Informatics Approaches for Developing and Organizing Chemical Descriptors

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Applying Exposure New Approach Methodologies to Chemical Risk Evaluation

International Society of Exposure Science

September 21, 2020

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

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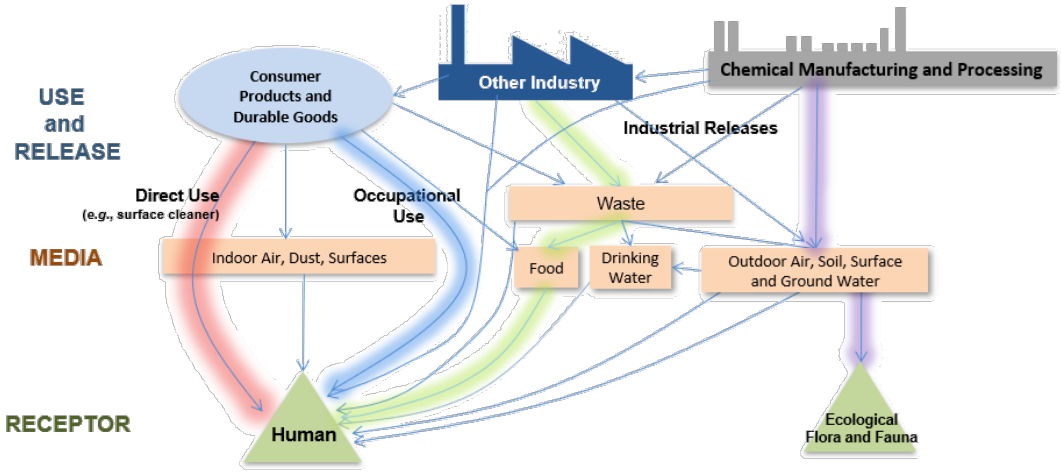
Chemical Descriptors

- How do we 'parameterize' exposure models for different pathways?
- In some cases may only know chemical structure.
- Critical information:
  - How and how much chemical mass is applied, used, or released
  - Physical chemical properties
- Chemical information should ideally be organized in a in a machine-readable format.



Exposure Pathway Classes:

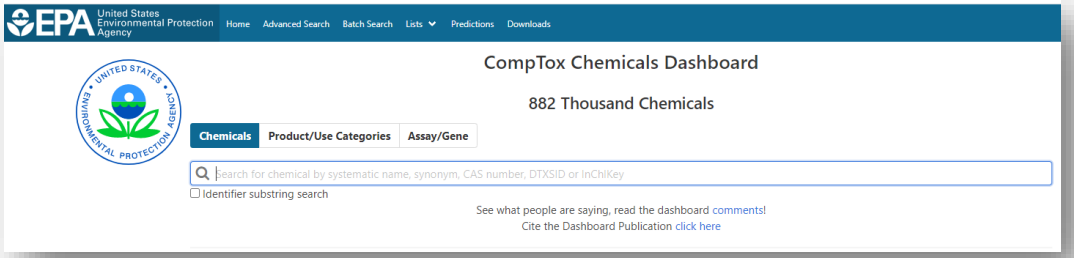
Consumer
Occupational
Ambient
Ecological

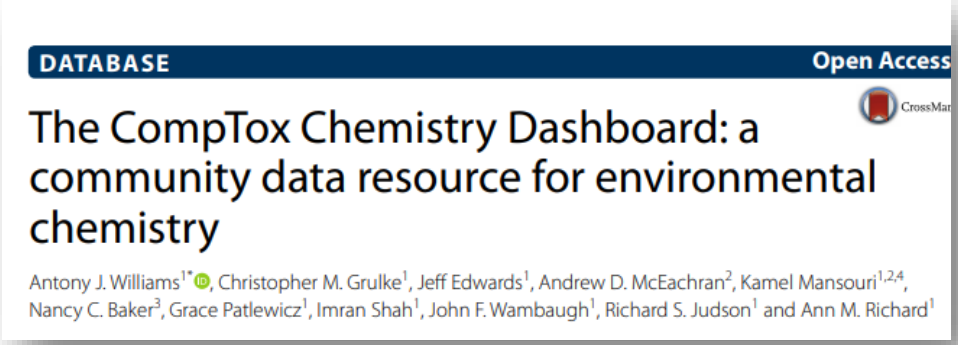
The CompTox Chemicals Dashboard

United States Environmental Protection Agency

- Delivers *high-quality, structure-curated, open data* to meet the various needs of the environmental sciences and computational toxicology communities
- Provides intrinsic property, toxicity, and exposure data for chemicals, in addition to tools supporting:
  - Chemical similarity analyses
  - Read-across of chemical toxicity
  - Real-time property modeling
  - Identification of chemicals in mass spectrometry
  - Literature searching and identification of other information resources
- 10th Release (July 2020): 882,000 chemicals

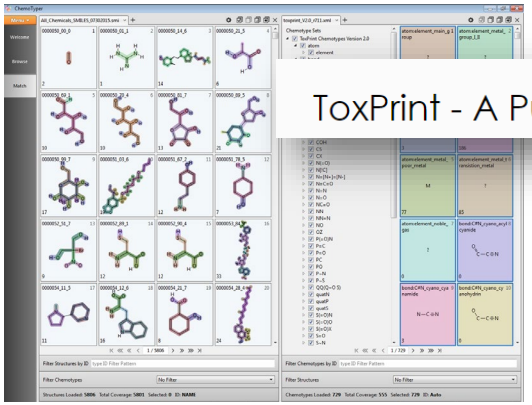
https://comptox.epa.gov/dashboard





Chemical Descriptors in the Dashboard

United States Environmental Protection Agency



ToxPrint - A Public Set of Chemotypes

- Molecular substructures

- Predicted EPA physical-chemical property data: Open Structure-Activity Relationship App ("OPERA")

Mansouri *et al. J Cheminform (2018) 10:10*
https://doi.org/10.1186/s13321-018-0263-1

Journal of Cheminformatics

RESEARCH ARTICLE Open Access

OPERA models for predicting physicochemical properties and environmental fate endpoints

Kamel Mansouri[1,2,3*], Chris M. Grulke[1], Richard S. Judson[1] and Antony J. Williams[1]

https://github.com/kmansouri/OPERA

- New descriptors containing information about ***chemical use***

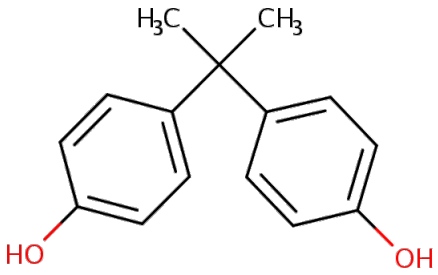
CPDat

Chemical and Products Database

Chemical Property Descriptors in the Dashboard

- Chemical information may be reported using a many different chemical identifiers
  - Different names
  - Regional spellings/ different languages
  - Multiple standard identifiers, e.g. active or retired Chemical Abstract Registration Numbers (CASRN), Beilstein Registry Number

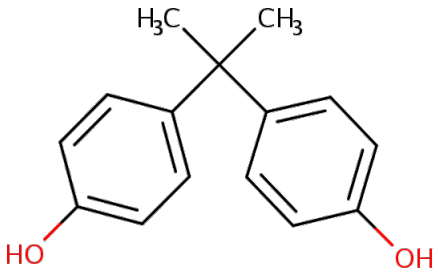
Bisphenol A



How Do We Deal with Chemical Synonomy?

- Chemical information may be reported using a many different chemical identifiers
  - Different names
  - Regional spellings/ different languages
  - Multiple standard identifiers, e.g. active or retired Chemical Abstract Registration Numbers (CASRN), Beilstein Registry Number

Bisphenol A

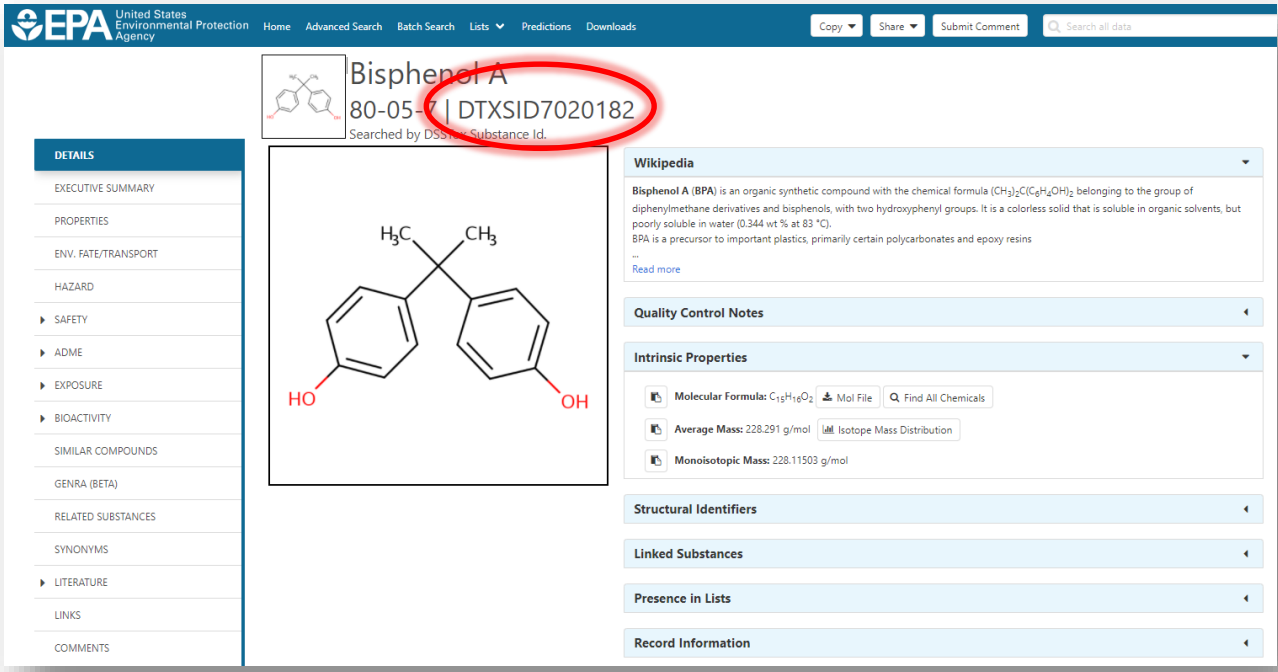


4,4'-(Propane-2,2-diyl)diphenol
Phenol, 4,4'-(1-methylethylidene)bis-
80-05-7
BPA
4,4'-Propane-2,2-diyldiphenol
Phenol, 4,4'-(1-methylethylidene)bis-
4-06-00-06717
(4,4'-Dihydroxydiphenyl)dimethylmethane
2,2-Bis(4'-hydroxyphenyl) propane
2,2'-Bis(4-hydroxyphenyl)propane
2,2-BIS-(4-HYDROXY-PHENYL)-PROPANE
2,2-Bis(4-hydroxyphenyl)propane
2,2-Bis(p-hydroxyphenyl)propane
2,2-Di(4-Hydroxyphenyl) Propane
2,2-DI(4-HYDROXYPHENYL)PROPANE
2,2-Di(4-phenylol)propane
4,4'-(1-Methylethylidene)bisphenol
4,4'-Bisphenol A
4,4'-DIHYDROXYPHENYL-2,2-PROPANE
4,4'-isopropilidendifenol
4,4'-Isopropylidendiphenol
4,4'-Isopropylidene bisphenol
4,4-ISOPROPYLIDENE DIPHENYL
4,4'-Isopropylidenebis[phenol]
4,4'-isopropylidenediphenol
4,4'-Methylethylidenebisphenol
Bis(4-hydroxyphenyl)dimethylmethane
Bis(p-hydroxyphenyl)propane

+100 more

DSSTox Substance Identifiers

- The Dashboard provides a unique DSSTox Substance Identifier (DTXSID) for each chemical
- Also provides a preferred name and CASRN
- DTXSIDs are unique substance identifiers, where a substance can be any single chemical, mixture, polymer
- Linked to unique chemical structures (DTXCIDs)
- Can be obtained for lists of chemicals using the Dashboard's Batch Search Utility (tutorial later)



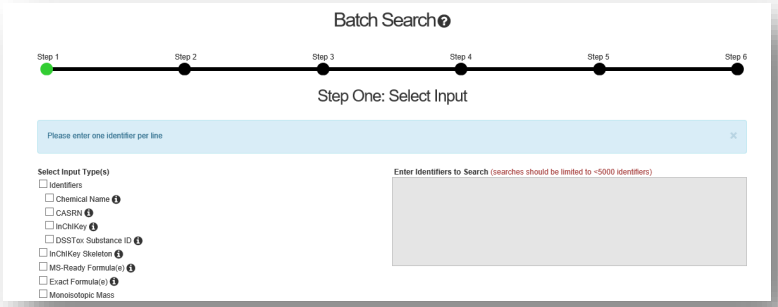
Example of Harmonizing Messy Chemical Identifier Data

United States Environmental Protection Agency

We recently curated chemical identifiers from 20 public biomonitoring and environmental surveillance data sources

- American Healthy Homes Survey
- California Air Monitoring Network
- California Air Resources Board (CARB)
- California Biomonitoring
- California Surface Water Database
- Canadian Health Measures Survey
- Comparative Toxicogenomics Database
- EPA Ambient Monitoring Technology Information Center – Air Toxics Data
- EPA Discharge Monitoring Report Data
- EPA Office of Water, National study of Chemical Residues in Lake Fish Tissue
- EPA Unregulated Contaminant Monitoring Rule
- FDA Total Diet Study
- Great Lakes Environmental Database
- ICES-Dome
- Information Platform for Chemical Monitoring Data
- Minnesota Biomonitoring
- National Atmospheric Deposition Program (Atmospheric Integrated Research Monitoring Network (AIRMoN)
- Targeted National Sewage Sludge Survey
- USDA National Residue Program
- USGS Monitoring Data –National Water Quality Monitoring Council
- OECD Monitoring Database

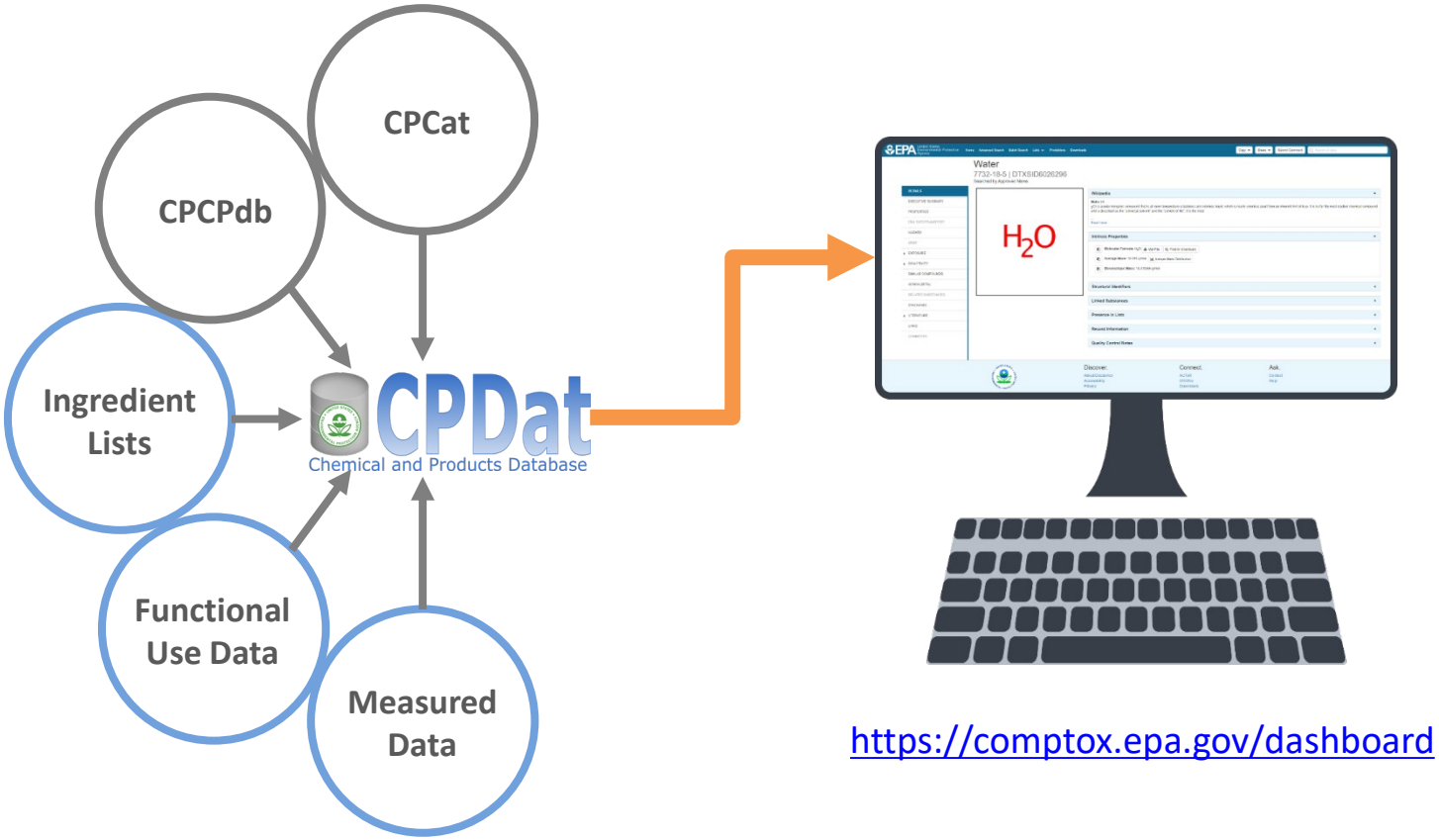
8168 *Unique reported chemical name/CASRN pairs*



INPUT	FOUND_BY	DTXSID	PREFERRED_NAME	CASRN
ethalfluralin	Approved Name	DTXSID8032386	Ethalfluralin	55283-68-6
butylate	Approved Name	DTXSID7023936	Butylate	2008-41-5
bifenthrin	Approved Name	DTXSID9020160	Bifenthrin	82657-04-3
ethoprop	Approved Name	DTXSID4032611	Ethoprop	13194-48-4
coumaphos	Approved Name	DTXSID2020347	Coumaphos	56-72-4
disulfoton	Approved Name	DTXSID0022018	Disulfoton	298-04-4
sulprofos	Approved Name	DTXSID8032675	Sulprofos	35400-43-2
tetrachlorvinphos	Synonym from Valid Source	DTXSID1032648	Z-Tetrachlorvinphos	22248-79-9
fenthion	Approved Name	DTXSID8020620	Fenthion	55-38-9
naled	Approved Name	DTXSID1024209	Naled	300-76-5
mevinphos	Approved Name	DTXSID7042481	Mevinphos	338-45-4
phorate	Approved Name	DTXSID4032459	Phorate	298-02-2
DDVP	Expert Validated Synonym	DTXSID5020449	Dichlorvos	62-73-7
cypermethrin	Approved Name	DTXSID1023998	Cypermethrin	52315-07-8
cyfluthrin	Approved Name	DTXSID5035957	Cyfluthrin	68359-37-5
diquat dibromide	Approved Name	DTXSID3024075	Diquat dibromide	85-00-7
methoprene	Approved Name	DTXSID8032627	Methoprene	40596-69-8
para-chloro-meta-cresol	Synonym from Valid Source	DTXSID4021717	4-Chloro-3-methylphenol	59-50-7
pentachlorophenol	Approved Name	DTXSID7021106	Pentachlorophenol	87-86-5
1,4-dichlorobenzene (p-DCB0	NO_MATCH	-	-	-
2,4-xylenol	Expert Validated Synonym	DTXSID2021864	2,4-Dimethylphenol	105-67-9

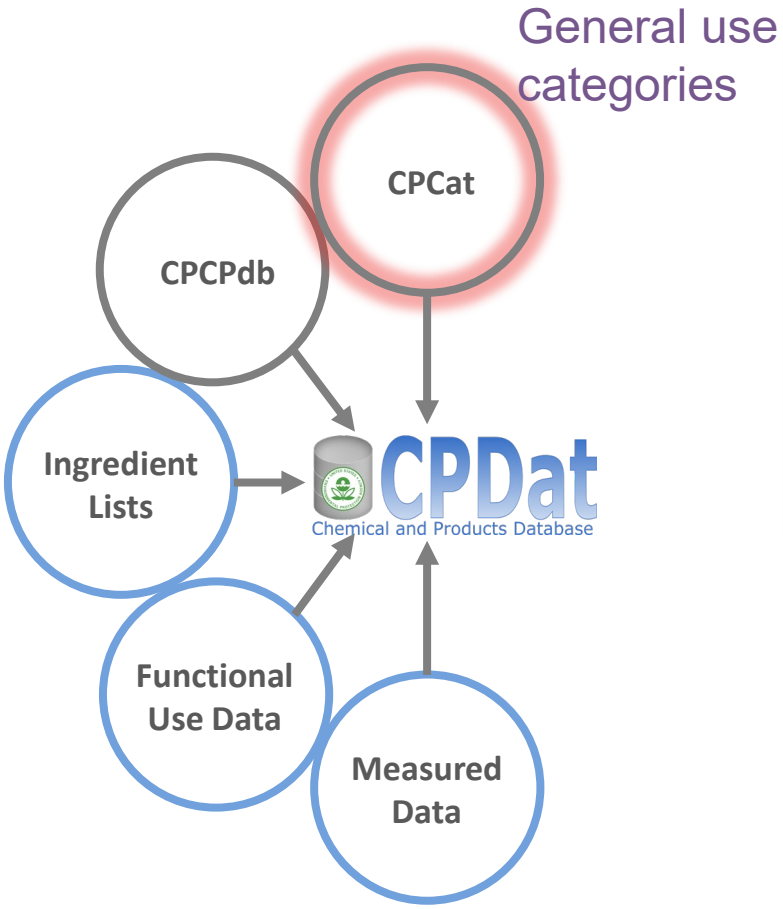
- ***4955*** could be identified as present in Dashboard
- ***1681*** substances with unique DTXSIDs
- Additional curation could catch more (e.g. parsing of names that include abbreviations in parentheses)

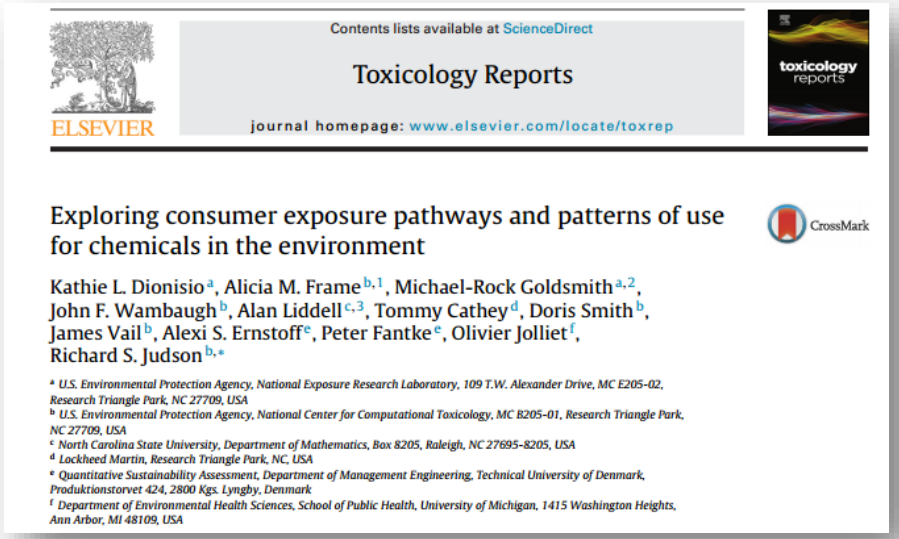
Chemical Use Descriptors



https://comptox.epa.gov/dashboard

Chemical Use Descriptors





Contents lists available at ScienceDirect

Toxicology Reports

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

ELSEVIER

toxicology reports

Exploring consumer exposure pathways and patterns of use for chemicals in the environment

CrossMark

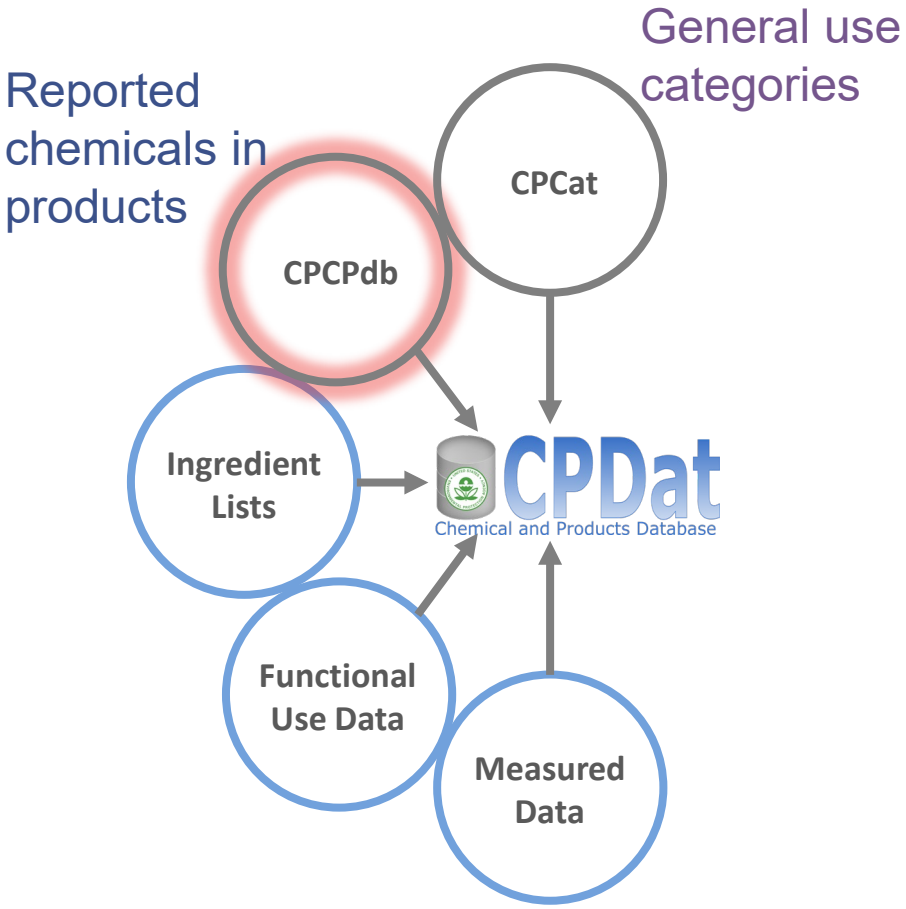
Kathie L. Dionisio[a], Alicia M. Frame[b,1], Michael-Rock Goldsmith[a,2], John F. Wambaugh[b], Alan Liddell[c,3], Tommy Cathey[d], Doris Smith[b], James Vail[b], Alexi S. Ernstoff[e], Peter Fantke[e], Olivier Jolliet[f], Richard S. Judson[b,*]

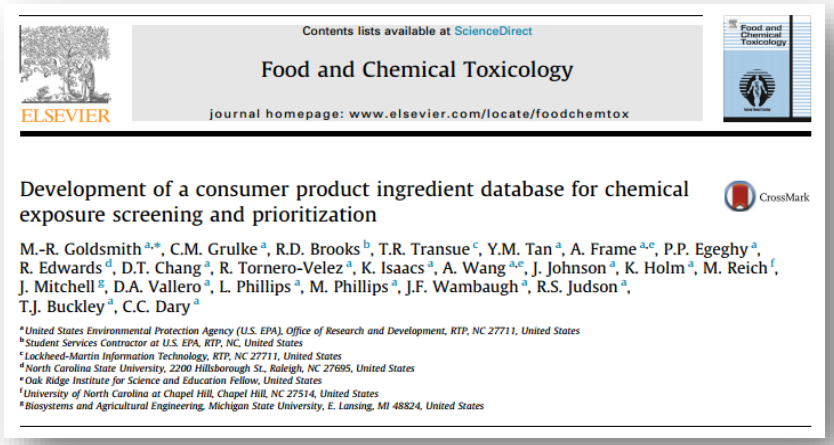
[a] U.S. Environmental Protection Agency, National Exposure Research Laboratory, 109 T.W. Alexander Drive, MC E205-02, Research Triangle Park, NC 27709, USA
[b] U.S. Environmental Protection Agency, National Center for Computational Toxicology, MC B205-01, Research Triangle Park, NC 27709, USA
[c] North Carolina State University, Department of Mathematics, Box 8205, Raleigh, NC 27695-8205, USA
[d] Lockheed Martin, Research Triangle Park, NC, USA
[e] Quantitative Sustainability Assessment, Department of Management Engineering, Technical University of Denmark, Produktionstorvet 424, 2800 Kgs. Lyngby, Denmark
[f] Department of Environmental Health Sciences, School of Public Health, University of Michigan, 1415 Washington Heights, Ann Arbor, MI 48109, USA

- Presence on other chemical lists
- Broad categorization of chemical use
  - Functional use
  - Therapeutic use
  - Consumer product-based use
  - Industrial process use
- Curated to a large number of relevant index terms

Chemical Use Descriptors

United States Environmental Protection Agency





Contents lists available at ScienceDirect

Food and Chemical Toxicology

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

Development of a consumer product ingredient database for chemical exposure screening and prioritization

M.-R. Goldsmith [a,*], C.M. Grulke [a], R.D. Brooks [b], T.R. Transue [c], Y.M. Tan [a], A. Frame [a,e], P.P. Egeghy [a], R. Edwards [d], D.T. Chang [a], R. Tornero-Velez [a], K. Isaacs [a], A. Wang [a,e], J. Johnson [a], K. Holm [a], M. Reich [f], J. Mitchell [g], D.A. Vallero [a], L. Phillips [a], M. Phillips [a], J.F. Wambaugh [a], R.S. Judson [a], T.J. Buckley [a], C.C. Dary [a]

[a] United States Environmental Protection Agency (U.S. EPA), Office of Research and Development, RTP, NC 27711, United States
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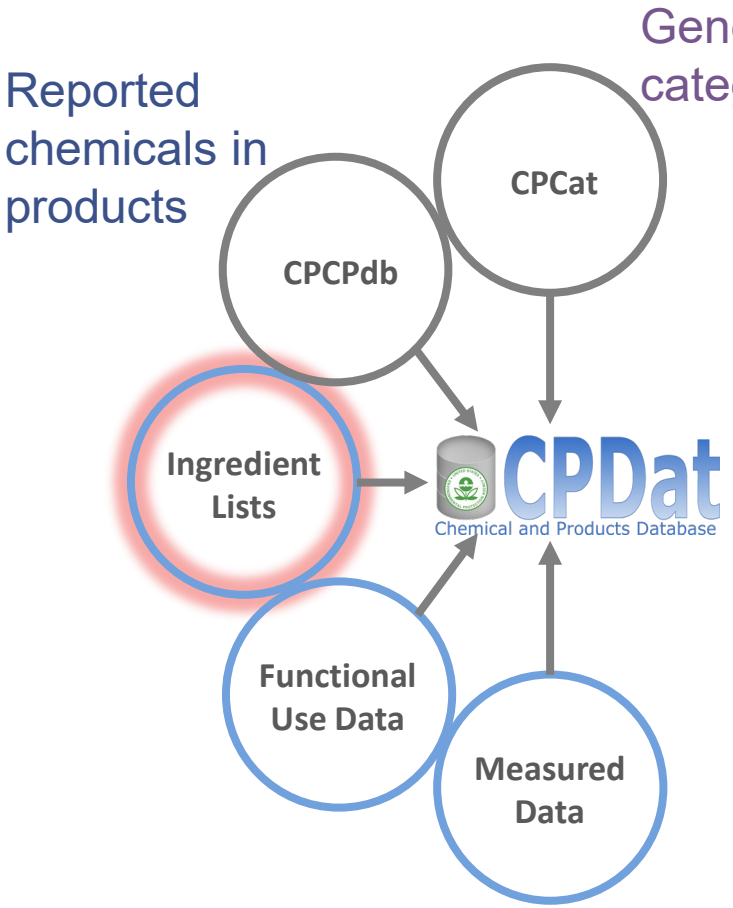
[c] Lockheed-Martin Information Technology, RTP, NC 27711, United States
[d] North Carolina State University, 2200 Hillsborough St., Raleigh, NC 27695, United States
[e] Oak Ridge Institute for Science and Education Fellow, United States
[f] University of North Carolina at Chapel Hill, Chapel Hill, NC 27514, United States
[g] Biosystems and Agricultural Engineering, Michigan State University, E. Lansing, MI 48824, United States

- MSDS-based composition information for consumer product formulations
  - Includes range of reported weight fraction
  - Provides quantitative input to consumer exposure models

Chemical Use Descriptors

United States Environmental Protection Agency



Journal of Exposure Science and Environmental Epidemiology (2017) 00, 1–7
© 2017 Nature America, Inc., part of Springer Nature. All rights reserved 1559-0631/17
www.nature.com/jes

ORIGINAL ARTICLE

Consumer product chemical weight fractions from ingredient lists

Kristin K. Isaacs[1], Katherine A. Phillips[1], Derya Biryol[1,2], Kathie L. Dionisio[1] and Paul S. Price[1]

Assessing human exposures to chemicals in consumer products requires composition information. However, comprehensive composition data for products in commerce are not generally available. Many consumer products have reported ingredient lists that are constructed using specific guidelines. A probabilistic model was developed to estimate quantitative weight fraction (WF) values that are consistent with the rank of an ingredient in the list, the number of reported ingredients, and labeling rules. The model provides the mean, median, and 95% upper and lower confidence limit WFs for ingredients of any rank in lists of any length. WFs predicted by the model compared favorably with those reported on Material Safety Data Sheets. Predictions for chemicals known to provide specific functions in products were also found to reasonably agree with reported WFs. The model was applied to a selection of publicly available ingredient lists, thereby estimating WFs for 1293 unique ingredients in 1123 products in 81 product categories. Predicted WFs, although less precise than reported values, can be estimated for large numbers of product–chemical combinations and thus provide a useful source of data for high-throughput or screening-level exposure assessments.

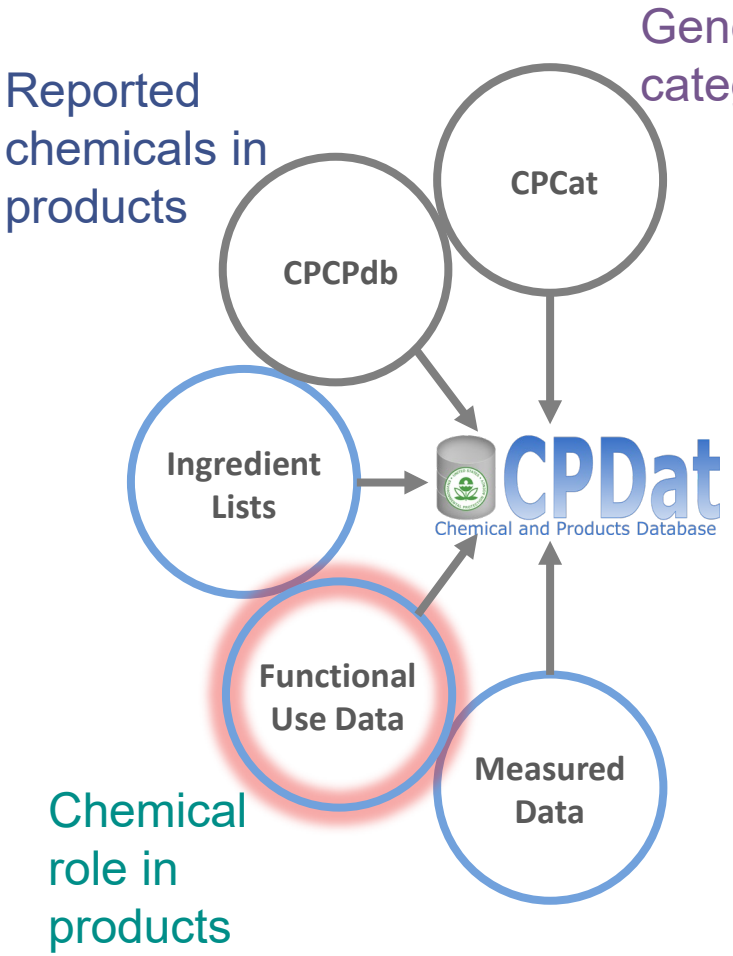
Journal of Exposure Science and Environmental Epidemiology advance online publication, 8 November 2017; doi:10.1038/jes.2017.29

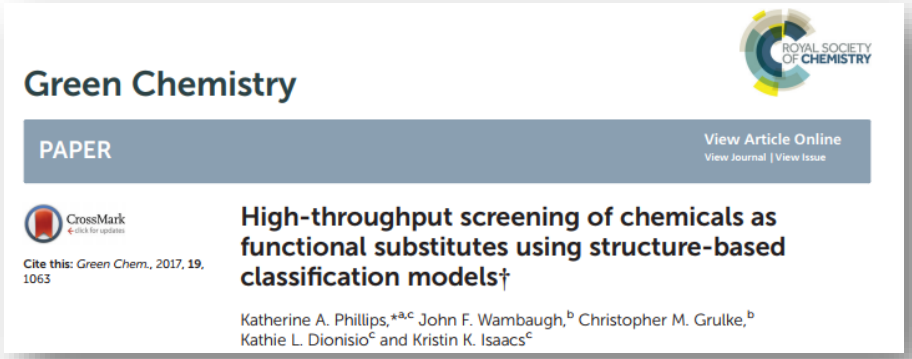
Keywords: consumer products; consumer exposures; ExpoCast; ingredients

- Chemical composition of consumer products from ingredient lists
  - Reported ingredients
  - Predicted weight fractions based on structured reporting rules

Chemical Use Descriptors

United States Environmental Protection Agency




Green Chemistry

PAPER

View Article Online
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CrossMark

Cite this: *Green Chem.*, 2017, **19**, 1063

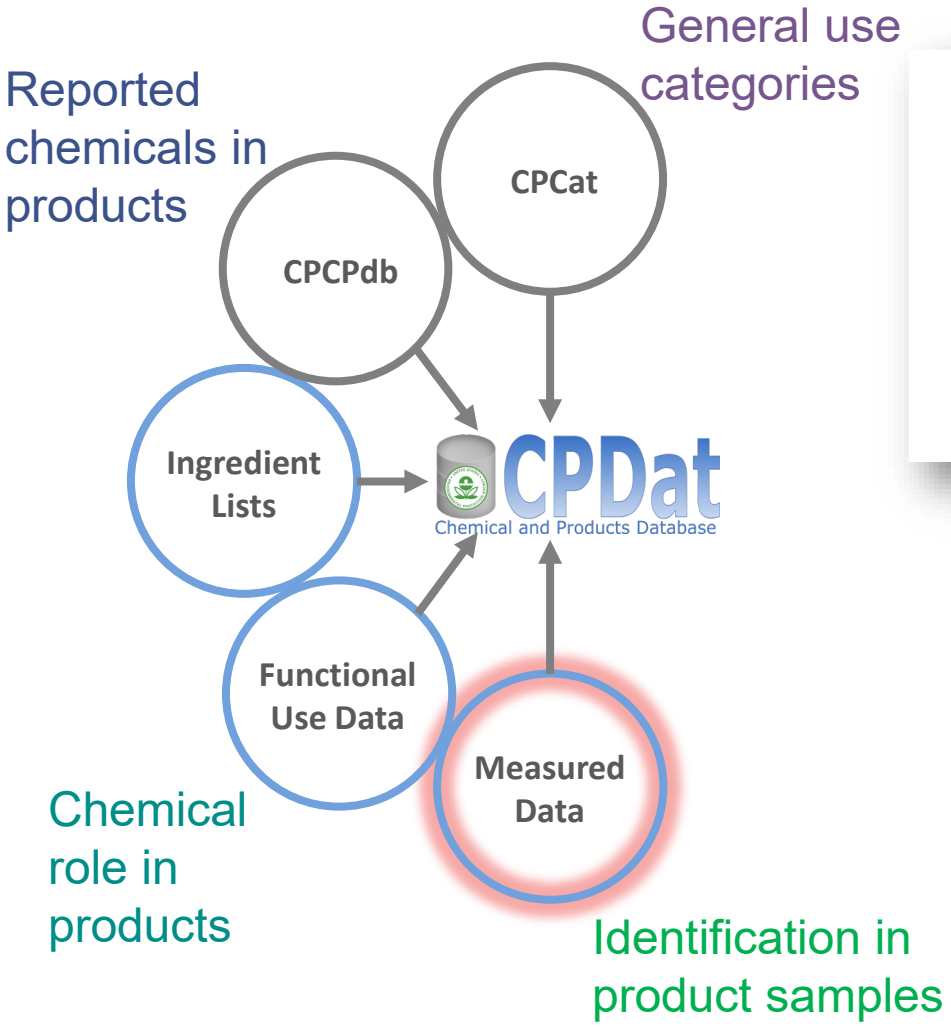
High-throughput screening of chemicals as functional substitutes using structure-based classification models†

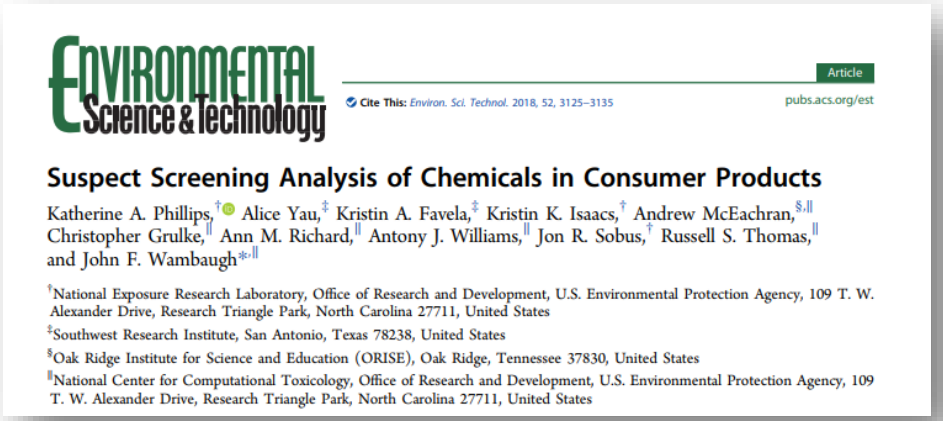
Katherine A. Phillips,*[a,c] John F. Wambaugh,[b] Christopher M. Grulke,[b] Kathie L. Dionisio[c] and Kristin K. Isaacs[c]

- Categorization by functional use
  - Reported functional use
  - Harmonized functional use
  - Predicted functional uses based on structure

Chemical Use Descriptors

United States Environmental Protection Agency





Environmental Science & Technology

Article

Cite This: *Environ. Sci. Technol.* 2018, 52, 3125−3135

pubs.acs.org/est

Suspect Screening Analysis of Chemicals in Consumer Products

Katherine A. Phillips,[†] Alice Yau,[‡] Kristin A. Favela,[‡] Kristin K. Isaacs,[†] Andrew McEachran,[§,∥] Christopher Grulke,[∥] Ann M. Richard,[∥] Antony J. Williams,[∥] Jon R. Sobus,[†] Russell S. Thomas,[∥] and John F. Wambaugh*[,∥]

[†]National Exposure Research Laboratory, Office of Research and Development, U.S. Environmental Protection Agency, 109 T. W. Alexander Drive, Research Triangle Park, North Carolina 27711, United States

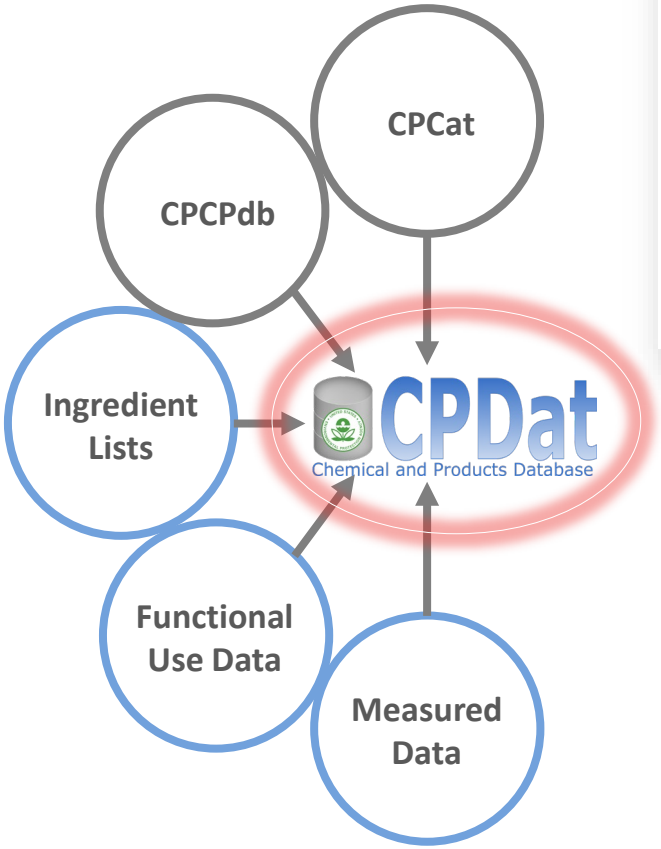
[‡]Southwest Research Institute, San Antonio, Texas 78238, United States

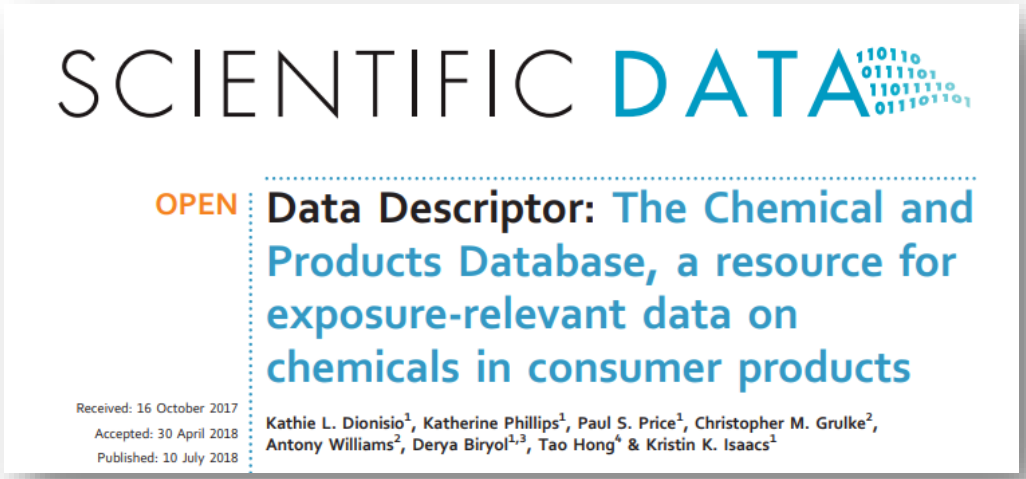
[§]Oak Ridge Institute for Science and Education (ORISE), Oak Ridge, Tennessee 37830, United States

[∥]National Center for Computational Toxicology, Office of Research and Development, U.S. Environmental Protection Agency, 109 T. W. Alexander Drive, Research Triangle Park, North Carolina 27711, United States

- Targeted and non-targeted measurement of chemicals in consumer products
  - Measured weight fractions
  - Confirmed presence
  - Tentative identification

Chemical Use Descriptors




SCIENTIFIC DATA

OPEN

Data Descriptor: The Chemical and Products Database, a resource for exposure-relevant data on chemicals in consumer products

Received: 16 October 2017
Accepted: 30 April 2018
Published: 10 July 2018

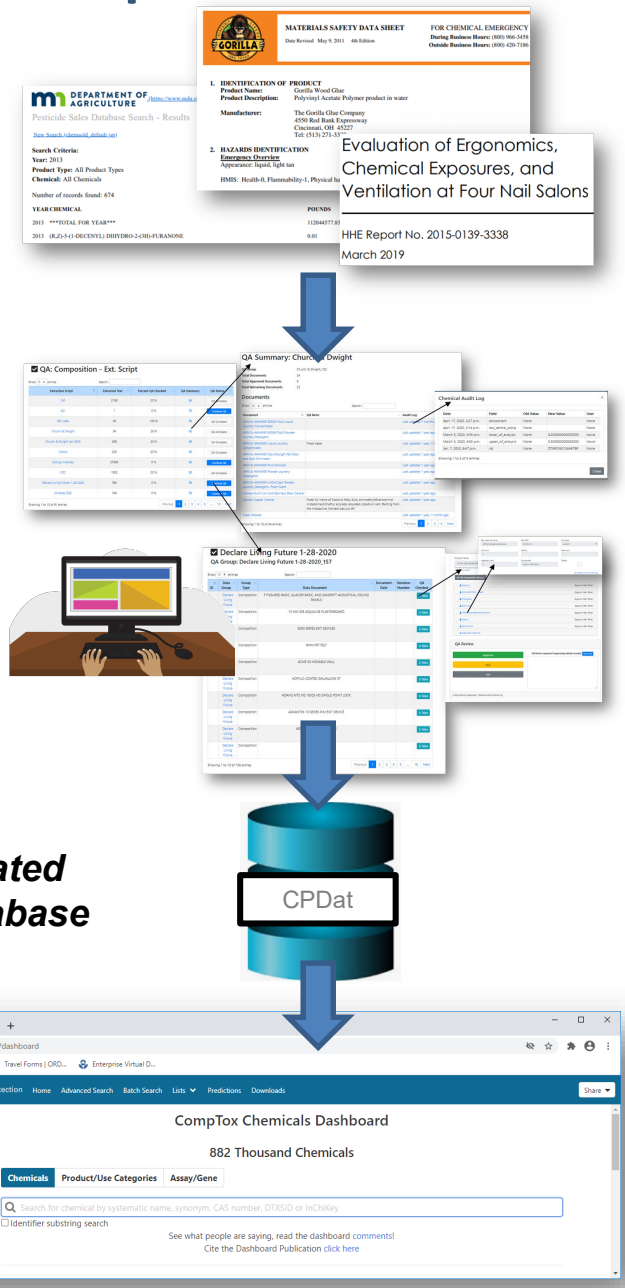
Kathie L. Dionisio[1], Katherine Phillips[1], Paul S. Price[1], Christopher M. Grulke[2], Antony Williams[2], Derya Biryol[1,3], Tao Hong[4] & Kristin K. Isaacs[1]

- Broad categorization of chemical use
- Comprehensive hierarchical categorization of chemical usage by consumer product type
- Functional use of chemicals
- Quantitative chemical composition for consumer products

Curation of Chemical Use Descriptors

United States Environmental Protection Agency

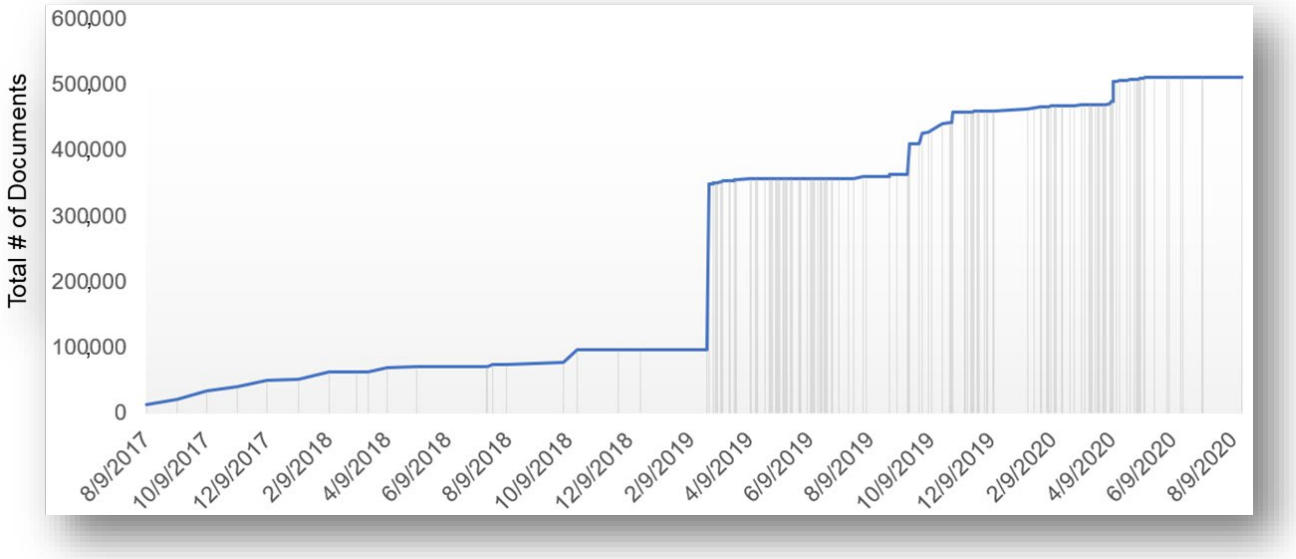
- We are using informatics approaches to obtain and curate additional chemical descriptor information
- Data from chemical use, monitoring, and release domains
- Public data sources: reports, open literature, databases
- Utilizing standard curation/QA procedures and tools



Chemical Descriptor NAMs

United States Environmental Protection Agency

Number of Documents in Factotum 2017-2020

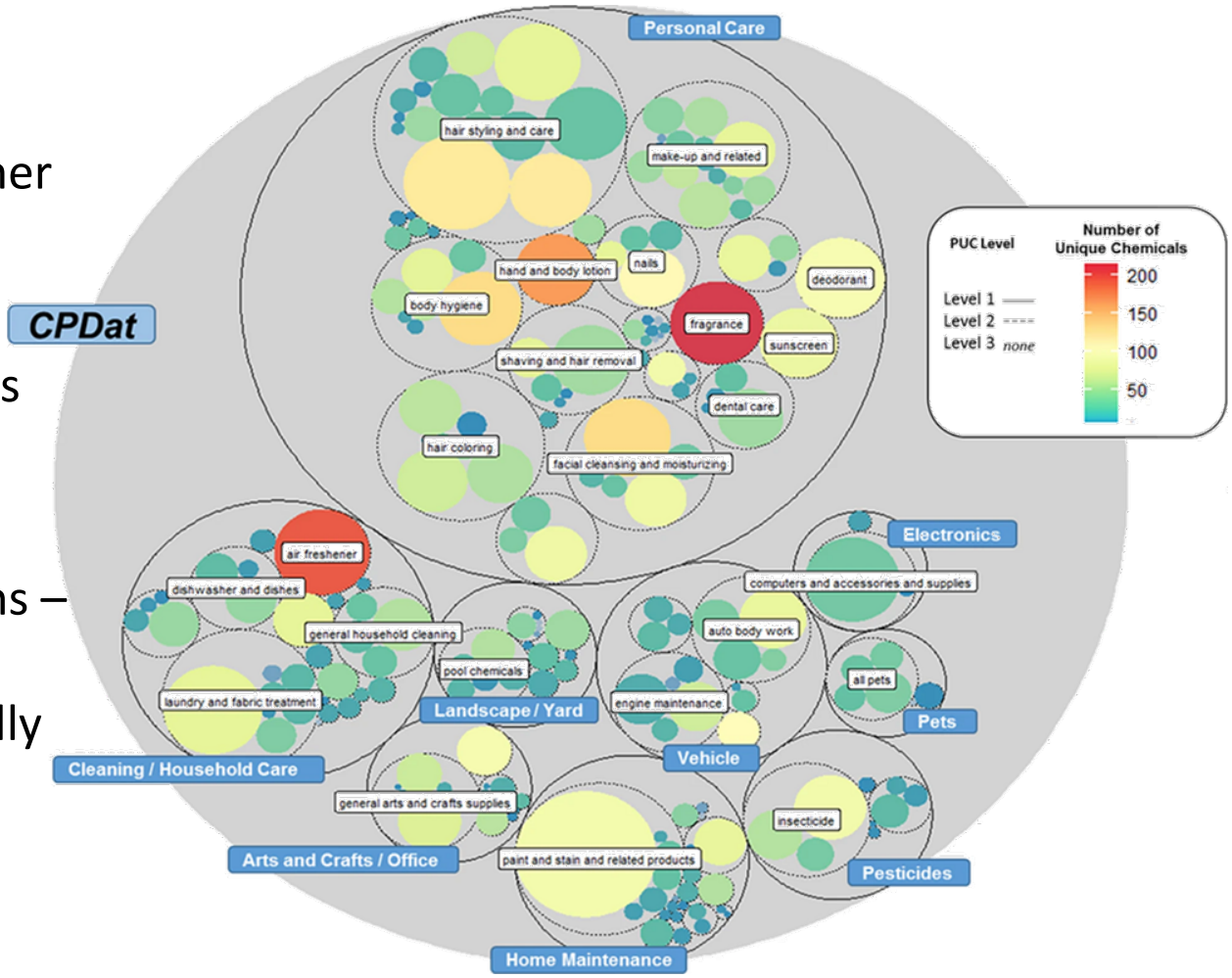


Group Type	Documents	Raw Chemical Records	Curated Chemical Records
Consumer Product Composition	473,271	3,738,350	1,791,250
Functional use	33,770	34,680	11,946
CPCat Categories	2,088	117,231	68,133
Occupational exposure	1,304	4,825	1078
Literature monitoring	1,175	966	In process
Habits and practices	202	NA	NA

Product categories in Factotum/CPDat

United States Environmental Protection Agency

- Allows for linking to consumer product exposure models
- Maps to habits and practices data
- Maps to exposure algorithms – if chemical and product are known, models can be rapidly and parameterized



Isaacs et al., 2019

Curation of Products to Consumer Product Categories

United States Environmental Protection Agency

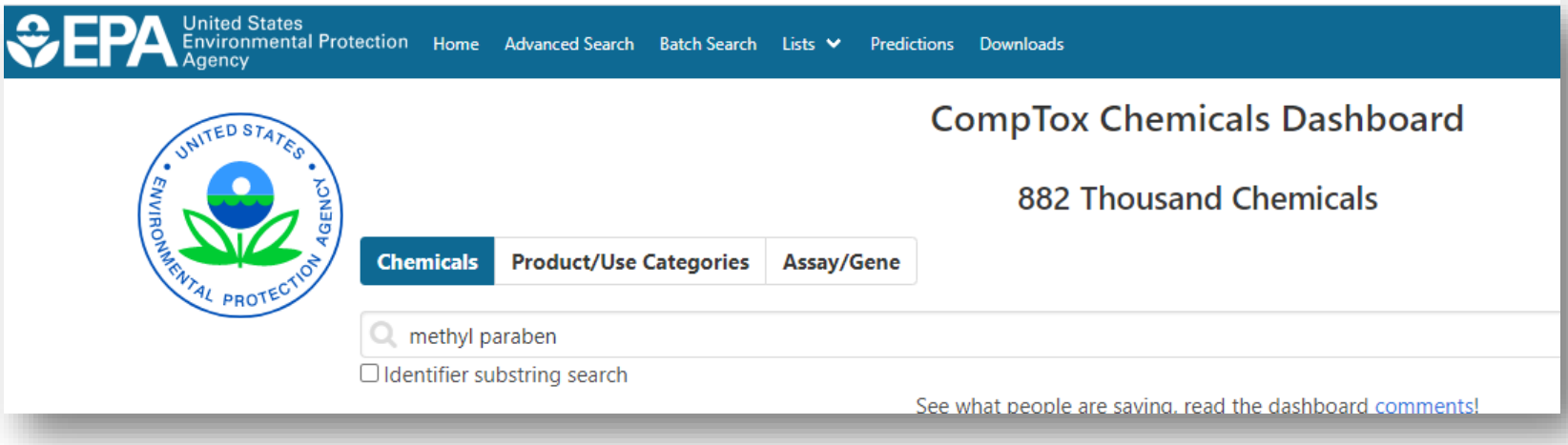
- Machine learning classifiers were built using the existing manually curated CPDat data as a training set
- Allowed for automated curation of new documents to Product Use Categories (PUCs) developed specifically for consumer exposure modeling.

New Product Data Documents (Safety Data Sheets (SDS, Ingredient lists, ingredient disclosures)

One-Vs-Rest Support Vector Machine Classifiers

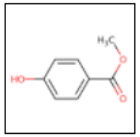
Automated assignment to Product Use Categories (PUCs, Isaacs et al. 2020)

Obtaining Descriptors Using the Dashboard



Obtaining Descriptors Using the Dashboard

United States Environmental Protection Agency

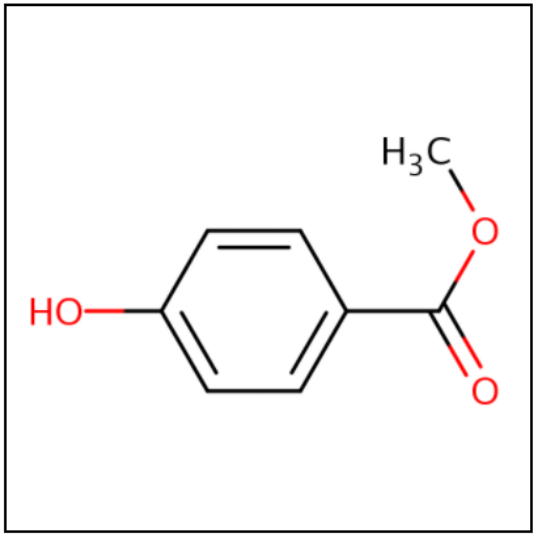


Methylparaben

99-76-3 | DTXSID4022529

Searched by Synonym from Valid Source.

- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- SAFETY
- ADME
- EXPOSURE
- BIOACTIVITY
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS
- LITERATURE
- LINKS
- COMMENTS



Wikipedia

Methylparaben, also **methyl paraben**, one of the parabens, is a preservative with the chemical formula $CH_3(C_6H_4(OH)COO)$. It is the methyl ester of *p*-hydroxybenzoic acid.

...

Read more

Quality Control Notes

Intrinsic Properties

Molecular Formula: $C_8H_8O_3$ | Mol File | Find All Chemicals

Average Mass: 152.149 g/mol | Isotope Mass Distribution

Monoisotopic Mass: 152.047344 g/mol

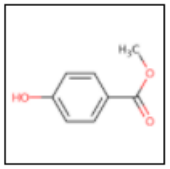
Structural Identifiers

Linked Substances

Presence in Lists

Record Information

Obtaining Descriptors Using the Dashboard



Methylparaben

99-76-3 | DTXSID4022529

Searched by Synonym from Valid Source.

Property

Vapor Pressure

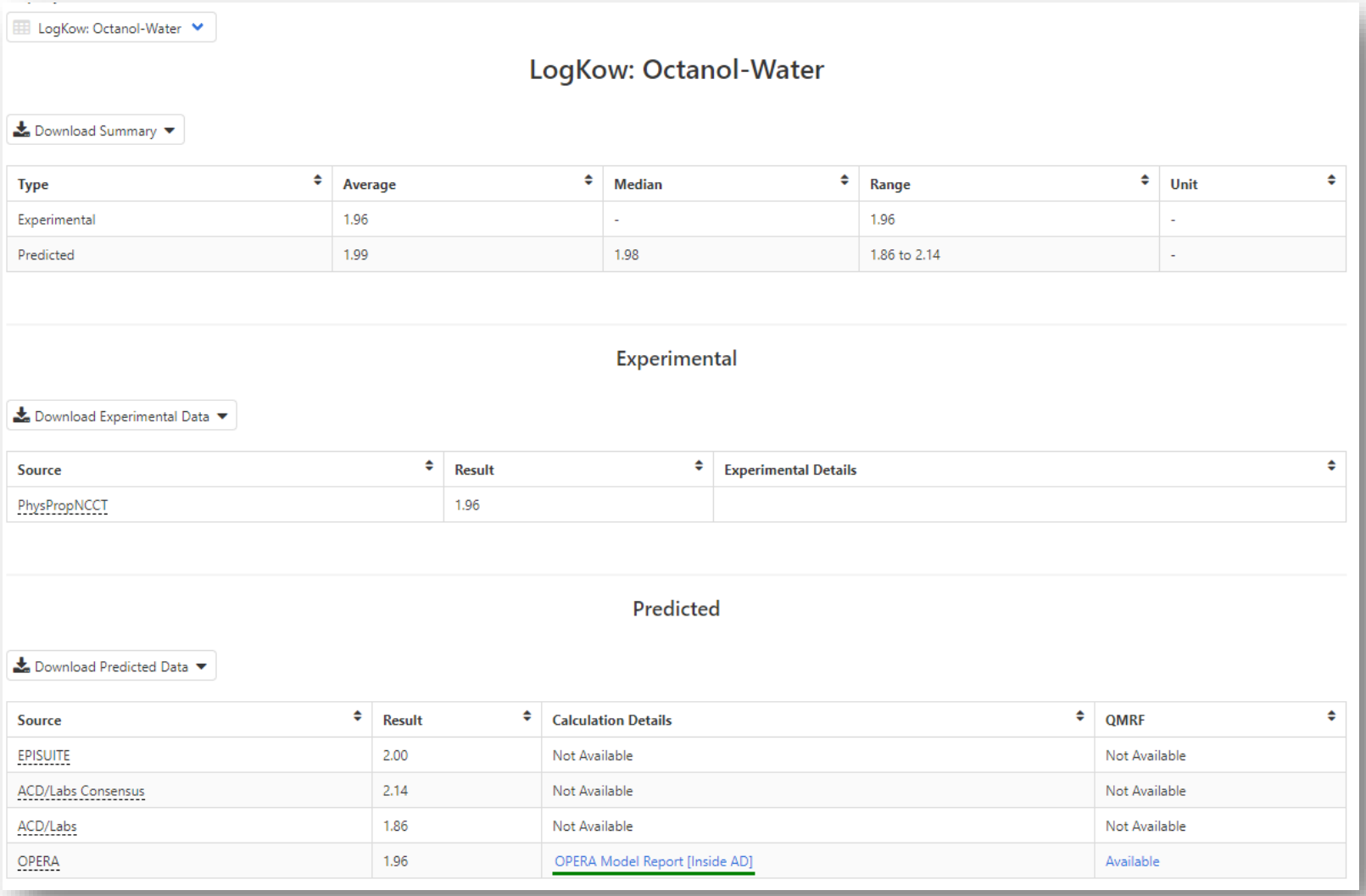
Summary

Download | Columns | Search query

Property	Experimental average	Predicted average	Experimental median	Predicted median	Experimental range	Predicted range	Unit
LogKow: Octanol-Water	1.96 (1)	1.99		1.98	1.96	1.86 to 2.14	-
Melting Point	128 (9)	83.7	127	69.4	126 to 131	51.5 to 130	°C
Boiling Point	278 (3)	261	280	260	275 to 280	252 to 273	°C
Water Solubility	1.73e-2 (4)	1.23	1.66e-2	2.82e-2	1.64e-2 to 1.97e-2	1.22e-2 to 4.86	mol/L
Flash Point	-	115		115	-	113 to 116	°C
Density	-	1.20		1.20	-	1.20 to 1.21	g/cm^3
Vapor Pressure	-	4.98e-3		5.55e-3	-	1.08e-3 to 8.32e-3	mmHg
Thermal Conductivity	-	150			-	150	mW/(m*K)
Viscosity	-	7.03			-	7.03	cP
Surface Tension	-	42.3		42.3	-	38.7 to 45.8	dyn/cm
Index of Refraction	-	1.55			-	1.55	-
Molar Refractivity	-	39.9			-	39.9	cm^3
Polarizability	-	15.8			-	15.8	Å^3

Obtaining Descriptors Using the Dashboard

United States Environmental Protection Agency



LogKow: Octanol-Water

LogKow: Octanol-Water

Download Summary

Type	Average	Median	Range	Unit
Experimental	1.96	-	1.96	-
Predicted	1.99	1.98	1.86 to 2.14	-

Experimental

Download Experimental Data

Source	Result	Experimental Details
PhysPropNCCT	1.96	

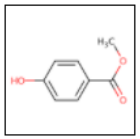
Predicted

Download Predicted Data

Source	Result	Calculation Details	QMRF
EPISUITE	2.00	Not Available	Not Available
ACD/Labs Consensus	2.14	Not Available	Not Available
ACD/Labs	1.86	Not Available	Not Available
OPERA	1.96	OPERA Model Report [Inside AD]	Available

Obtaining Descriptors Using the Dashboard

United States Environmental Protection Agency

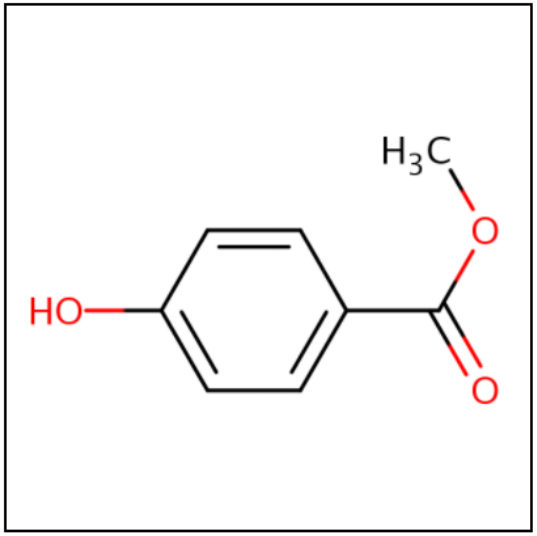


Methylparaben

99-76-3 | DTXSID4022529

Searched by Synonym from Valid Source.

- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- SAFETY
- ADME
- EXPOSURE
- BIOACTIVITY
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS
- LITERATURE
- LINKS
- COMMENTS



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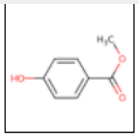

Methylparaben

99-76-3 | DTXSID4022529

Searched by Synonym from Valid Source.

- DETAILS
- EXECUTIVE SUMMARY
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- ADME
- EXPOSURE
  - PRODUCT & USE CATEGORIES
  - CHEMICAL WEIGHT FRACTION
  - CHEMICAL FUNCTIONAL USE
  - TOXICS RELEASE INVENTORY
  - MONITORING DATA
  - EXPOSURE PREDICTIONS
  - PRODUCTION VOLUME

Product and Use Categories (PUCs)

Download | Columns | 10 | Search query

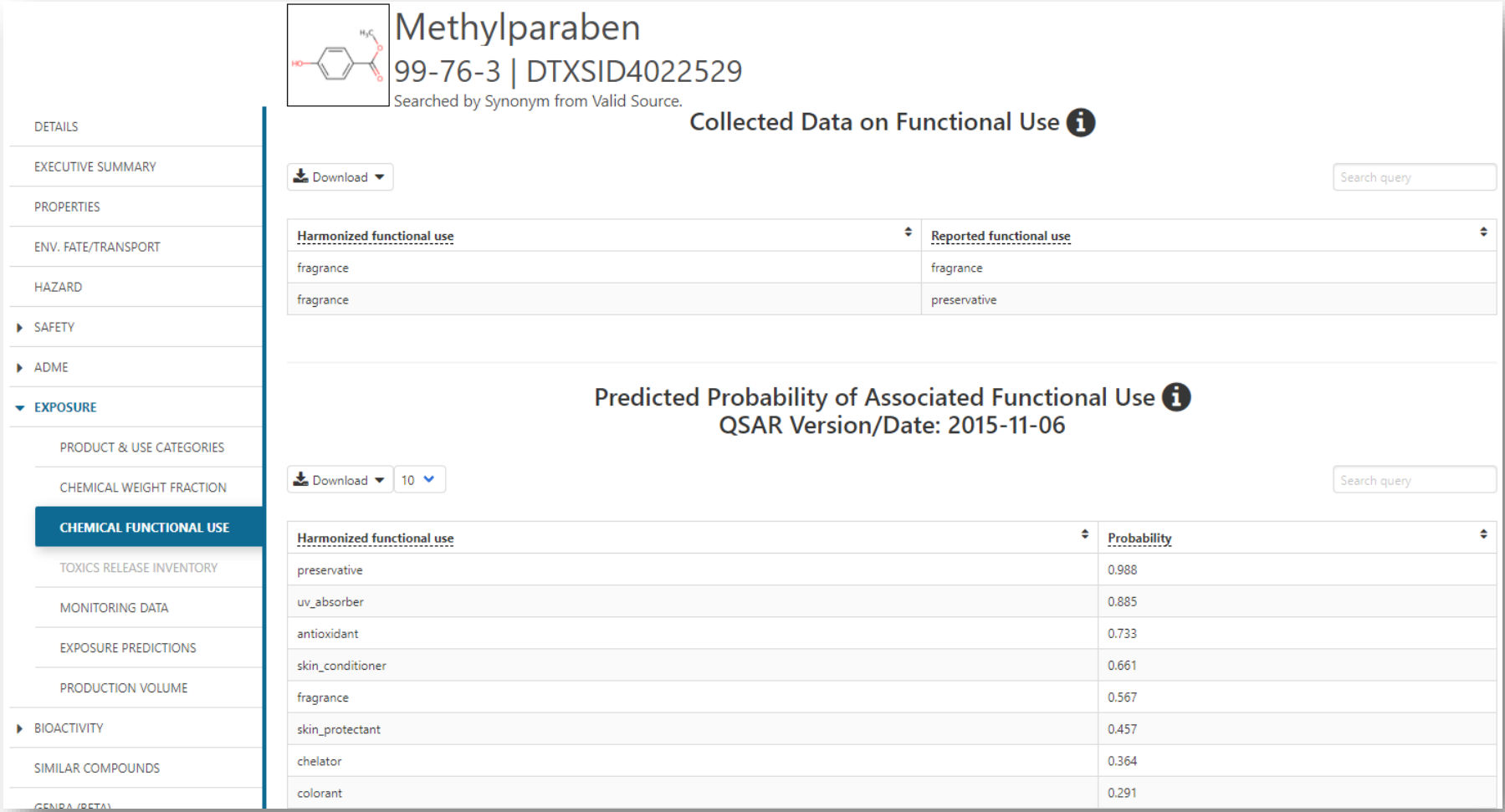
Product or Use Categorization	Categorization type	Number of Unique Products
hair styling and care:	PUC	1
hair styling and care: hair conditioner - leave-in	PUC	1
hair styling and care: hair conditioner	PUC	1
hair styling and care: hair styling	PUC	2
hair styling and care: lice shampoo	PUC	1
hair styling and care: shampoo	PUC	1
home office: pens and markers	PUC	2
inert_ingredient, Pesticides	CPCat Cassette	1
inert_ingredient, non_food_use, Pesticides	CPCat Cassette	1
make-up and related: eye liner	PUC	1

<< < 1 2 3 4 5 6 > >>

Showing 31 to 40 of 54 records

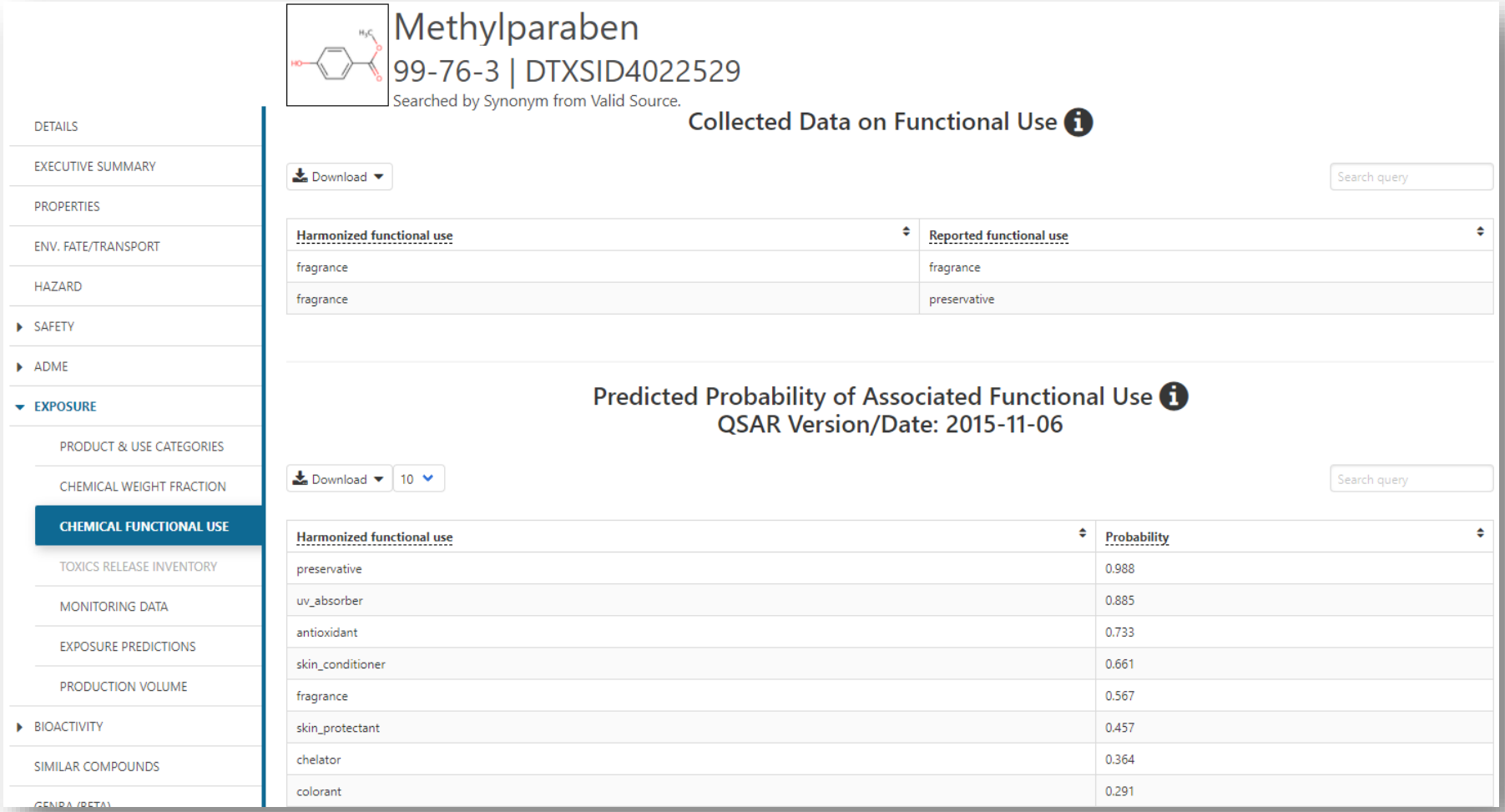
Obtaining Descriptors Using the Dashboard

United States Environmental Protection Agency

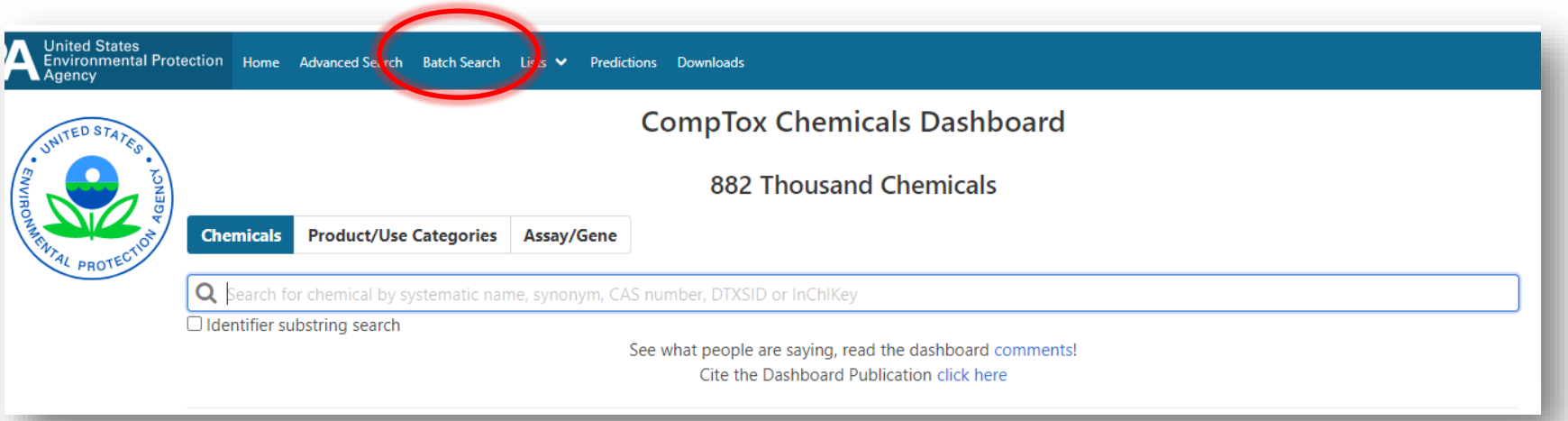


Obtaining Descriptors Using the Dashboard

United States Environmental Protection Agency

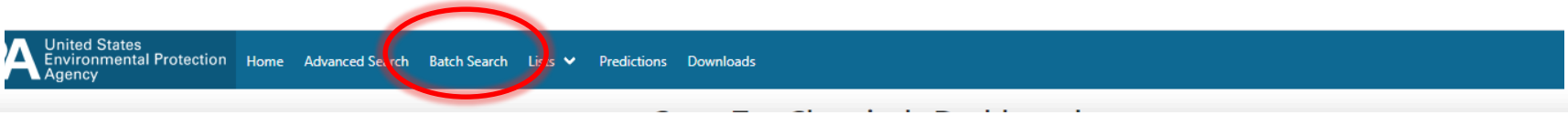


Obtaining Descriptors with Batch Search



Obtaining Descriptors with Batch Search

United States Environmental Protection Agency



Batch Search

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

Step One: Select Input

Please enter one identifier per line

Select Input Type(s)

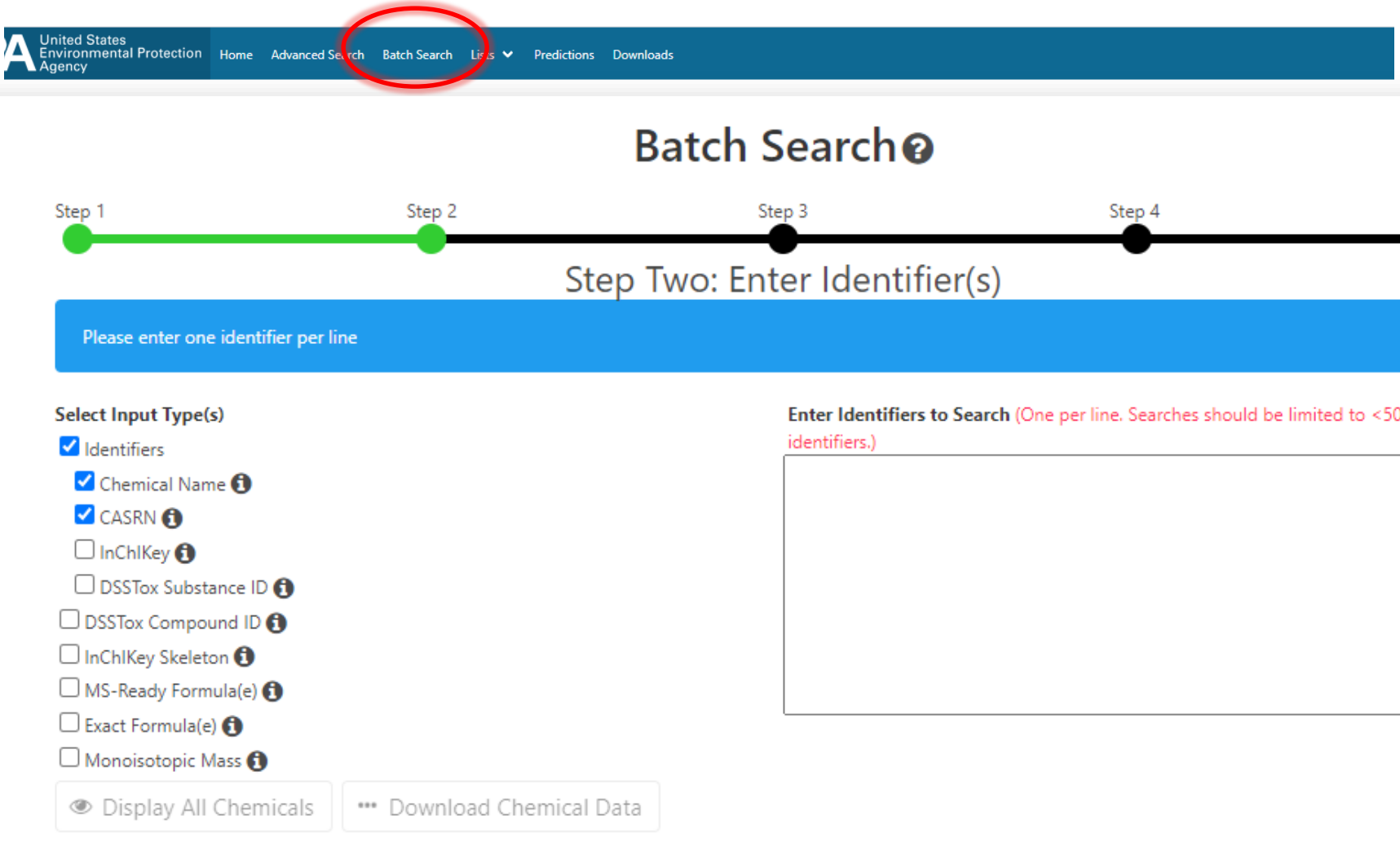
- Identifiers
  - Chemical Name
  - CASRN
  - InChIKey
  - DSSTox Substance ID
- DSSTox Compound ID
- InChIKey Skeleton
- MS-Ready Formula(e)
- Exact Formula(e)
- Monoisotopic Mass

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

Display All Chemicals | Download Chemical Data

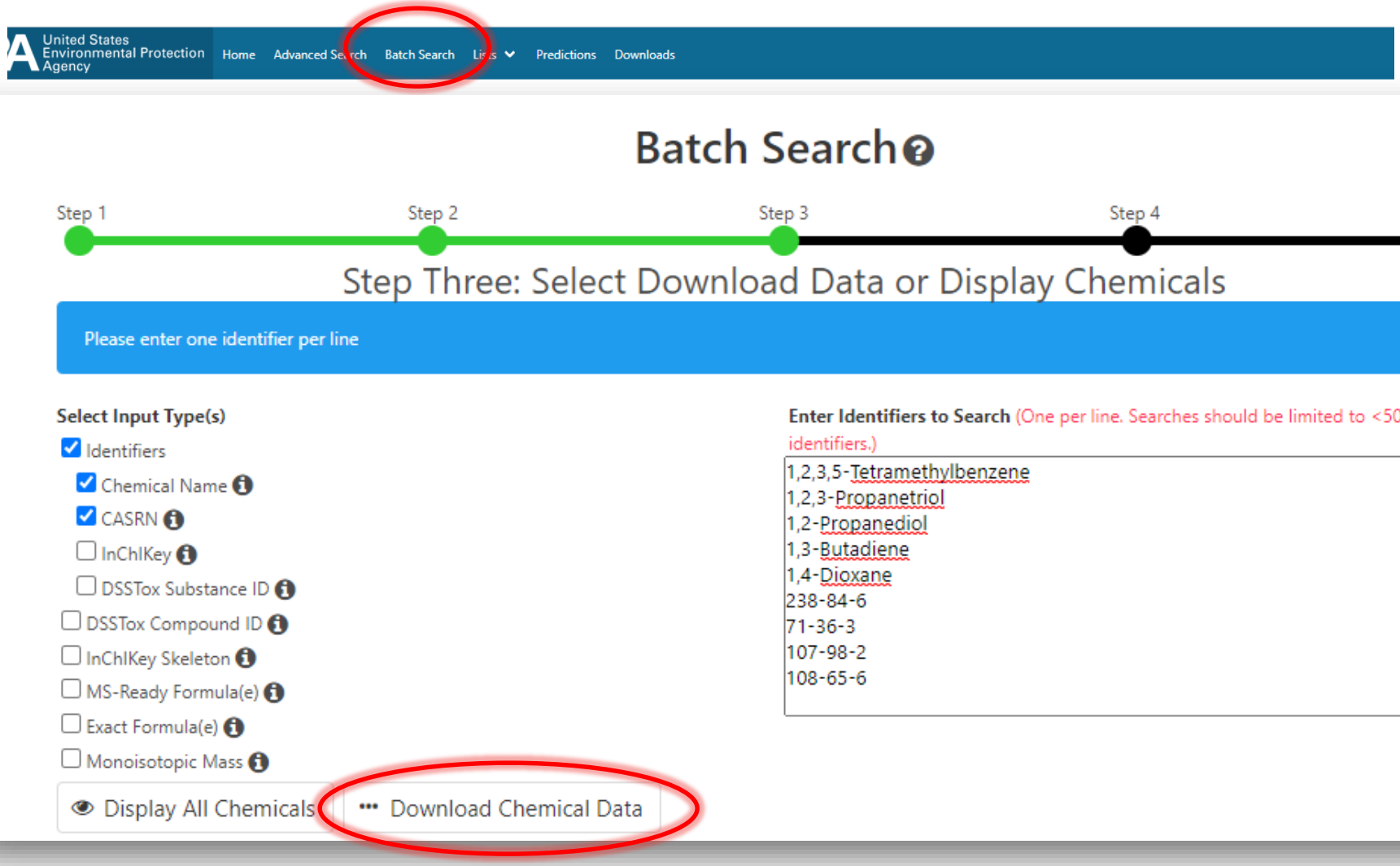
Obtaining Descriptors with Batch Search

United States Environmental Protection Agency

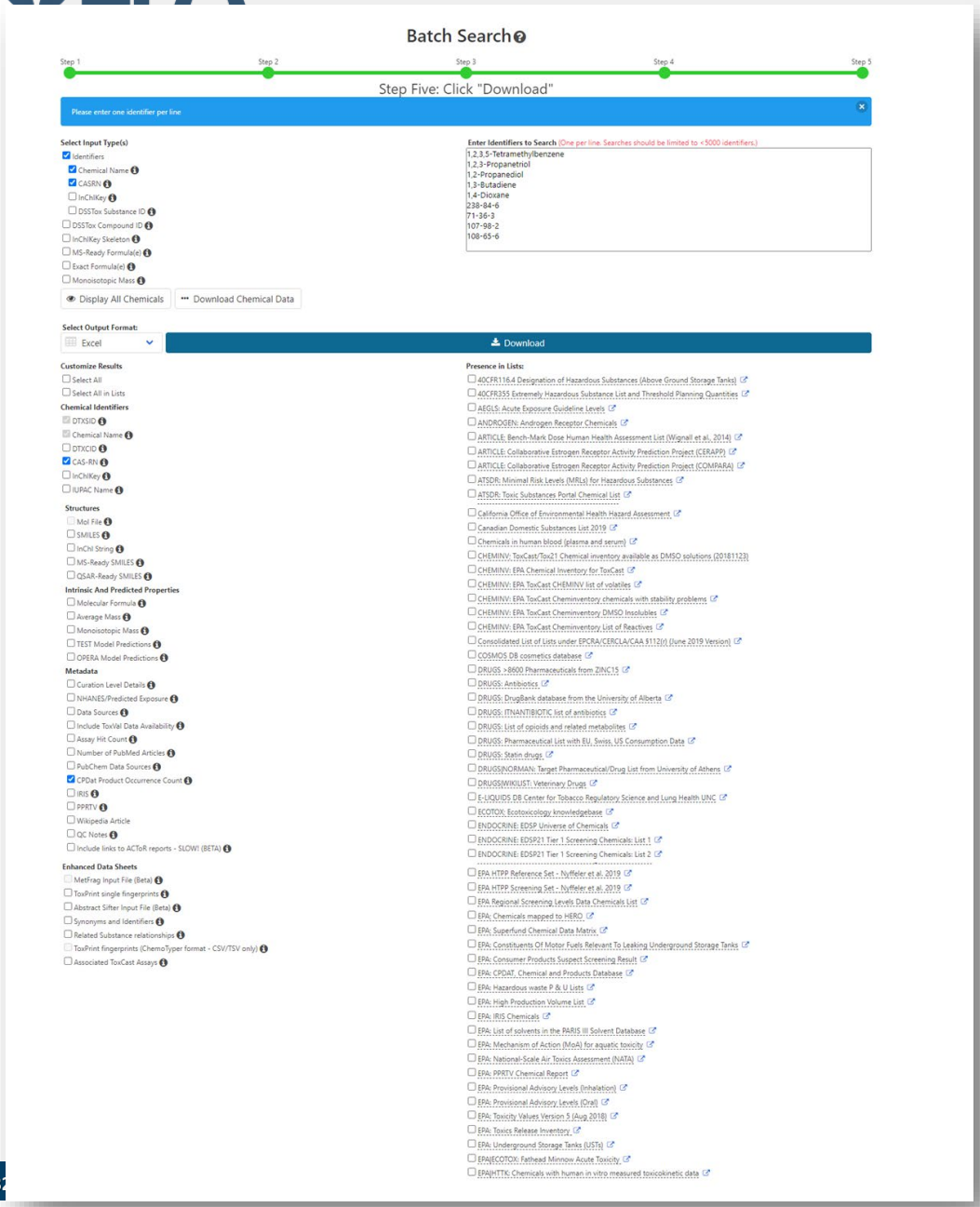


Obtaining Descriptors with Batch Search

United States Environmental Protection Agency

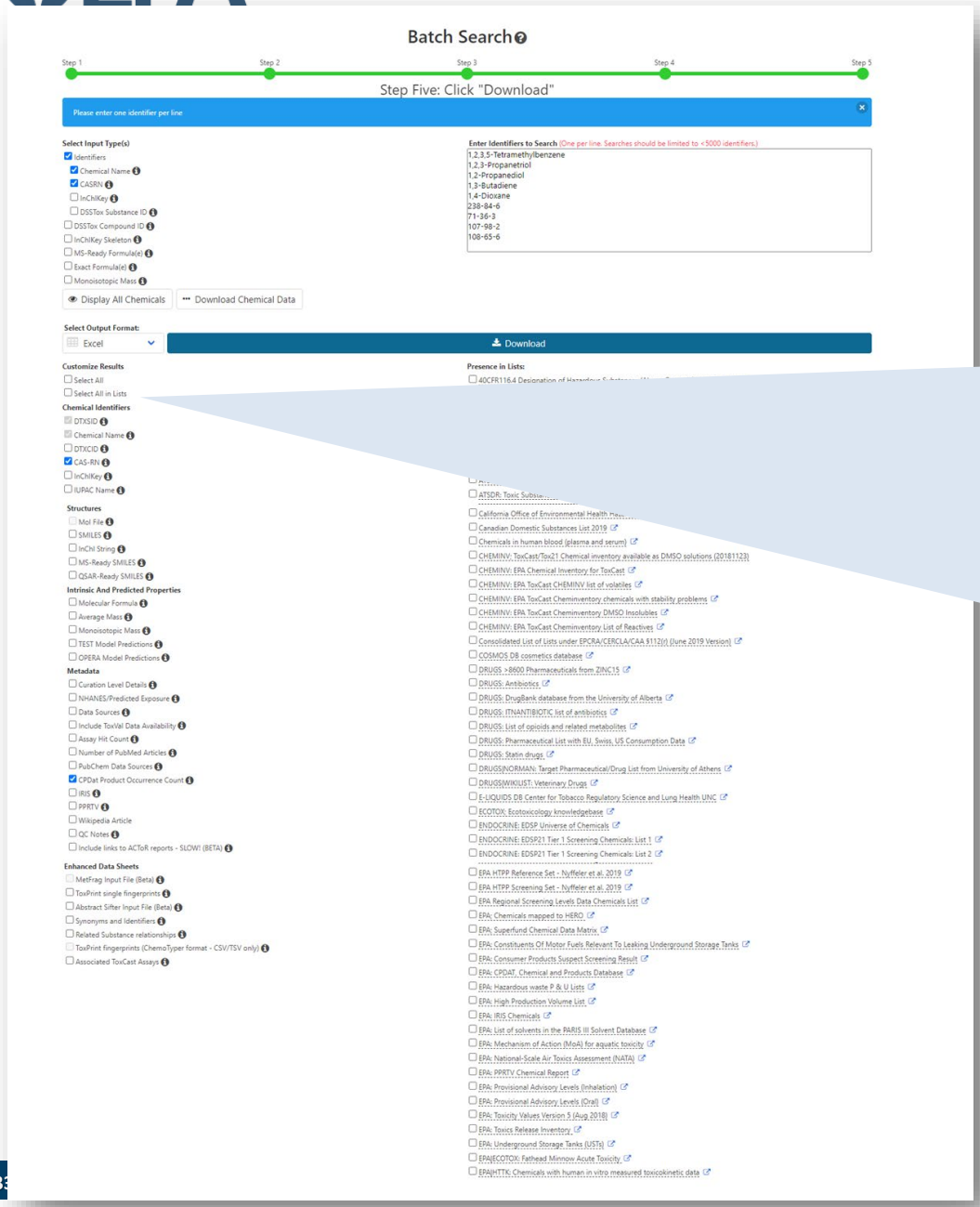


Obtaining Descriptors with Batch Search



Opens large panel of available chemical data for selection

Obtaining Descriptors with Batch Search



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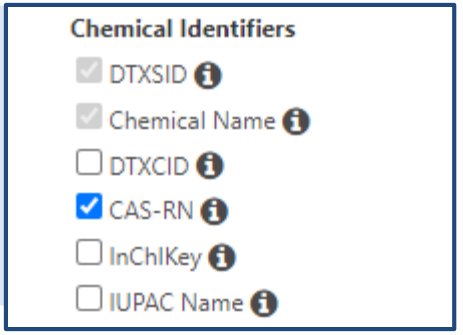

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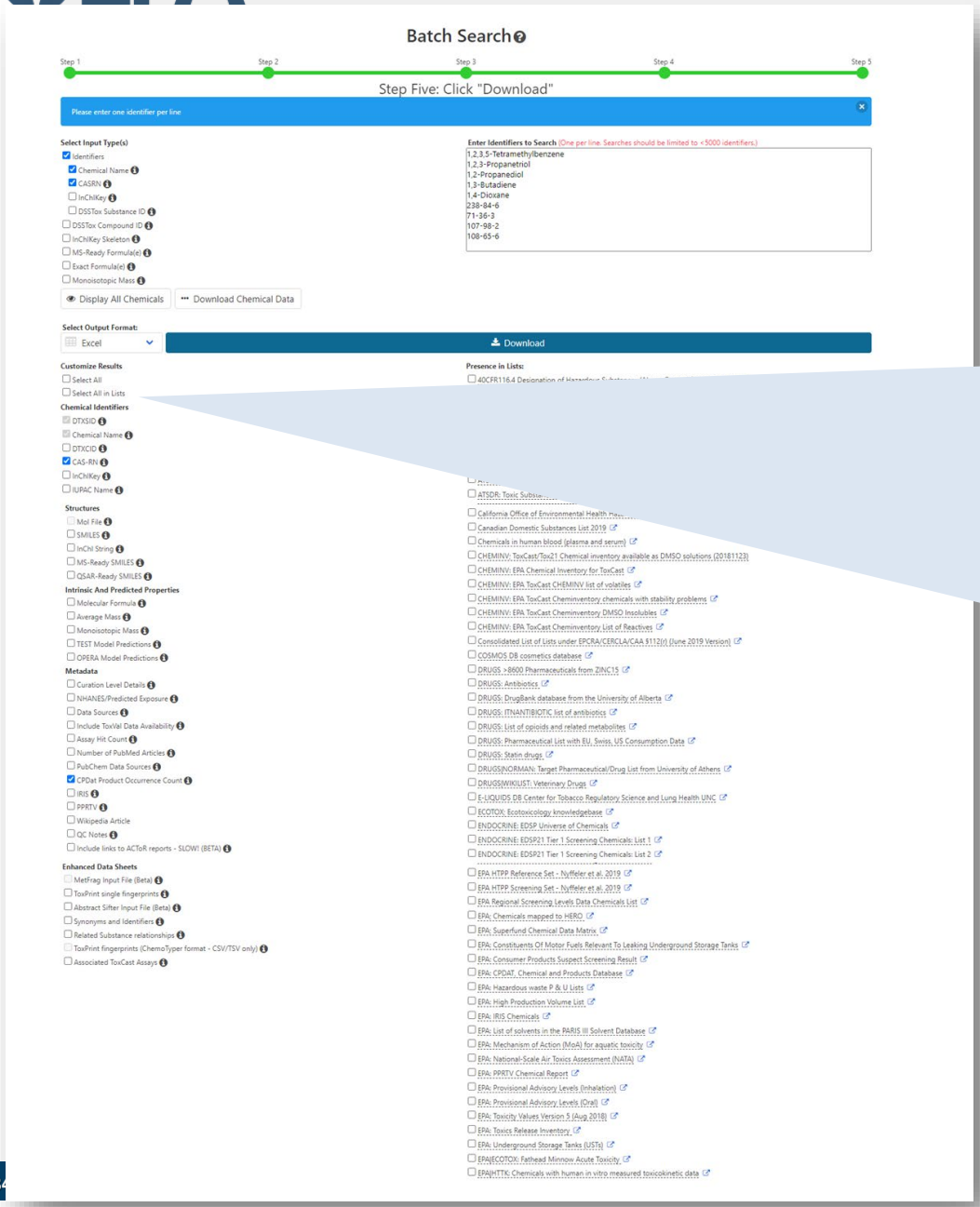

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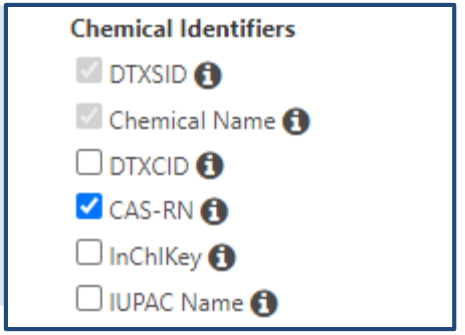

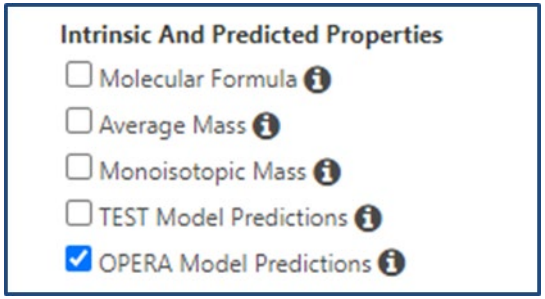

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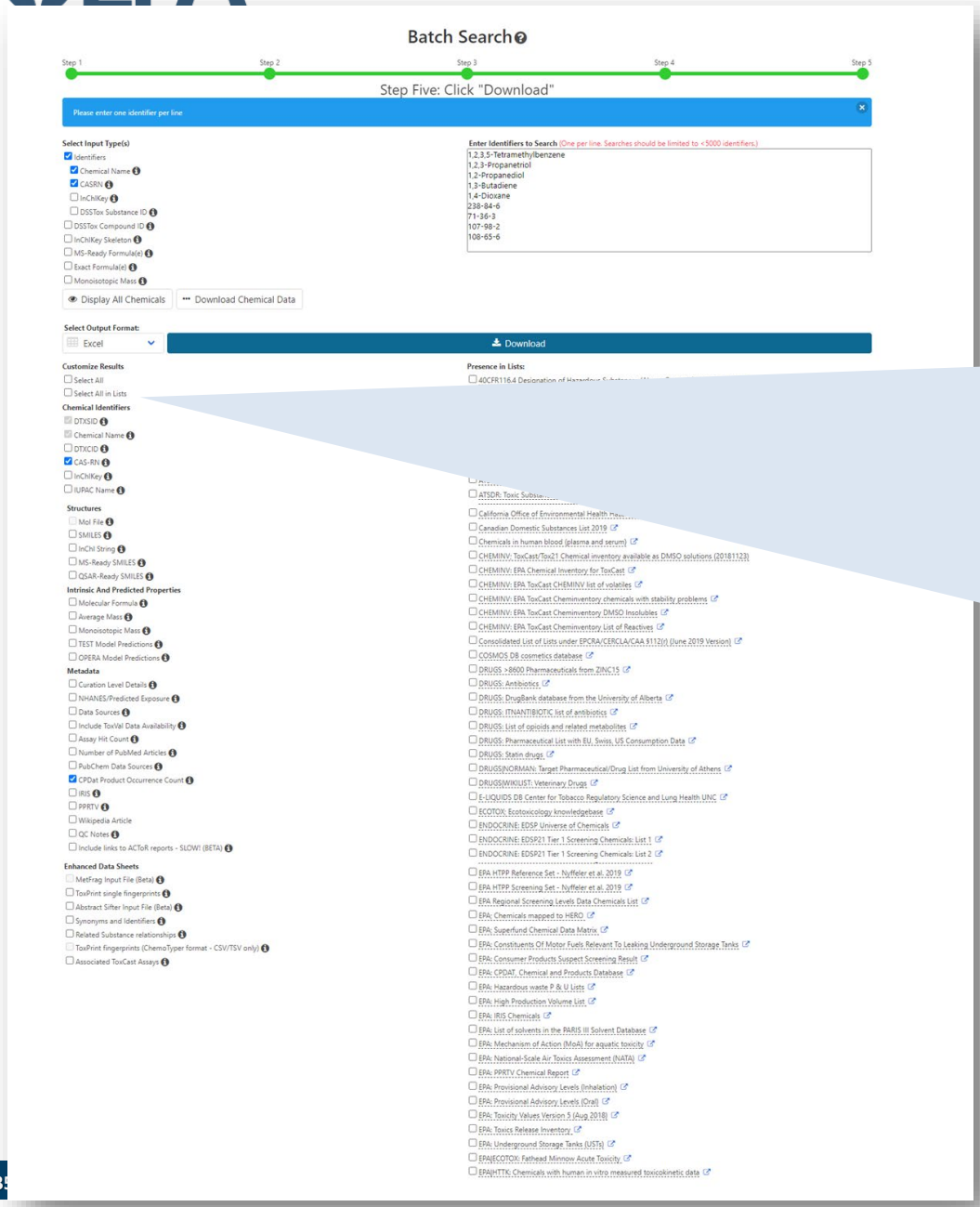

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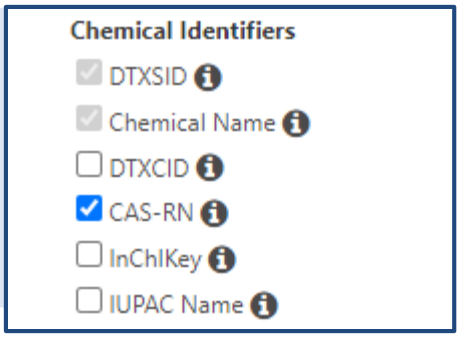

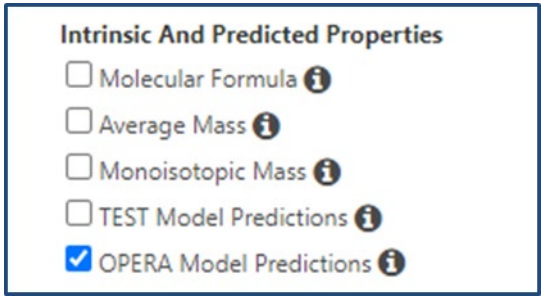

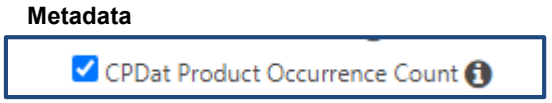

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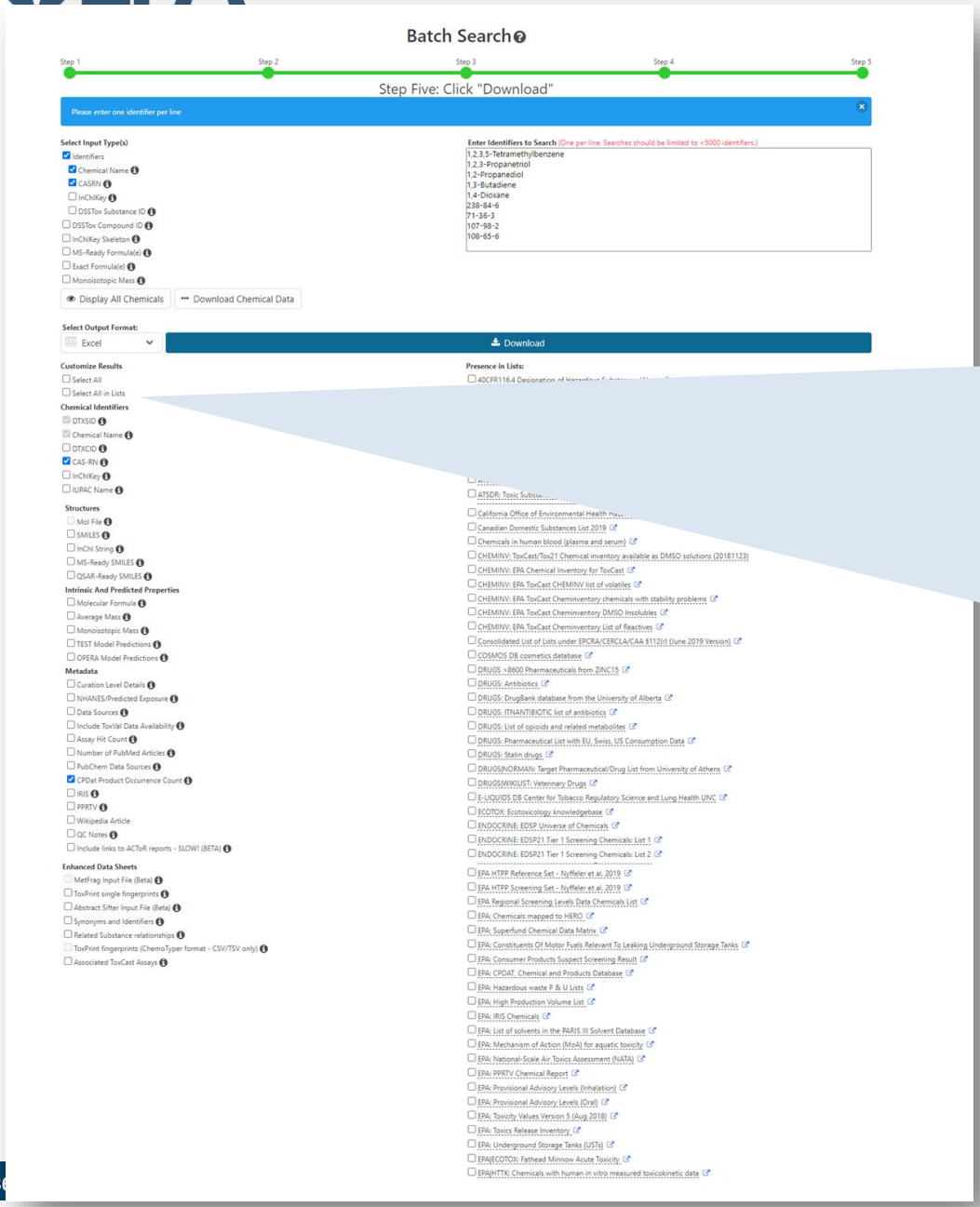

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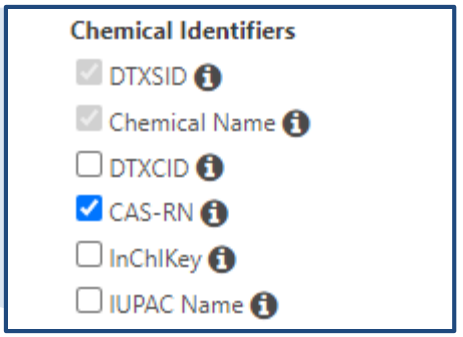

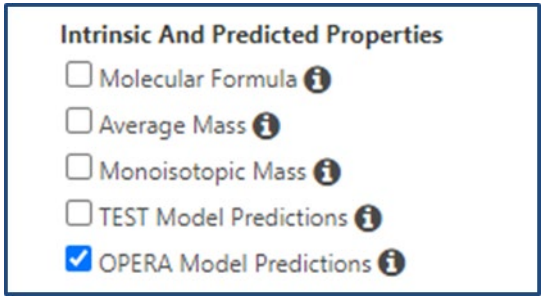

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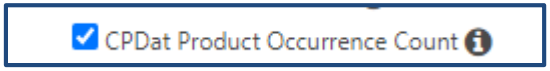
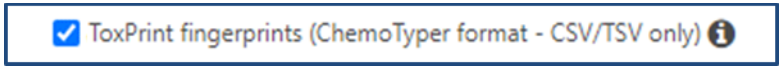
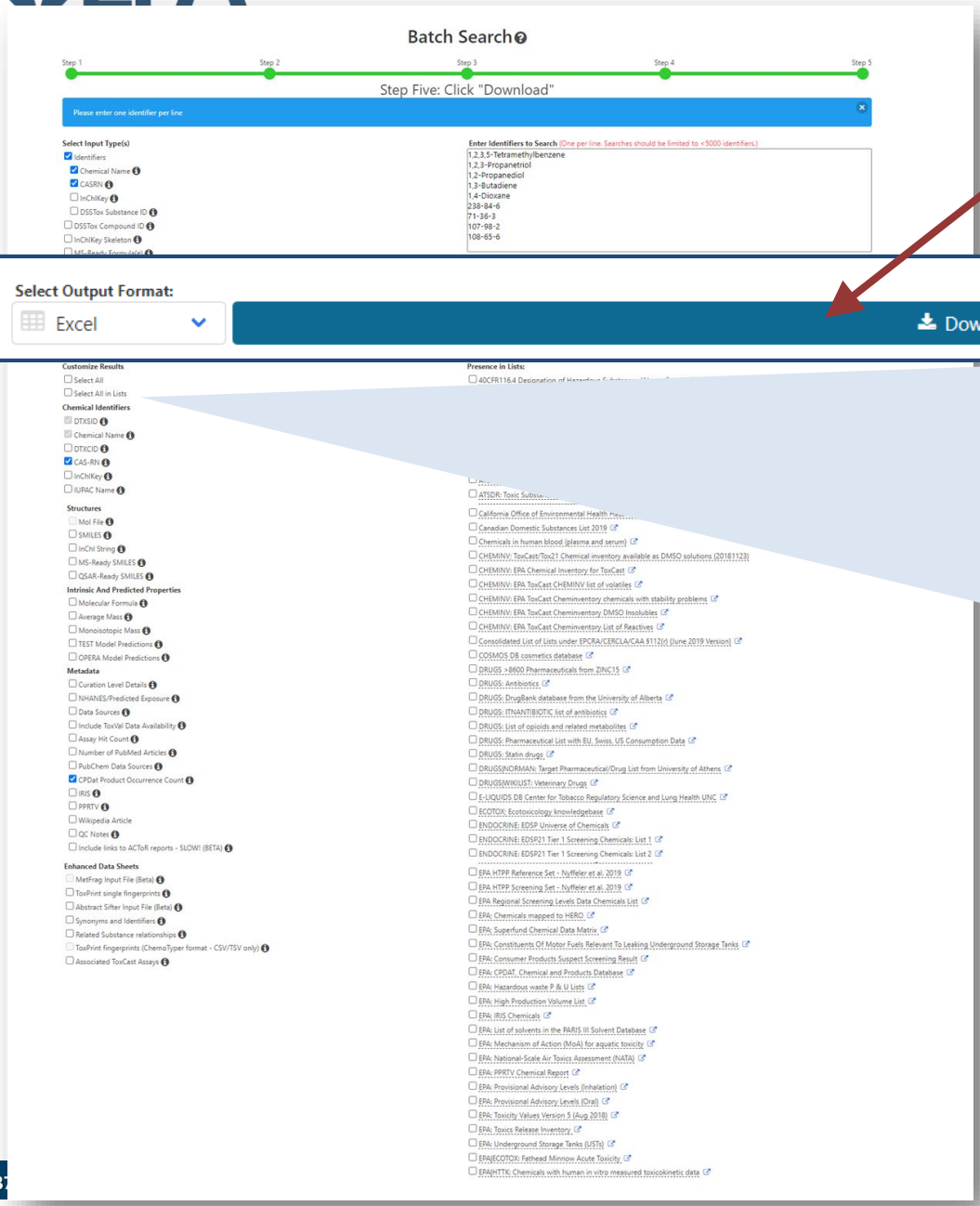


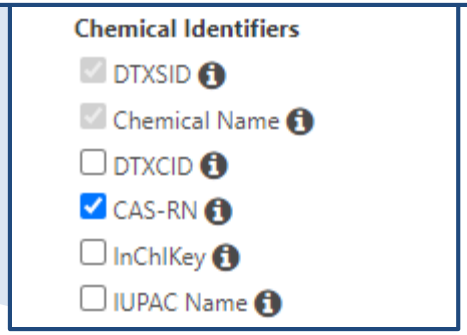
Enhanced Data Sheets

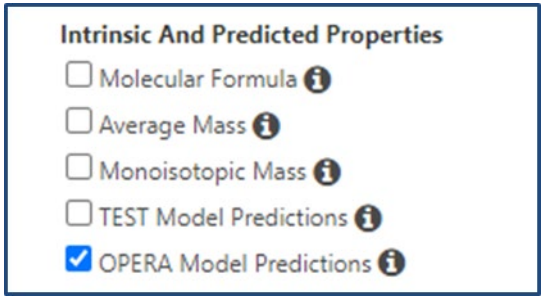


Obtaining Descriptors with Batch Search



Download Data to Excel, CSV, TSV files





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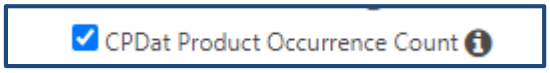

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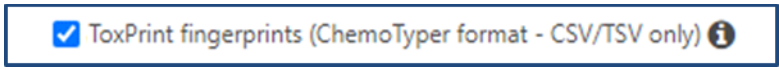
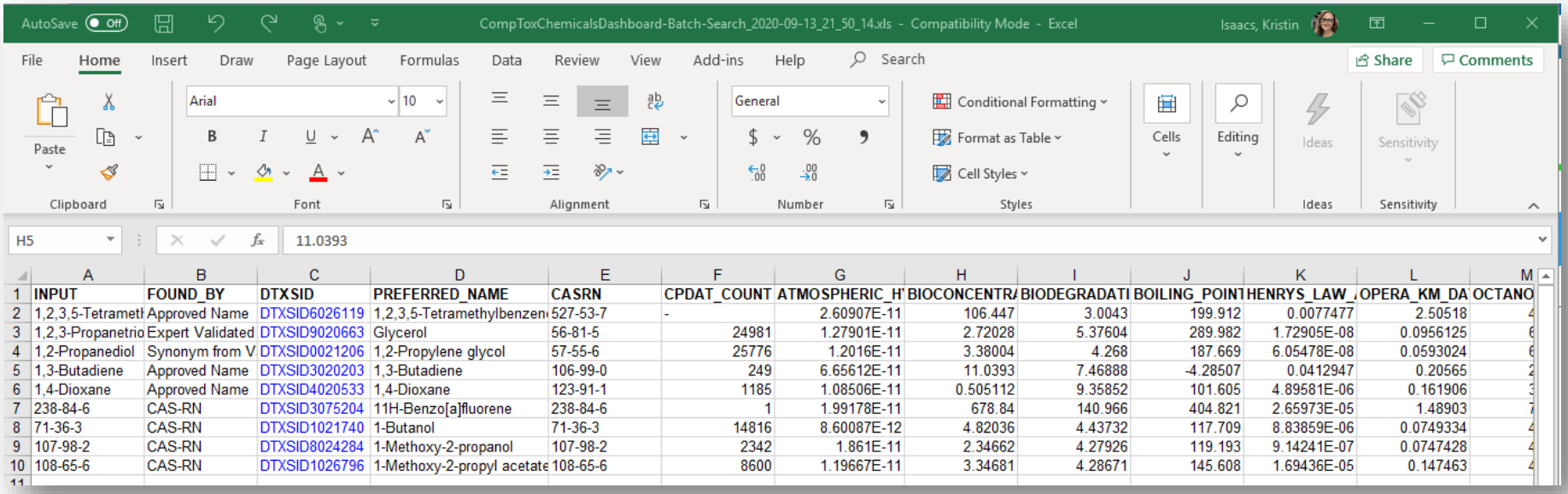


Obtaining Descriptors with Batch Search

United States Environmental Protection Agency

Downloaded File Contains Original Identifier, DTXSID, and selected datasets



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2	1,2,3,5-Tetrameth	Approved Name	DTXSID6026119	1,2,3,5-Tetramethylbenzen	527-53-7	-	2.60907E-11	106.447	3.0043	199.912	0.0077477	2.50518	4
3	1,2,3-Propanetrio	Expert Validated	DTXSID9020663	Glycerol	56-81-5	24981	1.27901E-11	2.72028	5.37604	289.982	1.72905E-08	0.0956125	6
4	1,2-Propanediol	Synonym from V	DTXSID0021206	1,2-Propylene glycol	57-55-6	25776	1.2016E-11	3.38004	4.268	187.669	6.05478E-08	0.0593024	6
5	1,3-Butadiene	Approved Name	DTXSID3020203	1,3-Butadiene	106-99-0	249	6.65612E-11	11.0393	7.46888	-4.28507	0.0412947	0.20565	2
6	1,4-Dioxane	Approved Name	DTXSID4020533	1,4-Dioxane	123-91-1	1185	1.08506E-11	0.505112	9.35852	101.605	4.89581E-06	0.161906	3
7	238-84-6	CAS-RN	DTXSID3075204	11H-Benzo[a]fluorene	238-84-6	1	1.99178E-11	678.84	140.966	404.821	2.65973E-05	1.48903	7
8	71-36-3	CAS-RN	DTXSID1021740	1-Butanol	71-36-3	14816	8.60087E-12	4.82036	4.43732	117.709	8.83859E-06	0.0749334	4
9	107-98-2	CAS-RN	DTXSID8024284	1-Methoxy-2-propanol	107-98-2	2342	1.861E-11	2.34662	4.27926	119.193	9.14241E-07	0.0747428	4
10	108-65-6	CAS-RN	DTXSID1026796	1-Methoxy-2-propyl acetate	108-65-6	8600	1.19667E-11	3.34681	4.28671	145.608	1.69436E-05	0.147463	4
11													

ExpoCast Project (Exposure Forecasting)

CCTE

Linda Adams
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Dan Dawson*
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Kathie Dionisio
Christopher Ecklund
Marina Evans
Peter Egeghy
Michael-Rock Goldsmith
Chris Grulke
Mike Hughes
Kristin Isaacs
Richard Judson
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Anna Kreutz*
Charles Lowe*
Seth Newton
Katherine Phillips
Paul Price
Tom Purucker
Ann Richard
Caroline Ring
Marci Smeltz*
Jon Sobus
Risa Sayre*
Mark Sfeir*
Mark Strynar
Zach Stanfield*
Rusty Thomas
Mike Tornero-Velez
Elin Ulrich
Dan Vallero
John Wambaugh
Barbara Wetmore
Antony Williams

CEMM

Xiaoyu Liu

CPHEA

Jane Ellen Simmons

CESER

David Meyer
Gerardo Ruiz-Mercado
Wes Ingwersen

***Trainees**

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Nisha Sipes
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ScitoVation
Chantel Nicolas
Silent Spring Institute
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Alice Yau
Kristin Favela
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Tox Strategies
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Beate Nicol
Cecilie Rendal
Ian Sorrell
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Hyeong-Moo Shin