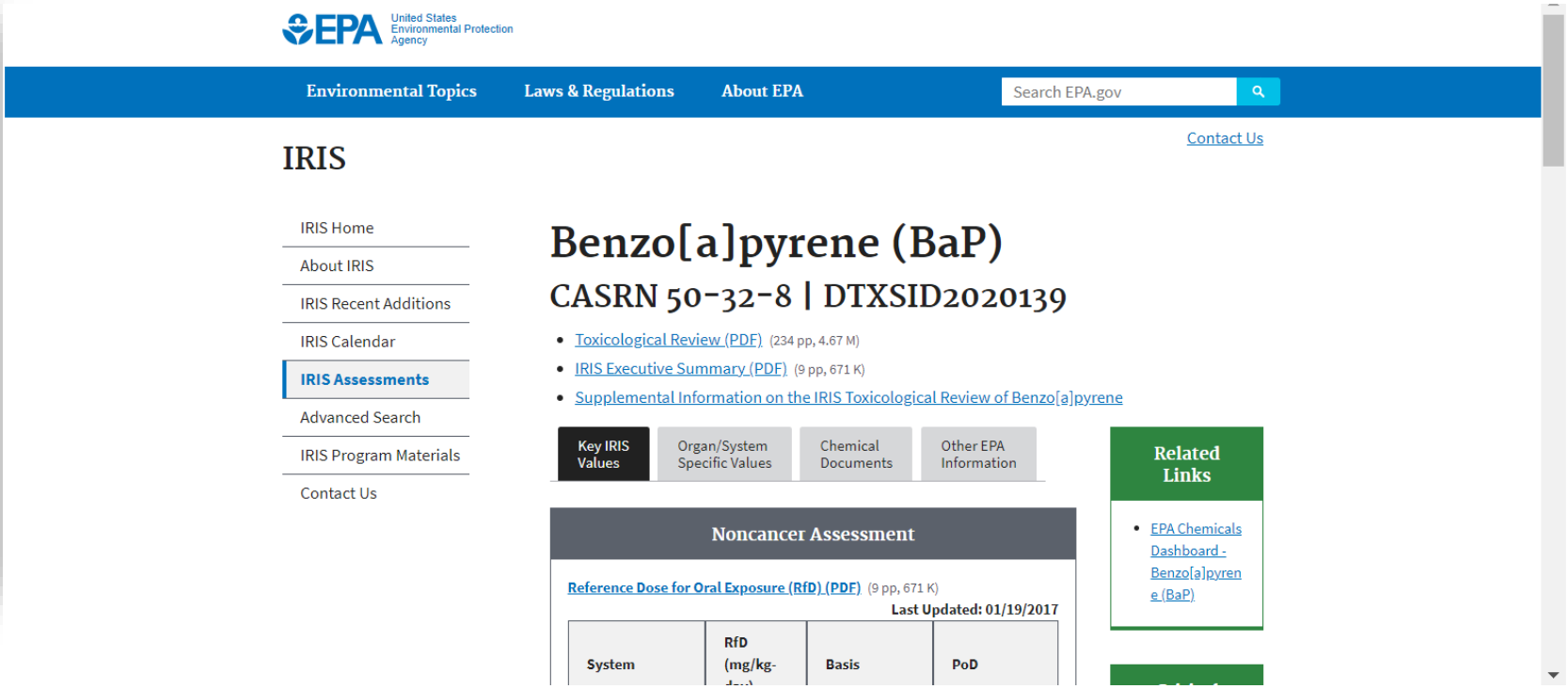
- We know how complex chemicals identifiers are…
  - CASRN(s)
  - Hundreds of names (maybe)
  - SMILES
  - InChIs
  - EINECS, EC numbers

- What can WE do to help you navigate the internet?

Identifiers are used in the app

- Identifiers are used to feed and link into “Literature”





Literature Searching

Benzo(a)pyrene

50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

Abstract Sifter

1) Select PubMed starting point query then 2) click on Retrieve.

Hazard

Retrieve Articles

- Select a Query Term
- Hazard
- Fate and Transport
- Metabolism/PK/PD
- Chemical Properties
- Exposure
- Mixtures
- Male Reproduction
- Androgen Disruption
- Female Reproduction
- GeneTox
- Cancer
- Clinical Trials
- Embryo and embryonic development
- Child (infant through adolescent)
- Dust and Exposure
- Food and Exposure
- Water and Exposure
- Algae
- Disaster / Emergency

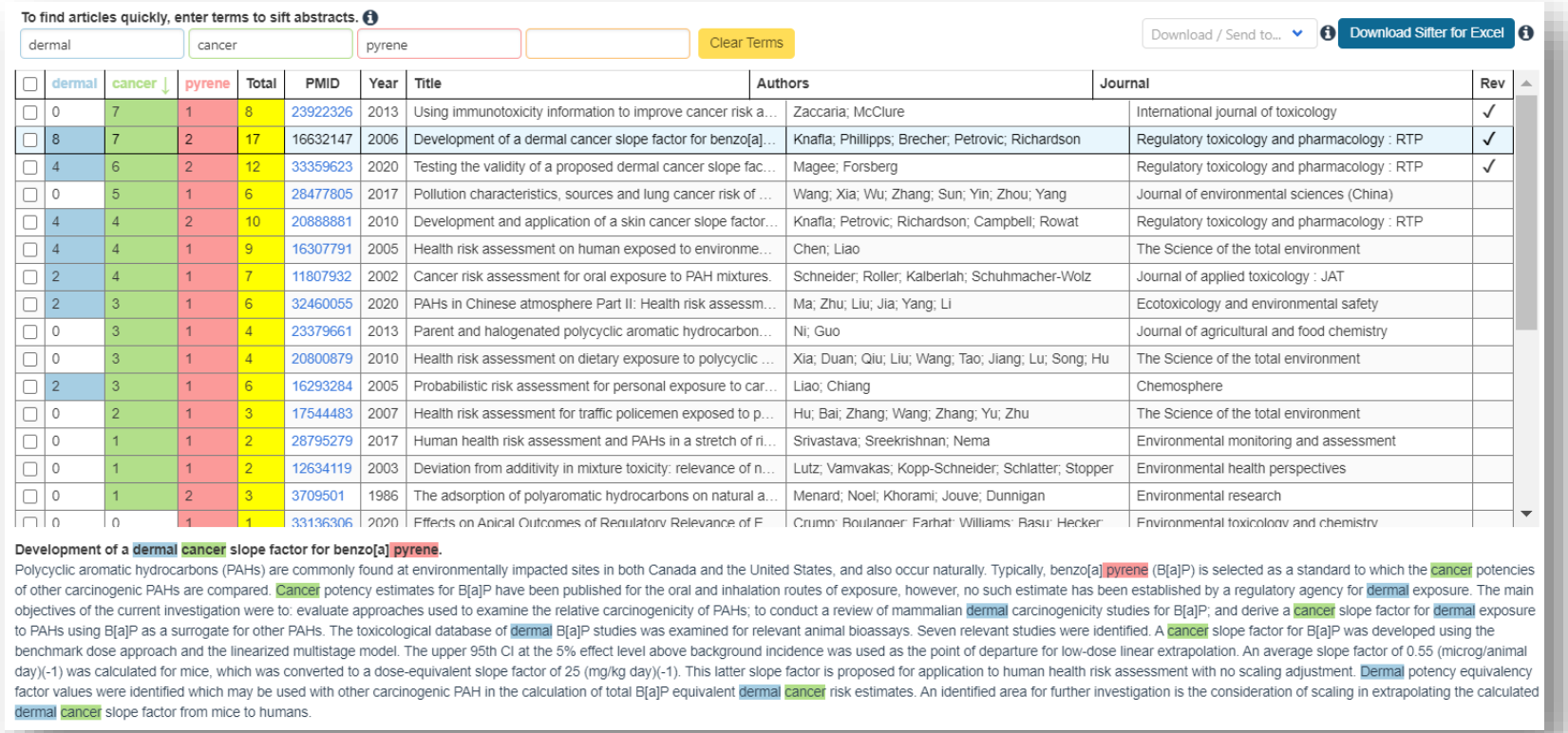
Optionally, edit the query before retrieving.

("50-32-8" OR "Benzo(a)pyrene") AND (NOAEL OR NOEL OR LOEL OR Rfd OR "reference dose" OR "reference concentration" OR "adverse effect level"[tiab] OR "cancer slope factor"[tiab])

- Real-time retrieval of data from PubMed ~30 million abstracts and growing)
- Choose from set of pre-defined queries
- Adjust and fine tune queries based on interests

Literature Searching

- "Sifting" of results using multiple terms
- Frequency counting terms
- Color highlighting of terms
- Download list to Excel
- Send list to PubMed for downloading ref. file
- Direct link via PubMed ID



To find articles quickly, enter terms to sift abstracts.

dermal | cancer | pyrene | Clear Terms | Download / Send to... | Download Sifter for Excel

	dermal	cancer ↓	pyrene	Total	PMID	Year	Title	Authors	Journal	Rev
	0	7	1	8	23922326	2013	Using immunotoxicity information to improve cancer risk a…	Zaccaria; McClure	International journal of toxicology	✓
	8	7	2	17	16632147	2006	Development of a dermal cancer slope factor for benzo[a]…	Knafla; Phillipps; Brecher; Petrovic; Richardson	Regulatory toxicology and pharmacology : RTP	✓
	4	6	2	12	33359623	2020	Testing the validity of a proposed dermal cancer slope fac…	Magee; Forsberg	Regulatory toxicology and pharmacology : RTP	✓
	0	5	1	6	28477805	2017	Pollution characteristics, sources and lung cancer risk of …	Wang; Xia; Wu; Zhang; Sun; Yin; Zhou; Yang	Journal of environmental sciences (China)	
	4	4	2	10	20888881	2010	Development and application of a skin cancer slope factor…	Knafla; Petrovic; Richardson; Campbell; Rowat	Regulatory toxicology and pharmacology : RTP	
	4	4	1	9	16307791	2005	Health risk assessment on human exposed to environme…	Chen; Liao	The Science of the total environment	
	2	4	1	7	11807932	2002	Cancer risk assessment for oral exposure to PAH mixtures.	Schneider; Roller; Kalberlah; Schuhmacher-Wolz	Journal of applied toxicology : JAT	
	2	3	1	6	32460055	2020	PAHs in Chinese atmosphere Part II: Health risk assessm…	Ma; Zhu; Liu; Jia; Yang; Li	Ecotoxicology and environmental safety	
	0	3	1	4	23379661	2013	Parent and halogenated polycyclic aromatic hydrocarbon…	Ni; Guo	Journal of agricultural and food chemistry	
	0	3	1	4	20800879	2010	Health risk assessment on dietary exposure to polycyclic …	Xia; Duan; Qiu; Liu; Wang; Tao; Jiang; Lu; Song; Hu	The Science of the total environment	
	2	3	1	6	16293284	2005	Probabilistic risk assessment for personal exposure to car…	Liao; Chiang	Chemosphere	
	0	2	1	3	17544483	2007	Health risk assessment for traffic policemen exposed to p…	Hu; Bai; Zhang; Wang; Zhang; Yu; Zhu	The Science of the total environment	
	0	1	1	2	28795279	2017	Human health risk assessment and PAHs in a stretch of ri…	Srivastava; Sreekrishnan; Nema	Environmental monitoring and assessment	
	0	1	1	2	12634119	2003	Deviation from additivity in mixture toxicity: relevance of n…	Lutz; Vamvakas; Kopp-Schneider; Schlatter; Stopper	Environmental health perspectives	
	0	1	2	3	3709501	1986	The adsorption of polyaromatic hydrocarbons on natural a…	Menard; Noel; Khorami; Jouve; Dunnigan	Environmental research	
	0	0	1	1	33136306	2020	Effects on Apical Outcomes of Regulatory Relevance of E…	Crump; Boulanger; Farhat; Williams; Basu; Hecker	Environmental toxicology and chemistry	

Development of a dermal cancer slope factor for benzo[a] pyrene.

Polycyclic aromatic hydrocarbons (PAHs) are commonly found at environmentally impacted sites in both Canada and the United States, and also occur naturally. Typically, benzo[a] pyrene (B[a]P) is selected as a standard to which the cancer potencies of other carcinogenic PAHs are compared. Cancer potency estimates for B[a]P have been published for the oral and inhalation routes of exposure, however, no such estimate has been established by a regulatory agency for dermal exposure. The main objectives of the current investigation were to: evaluate approaches used to examine the relative carcinogenicity of PAHs; to conduct a review of mammalian dermal carcinogenicity studies for B[a]P; and derive a cancer slope factor for dermal exposure to PAHs using B[a]P as a surrogate for other PAHs. The toxicological database of dermal B[a]P studies was examined for relevant animal bioassays. Seven relevant studies were identified. A cancer slope factor for B[a]P was developed using the benchmark dose approach and the linearized multistage model. The upper 95th CI at the 5% effect level above background incidence was used as the point of departure for low-dose linear extrapolation. An average slope factor of 0.55 (microg/animal day)(-1) was calculated for mice, which was converted to a dose-equivalent slope factor of 25 (mg/kg day)(-1). This latter slope factor is proposed for application to human health risk assessment with no scaling adjustment. Dermal potency equivalency factor values were identified which may be used with other carcinogenic PAH in the calculation of total B[a]P equivalent dermal cancer risk estimates. An identified area for further investigation is the consideration of scaling in extrapolating the calculated dermal cancer slope factor from mice to humans.

External Links – Also use Identifiers
Names, CASRN, PubChem IDs, InChIs…

Benzo(a)pyrene

50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

General

- EPA Substance Registry Service
- PubChem
- Chemspider
- CPCat
- DrugBank
- Wikipedia
- MSDS Lookup
- ChEMBL
- ToxPlanet
- ACS Reagent Chemicals
- Wolfram Alpha
- ECHA Infocard
- ChemAgora
- Consumer Product Information Database
- ChEBI
- NIST Chemistry Webbook
- WEBWISER
- PubChem Safety Sheet
- Consumer Product Information Database
- PubChem: Chemical Vendors

Toxicology

- ACToR
- DrugPortal
- CCRIS
- ChemView
- CTD
- eChemPortal
- Gene-Tox
- HSDB
- ACToR PDF Report
- CREST
- National Air Toxics Assessment
- ECOTOX
- ChemView
- Chemical Checker
- BindingDB
- CalEPA OEHHA
- NIOSH IDLH Values
- LactMed
- ECOTOX

Publications

- Toxline
- PPRTVWEB
- PubMed
- IRIS Assessments
- EPA HERO
- NIOSH Skin Notation Profiles
- NIOSH Pocket Guide
- RSC Publications
- BioCaddie DataMed
- Springer Materials
- Bielefeld Academic Search Engine
- CORE Literature Search
- Google Books (Text Search)
- Google Patents (Text search)
- Google Scholar (Text search)
- Google Patents (Structure search)
- Google Books (Structure Search)
- Google Scholar (Structure search)
- Federal Register

Analytical

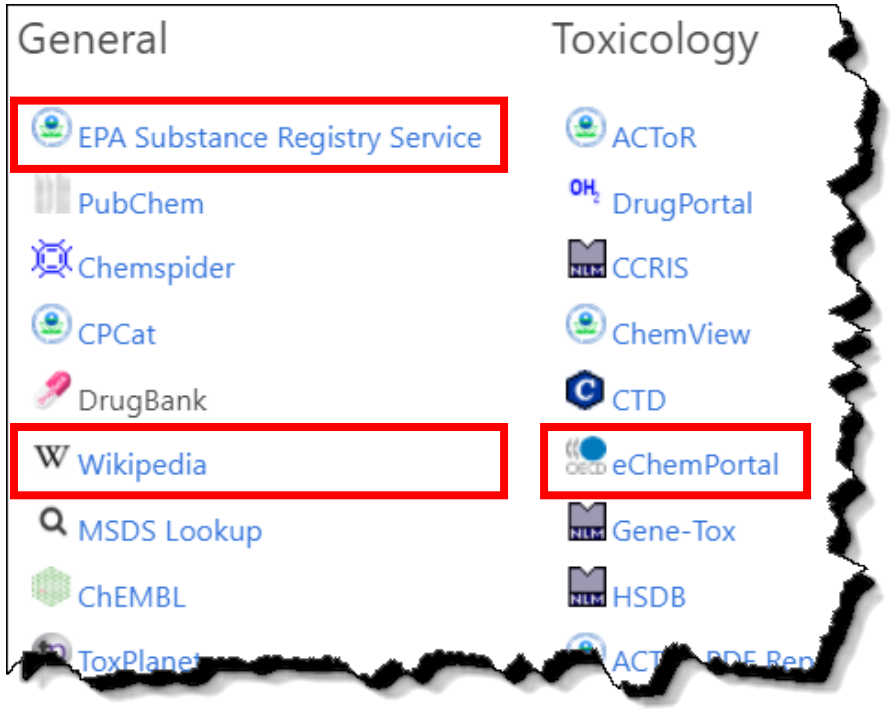
- RSC Analytical Abstracts
- Tox21 Analytical Data
- MONA: MassBank North America
- mzCloud
- NIST IR Spectrum
- NIST MS Spectrum
- MassBank
- NIST Antoine Constants
- IR Spectra on PubChem
- NIST Kovats Index values
- Protein DataBank
- National Environmental Methods Index

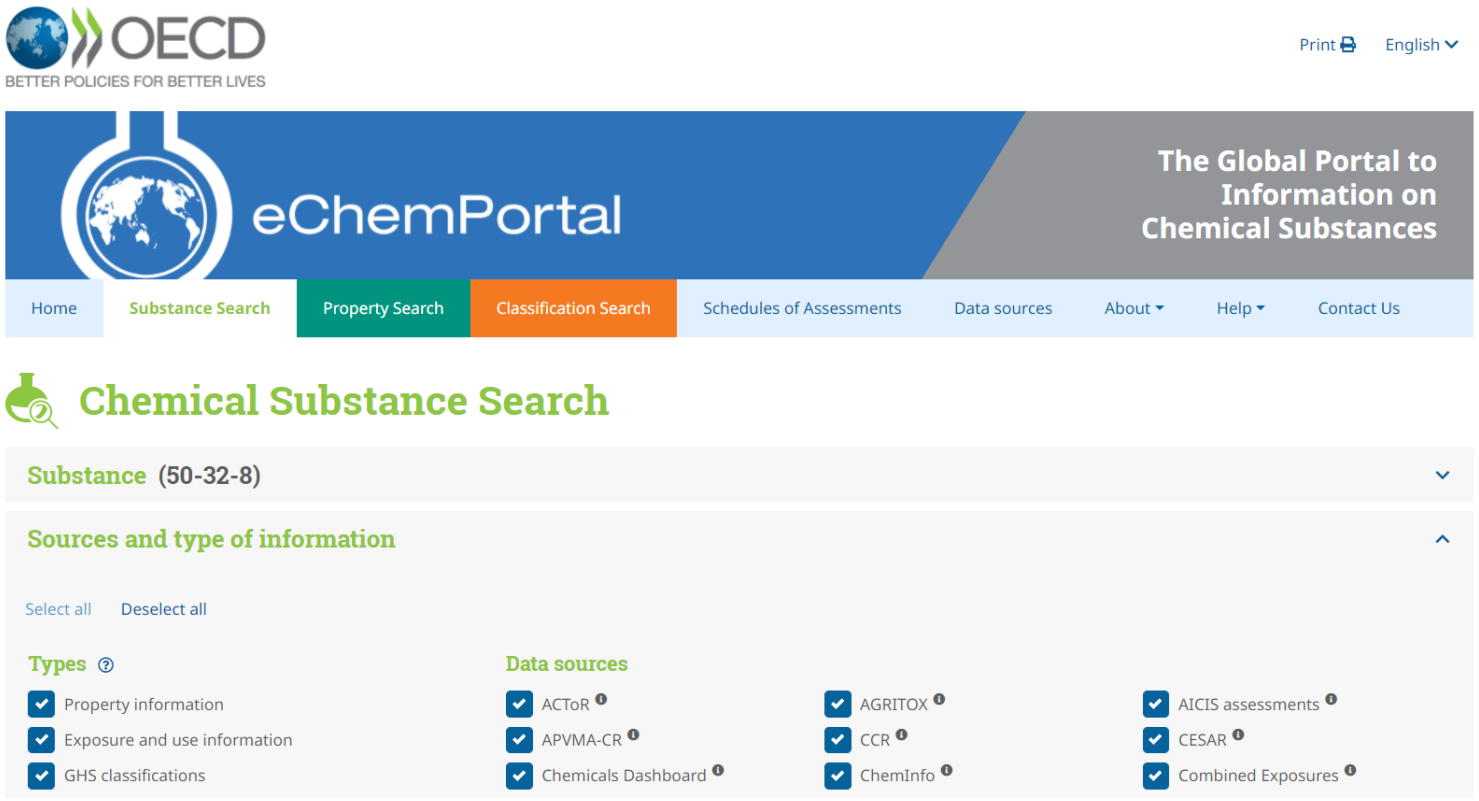
Prediction

- 2D NMR HSQC/HMBC Prediction
- Carbon-13 NMR Prediction
- Proton NMR Prediction
- ChemRTP Predictor
- LSERD

External Links

- Links to ~90 websites providing access to additional data on the chemical of interest





EPA
United States
Environmental Protection
Agency

Chemical Lists and Categories

PFAS lists of Chemicals

EPA United States Environmental Protection Agency

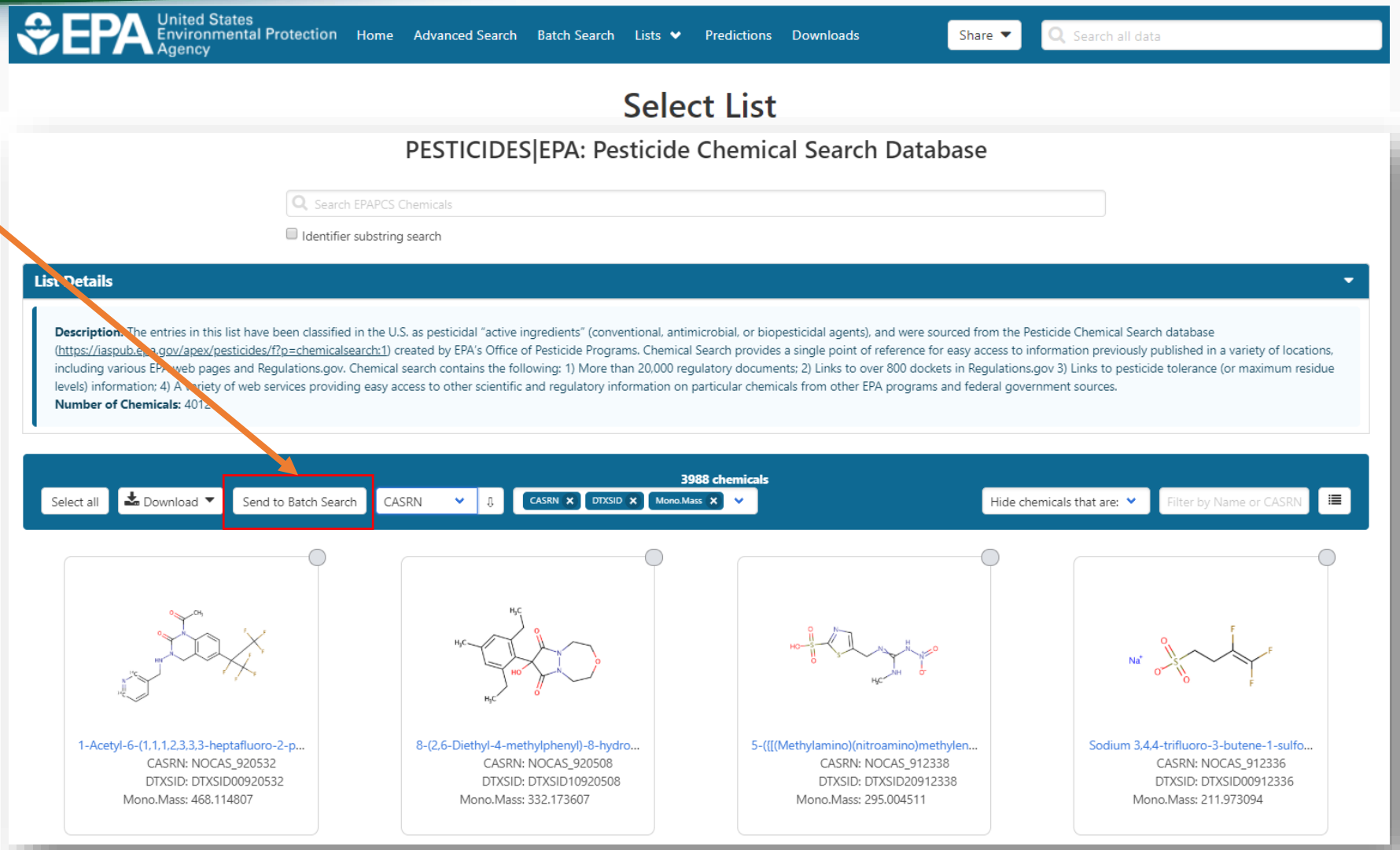
Select List

Download | Columns | PFAS | Copy Filtered Lists URL

List Acronym	List Name	Last Updated	Number of Chemicals	List Description
EPAPFAS75S1	PFAS|EPA: List of 75 Test Samples (Set 1)	2018-06-29	74	PFAS list corresponds to 75 samples (Set 1) submitted for initial testing screens conducted by EPA researchers in collaboration with researchers at the National Toxicology Program.
EPAPFAS75S2	PFAS|EPA: List of 75 Test Samples (Set 2)	2019-02-21	75	PFAS list corresponds to a second set of 75 samples (Set 2) submitted for testing screens conducted by EPA researchers in collaboration with researchers at the National Toxicology Program.
EPAPFASCAT	PFAS|EPA Structure-based Categories	2018-06-29	64	List of registered DSSTox "category substances" representing PFAS categories created using ChemAxon's Markush structure-based query representations.
EPAPFASINSOL	PFAS|EPA: Chemical Inventory Insoluble in DMSO	2018-06-29	43	PFAS chemicals included in EPA's expanded ToxCast chemical inventory found to be insoluble in DMSO above 5mM.
EPAPFASINV	PFAS|EPA: ToxCast Chemical Inventory	2018-06-29	430	PFAS chemicals included in EPA's expanded ToxCast chemical inventory and available for testing.
EPAPFASRL	PFAS|EPA: Cross-Agency Research List	2017-11-16	199	EPAPFASRL is a manually curated listing of mainly straight-chain and branched PFAS (Per- & Poly-fluorinated alkyl substances) compiled from various internal, literature and public sources by EPA researchers and program office representatives.
PFASKEMI	PFAS: List from the Swedish Chemicals Agency (KEMI) Report	2017-02-09	2416	Perfluorinated substances from a Swedish Chemicals Agency (KEMI) Report on the occurrence and use of highly fluorinated substances.
PFASMASTER	PFAS Master List of PFAS Substances	2018-07-26	5061	PFASMASTER is a consolidated list of PFAS substances spanning and bounded by the below lists of current interest to researchers and regulators worldwide.
PFASOECD	PFAS: Listed in OECD Global Database	2018-05-16	4729	OECD released a New Comprehensive Global Database of Per- and Polyfluoroalkyl Substances, (PFASs) listing more than 4700 new PFAS
PFASTRIER	PFAS Community-Compiled List (Trier et al., 2015)	2017-07-16	597	PFASTRIER community-compiled public listing of PFAS (Trier et al, 2015)

Curated List of Pesticides

- Find list of interest
- Select list and send to batch



Batch Searching

- Singleton searches are great but…
- …we generally want data on LOTS of chemicals!

- Typical questions
  - What are the structures for a set of chemical names? Set of CASRNs?
  - Can I get chemical lists in Excel files? As a list of SMILES strings? Can I get an SDF file?
  - Can I include predicted properties in the download file? OPERA? TEST?
  - Are “these chemicals” screened in Toxcast?
  - I’m a mass spectrometrist and need masses and formulae for a list of chemicals

Access data *en masse* for thousands of chemicals….

EPA United States Environmental Protection Agency

EPA United States Environmental Protection Agency | Home | Advanced Search | Batch Search | Lists | Predictions | Downloads | Share | Search all data

Batch Search

Step 1 — Step 2 — Step 3 — Step 4 — Step 5

Step Three: Select Download Data or Display Chemicals

Please enter one identifier per line

Select Input Type(s)

- [x] Identifiers
  - [x] Chemical Name
  - [x] CASRN
  - [ ] InChIKey
  - [ ] DSSTox Substance ID
- [ ] DSSTox Compound ID
- [ ] InChIKey Skeleton
- [ ] MS-Ready Formula(e)
- [ ] Exact Formula(e)
- [ ] Monoisotopic Mass

Enter Identifiers to Search (One per line. Searches should be limited to <5000 identifiers.)

```
Sodium azide
O,O-Dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] phosphorodithioate
(Trichloromethyl)benzene
100-44-7
(Chloromethyl)benzene
98-07-7
111-44-4
1-Chloro-2-(2-chloroethoxy)ethane
Chloro(chloromethoxy)methane
2-(Butan-2-yl)-4,6-dinitrophenol
```

Display All Chemicals | Download Chemical Data

Select Output Format and Content

United States Environmental Protection Agency

Step Four: Select Data Output Format and Choose Data Fields to Download

Select Output Format:

Excel

Download

Customize Results

- [ ] Select All
- [ ] Select All in Lists

Chemical Identifiers

- [x] DTXSID
- [x] 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

Metadata

- [ ] Curation Level Details
- [ ] NHANES/Predicted Exposure
- [ ] Data Sources
- [ ] Include ToxVal Data Availability
- [ ] Assay Hit Count
- [ ] Number of PubMed Articles
- [ ] PubChem Data Sources
- [ ] CPDat Product Occurrence Count
- [ ] IRIS
- [ ] PPRTV
- [ ] Wikipedia Article
- [ ] QC Notes
- [ ] Include links to ACToR reports - SLOW! (BETA)

Presence in Lists:

- [ ] 40CFR116.4 Designation of Hazardous Substances (Above Ground Storage Tanks)
- [ ] 40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities
- [ ] AEGLS: Acute Exposure Guideline Levels
- [ ] ANDROGEN: Androgen Receptor Chemicals
- [ ] ARTICLE; Bench-Mark Dose Human Health Assessment List (Wignall et al., 2014)
- [ ] ARTICLE: Collaborative Estrogen Receptor Activity Prediction Project (CERAPP)
- [ ] ARTICLE: Collaborative Estrogen Receptor Activity Prediction Project (COMPARA)
- [ ] ATSDR Toxicological Profiles
- [ ] ATSDR: Minimal Risk Levels (MRLs) for Hazardous Substances
- [ ] ATSDR: Toxic Substances Portal Chemical List
- [ ] California Office of Environmental Health Hazard Assessment
- [ ] Canadian Domestic Substances List 2019
- [ ] CATEGORY: Amino acids
- [ ] CATEGORY: Color Index dyes
- [ ] CATEGORY: Flame Retardants

Batch Search CASRNs

EPA United States Environmental Protection Agency

Batch Search

Step 1 — Step 2 — Step 3 — Step 4 — Step 5

Step Four: Select Data Output Format and Choose Data Fields to Download

Please enter one identifier per line

Chemical Identifiers
- [x] DTXSID
- [x] Chemical Name
- [ ] DTXCID
- [x] CAS-RN
- [x] InChIKey
- [x] IUPAC Name

Structures
- [ ] Mol File
- [ ] SMILES
- [ ] InChI String
- [x] MS-Ready SMILES
- [ ] QSAR-Ready SMILES

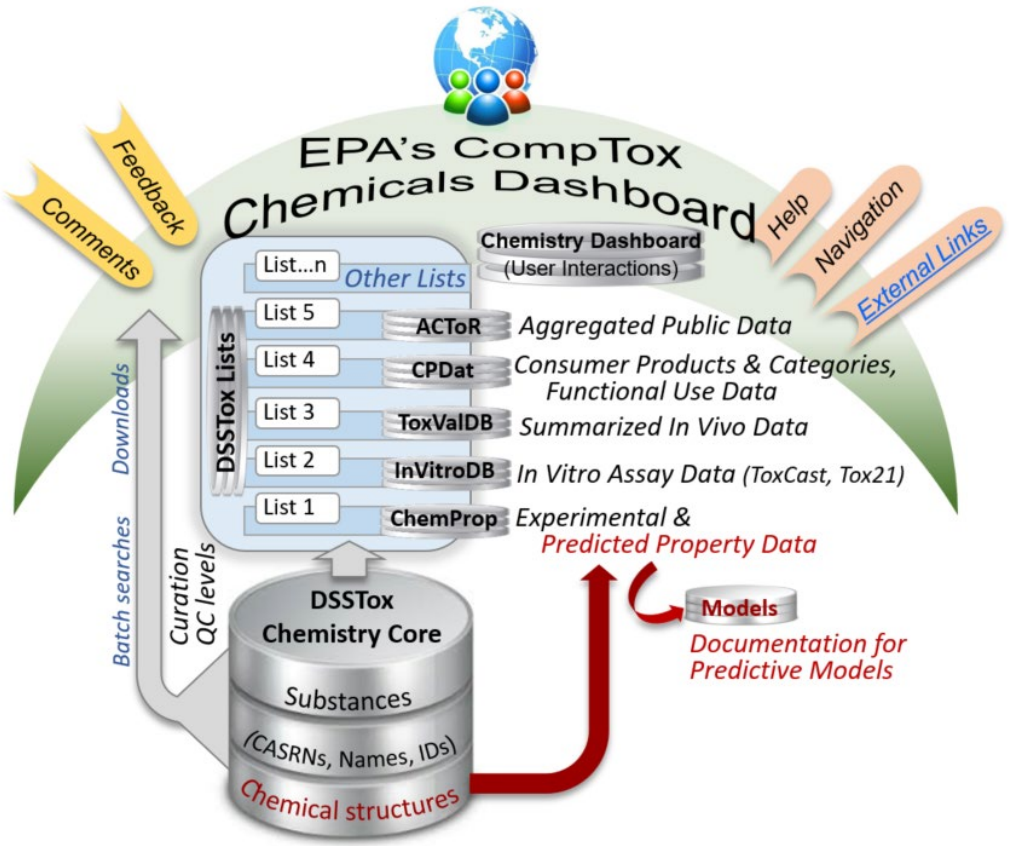
Intrinsic And Predicted Properties
- [x] Molecular Formula
- [ ] Average Mass
- [ ] Monoisotopic Mass
- [ ] TEST Model Predictions
- [x] OPERA Model Predictions

Metadata
- [ ] Curation Level Details
- [ ] NHANES/Predicted Exposure
- [ ] Data Sources
- [x] Include ToxVal Data Availability
- [x] Assay Hit Count
- [x] Number of PubMed Articles

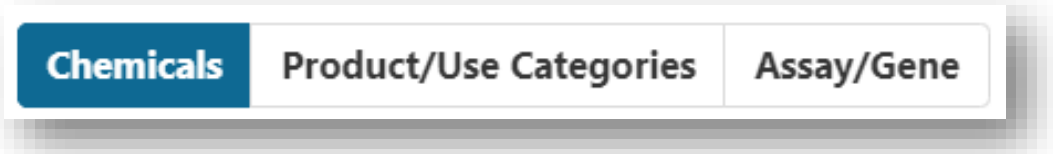
	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	INPUT	FOUND_BY	DTXSID	PREFERRE	CASRN	INCHIKEY	IUPAC_NAI	MOLECULA	TOXVAL_D	TOXCAST_	TOXCAST_	MS_READY	NUMBER_C	IRIS_LINK	PPRTV_LIN	ATMOSPHE	BIOCONCE
2	534-52-1	CAS-RN	DTXSID10	2-Methyl-4,6	534-52-1	ZXVONLUN	2-Methyl-4,6	C7H6N2O5	Y	27.56	261/947	CC1=C(O)C	179	-	Y	1.571E-12	2.88959
3	115-21-9	CAS-RN	DTXSID70	Ethyl silicon	115-21-9	ZOYFEXPF	Trichloro(eth	C2H5Cl3Si	Y	-	-	-	-	-	-	8.289E-12	13.9658
4	111-44-4	CAS-RN	DTXSID90	Bis(2-chloro	111-44-4	ZNSMNVML	1-Chloro-2-(	C4H8Cl2O	Y	1.12	10/891	ClCCOCCCl	12	Y	-	2.647E-12	9.99608
5	2763-96-4	CAS-RN	DTXSID50	Muscimol	2763-96-4	ZJQHPWUV	5-(Aminome	C4H6N2O2	Y	-	-	NCC1=CC((	4308	-	-	1.179E-10	5.05695
6	1464-53-5	CAS-RN	DTXSID00	2,2'-Bioxiran	1464-53-5	ZFIVKAOQE	2,2'-Bioxiran	C4H6O2	Y	-	-	C1OC1C1C	363	-	-	4.383E-12	1.27107
7	22224-92-6	CAS-RN	DTXSID30	Fenamiphos	22224-92-	ZCJPOPBZI	Ethyl 3-meth	C13H22NO3	Y	10.8	105/972	CCOP(=O)(	58	Y	-	1.66E-11	2.3394
8	359-06-8	CAS-RN	DTXSID40	Fluoroacetyl	359-06-8	ZBHDTYQJ	Fluoroacetyl	C2H2ClFO	Y	-	-	FCC(Cl)=O	-	-	-	3.513E-13	4.49379
9	5344-82-1	CAS-RN	DTXSID40	1-(o-Chlorop	5344-82-1	YZUKKTCD	N-(2-Chloro	C7H7ClN2S	Y	-	-	NC(=S)NC1	-	-	-	2.482E-11	9.95206
10	7446-18-6	CAS-RN	DTXSID10	Thallium (I) s	7446-18-6	YTQVHRVI	Dithallium(1+	O4STl2	Y	-	-	-	34	Y	Y	-	-
11	62207-76-5	CAS-RN	DTXSID40	Bis(3-fluoros	62207-76-	YRZXYIHD	-	C16H14CoF	Y	-	-	-	-	-	-	-	-
12	66-81-9	CAS-RN	DTXSID60	Cycloheximi	66-81-9	YPHMISFO	4-{(2R)-2-[(1	C15H23NO4	Y	32.27	294/911	CC1CC(C)C	18709	-	-	1.756E-11	2.81761
13	106-96-7	CAS-RN	DTXSID30	Propargyl br	106-96-7	YORCIIVHU	3-Bromopro	C3H3Br	Y	-	-	BrCC#C	-	-	-	1.069E-11	10.4968
14	315-18-4	CAS-RN	DTXSID70	Mexacarbat	315-18-4	YNEVBPNZ	4-(Dimethyla	C12H18N2O	Y	5.11	12/235	CNC(=O)OC	27	-	-	1.447E-11	26.2914
15	110-00-9	CAS-RN	DTXSID60	Furan	110-00-9	YLQBMQCU	Furan	C4H4O	Y	0.0	0/235	O1C=CC=C	919	Y	-	4.019E-11	5.01648
16	3037-72-7	CAS-RN	DTXSID20	4-(diethoxyn	3037-72-7	YHFFINXFN	4-[Diethoxy(	C9H23NO2S	Y	-	-	-	-	-	-	5.95E-12	6.71292
17	75-44-5	CAS-RN	DTXSID00	Phosgene	75-44-5	YGYAWVDI	Carbonyl dic	CCl2O	Y	-	-	ClC(Cl)=O	489	Y	-	9.994E-16	13.0711
18	2032-65-7	CAS-RN	DTXSID30	Methiocarb	2032-65-7	YFBPRJGD	3,5-Dimethy	C11H15NO2	Y	18.14	88/485	CNC(=O)OC	65	-	-	1.446E-11	34.1692
19	2778-04-3	CAS-RN	DTXSID20	Endothion	2778-04-3	YCAGGFXS	S-[(5-Metho	C9H13O6PS	Y	-	-	COC1=COC	-	-	-	4.355E-11	1.18341
20	12108-13-3	CAS-RN	DTXSID90	(Methylcyclc	12108-13-	YASXMYPV	Tricarbonyl(	C9H7MnO3	Y	2.56	11/430	-	68	-	-	-	-
21	7803-51-2	CAS-RN	DTXSID20	Phosphine	7803-51-2	XYFCBTPG	Phosphane	H3P	Y	-	-	-	928	Y	-	-	-
22	107-18-6	CAS-RN	DTXSID80	Allyl alcohol	107-18-6	XXROGKLT	Prop-2-en-1	C3H6O	Y	3.99	17/426	OCC=C	627	Y	Y	2.592E-11	4.03901
23	108-05-4	CAS-RN	DTXSID30	Vinyl acetate	108-05-4	XTXRWKRV	Ethenyl acet	C4H6O2	Y	1.7	4/235	CC(=O)OC=	206	Y	-	2.5E-11	5.52157
24	19624-22-7	CAS-RN	DTXSID10	Pentaborane	19624-22-	XPIBKKWN	-	B5H9	Y	-	-	-	-	-	-	-	-
25	75-74-1	CAS-RN	DTXSID00	Tetramethyl	75-74-1	XOOGZRUI	Tetramethyl	C4H12Pb	Y	-	-	C[Pb](C)(C)	24	-	-	-	-

Worksheet1

Summary and Conclusion



- CompTox Chemicals Dashboard - a central hub for environmental data
  - ~900k chemical substances
  - Integrating property data, hazard data, exposure data, *in vitro* bioactivity data
  - Interrogation of bioactivity data -
  - Multiple types of searches



  - Batch search for thousands of chemicals
  - Real-time property and toxicity predictions
  - Downloadable files – CSV, TSV and Excel

References

- The CompTox Chemistry Dashboard: a community data resource for environmental chemistry, *J. Cheminformatics*, **9**, 61 (2017)
- EPA's DSSTox database: History of development of a curated chemistry resource supporting computational toxicology research, *Comp. Tox.* **12**, 100096 (2019)
- OPERA models for predicting physicochemical properties and environmental fate endpoints, *J. Cheminformatics*, **10**, 10 (2018)
- Screening Chemicals for Estrogen Receptor Bioactivity Using a Computational Model, *Environ. Sci. Technol.* **49**, 8804-8814 (2015)
- ToxCast Chemical Landscape: Paving the Road to 21st Century Toxicology, *Chem. Res. Toxicol.* **29**, 1225-51 (2016)
- Development and Validation of a Computational Model for Androgen Receptor Activity, *Chem. Res. Toxicol.* **30**, 946-964 (2017)
- CERAPP: Collaborative Estrogen Receptor Activity Prediction Project, *Environ. Health Perspect*. **124**, 1023 (2016)
- Abstract Sifter: a comprehensive front-end system to PubMed, *F1000,* **6**, 2164 (2017)

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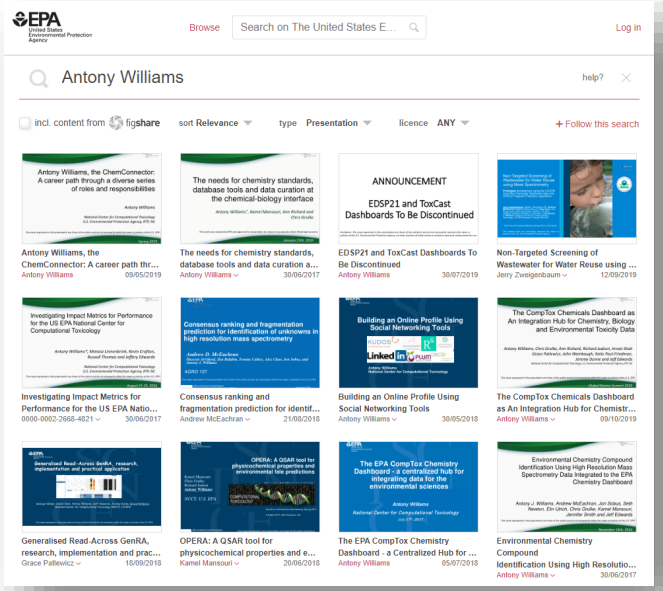
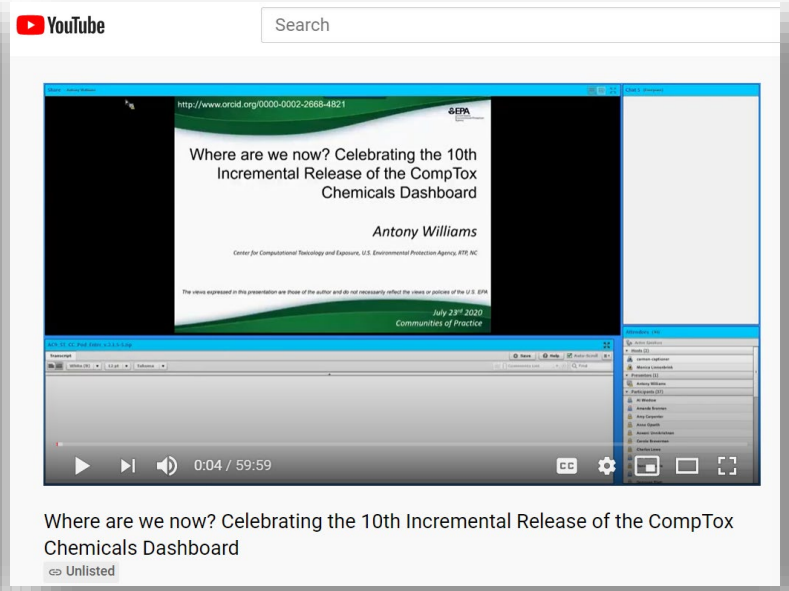
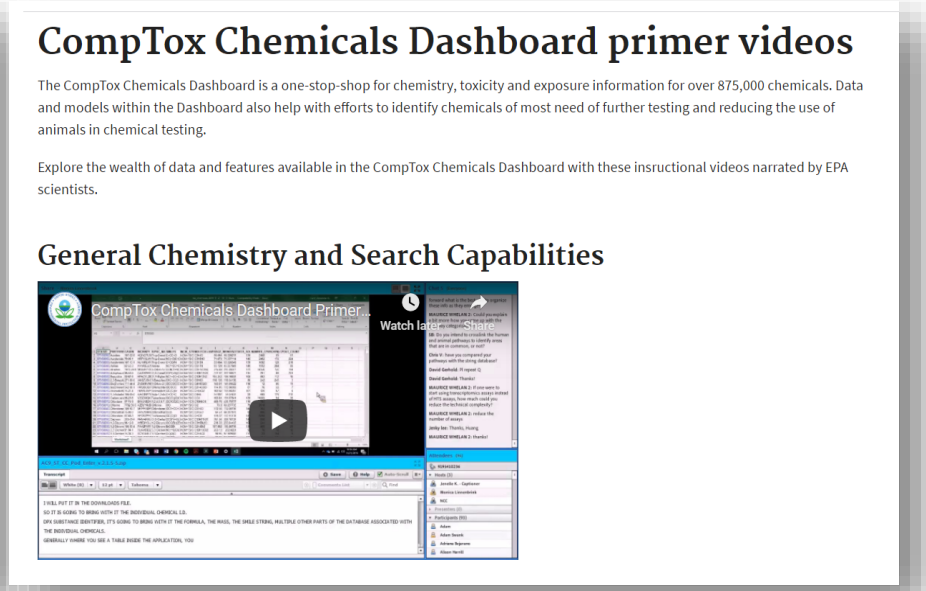
- Lots of resources available
  - Presentations: https://tinyurl.com/w5hqs55
  - Communities of Practice Videos: https://rb.gy/qsbno1
  - Manual: https://rb.gy/4fgydc
  - Latest News: https://comptox.epa.gov/dashboard/news_info







Acknowledgments

- Contact: Williams.Antony@epa.gov
- Feedback and follow-up is welcomed! Your questions help
- The dashboard is based on the efforts of many more team members than us. Many collaborators provide data also.

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