Introducing EPA'S Chemical Exposure Knowledgebase

Sakshi Handa, Kristin Isaacs, Katherine Phillips

CCTE NAMs Training Workshop

Research Triangle Park, NC

April 24 – 25, 2024

Disclaimer: The views expressed in this presentation are those of the authors and do not necessarily reflect the views or policies of the United States EPA. Mention of trade names or commercial products does constitute endorsement or recommendation for use.

THANK YOU!!

U.S. EPA

Peter Egeghy
Colleen Elonen
Kenta Baron-Furuyama
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ChemExpo

Email
chemexpo.support@epa.gov
with questions and comments

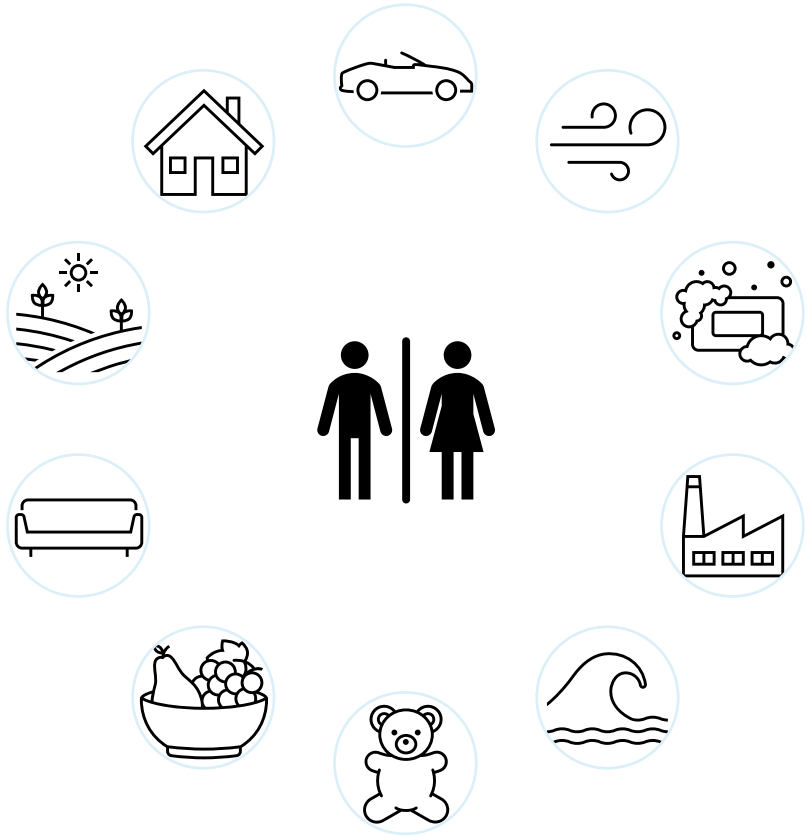
Session Overview

- Background/Motivation
- What is CPDat?
- How is CPDat accessed?
- ChemExpo Demo

Background

Chemical Exposure

- Humans interact with thousands of chemicals on a regular basis
- We often don’t know precisely…
  - …which chemicals we contact in our everyday lives
  - …the quantities of those chemicals
  - …the ultimate fate of those chemicals in our bodies
- Tools developed for Computational Exposure Science allow us to characterize our potential exposure to many chemicals along many exposure pathways



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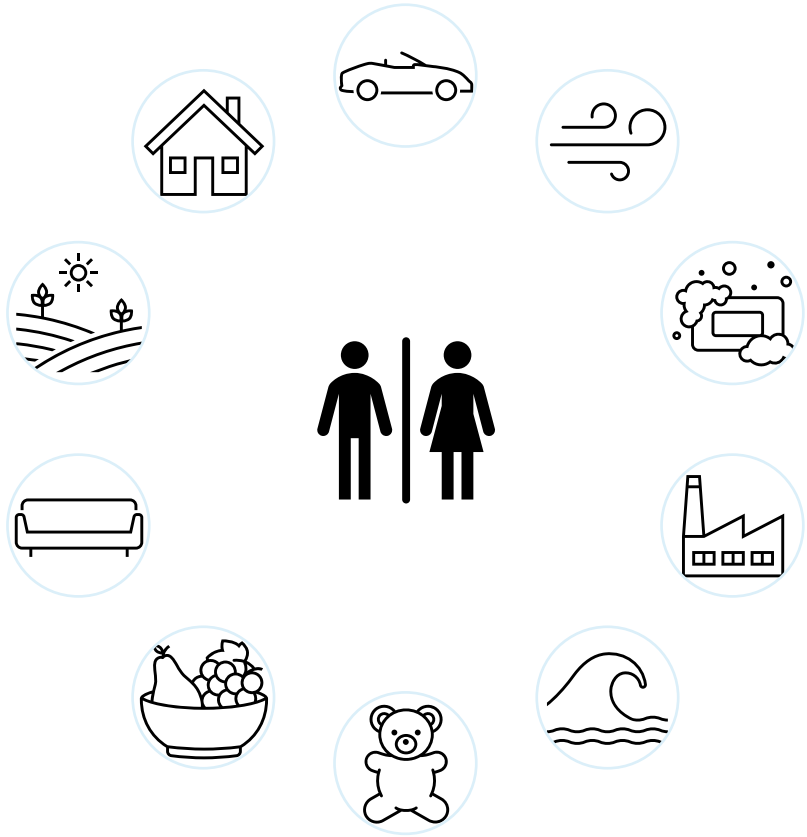
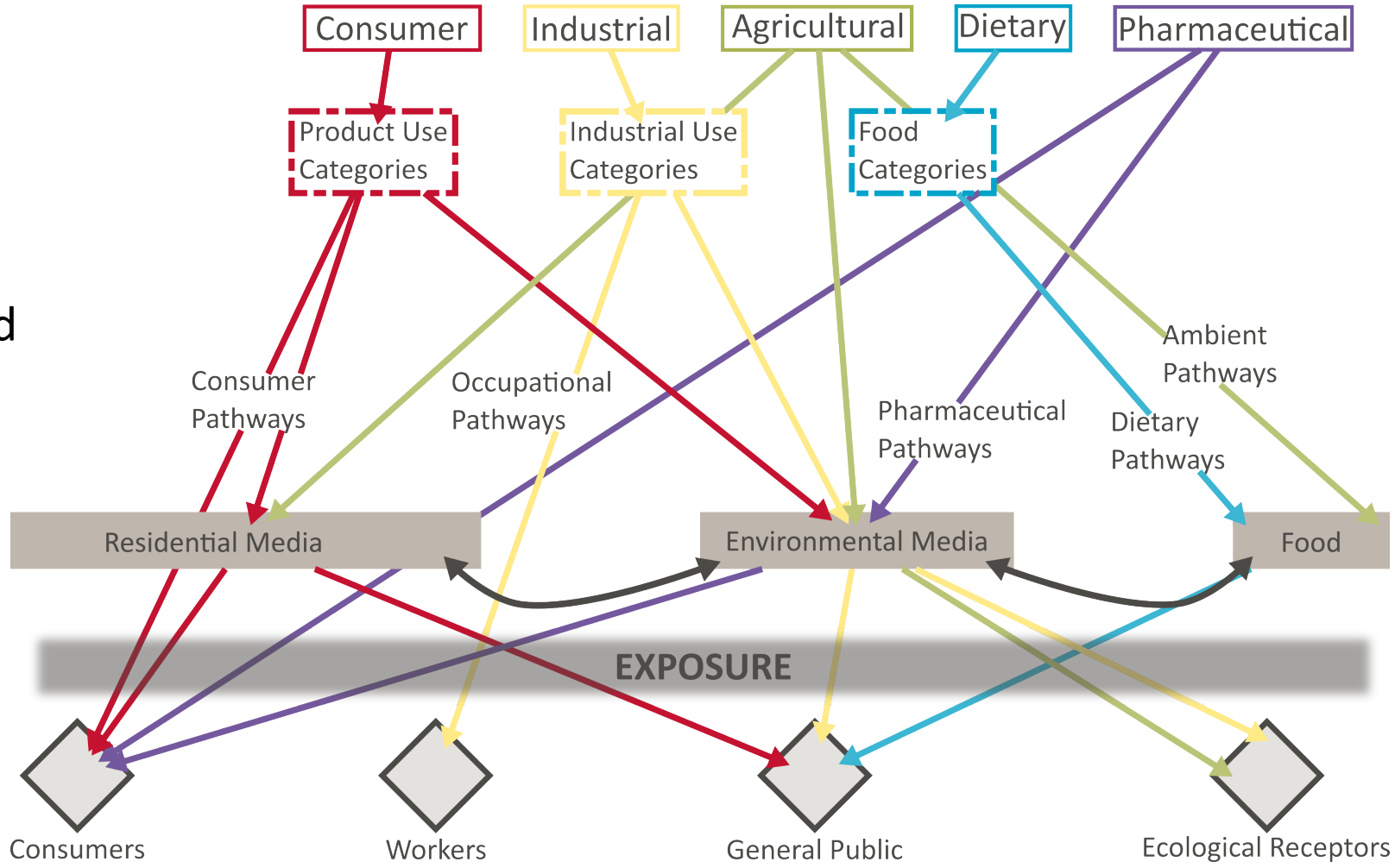


Exposure Pathways:

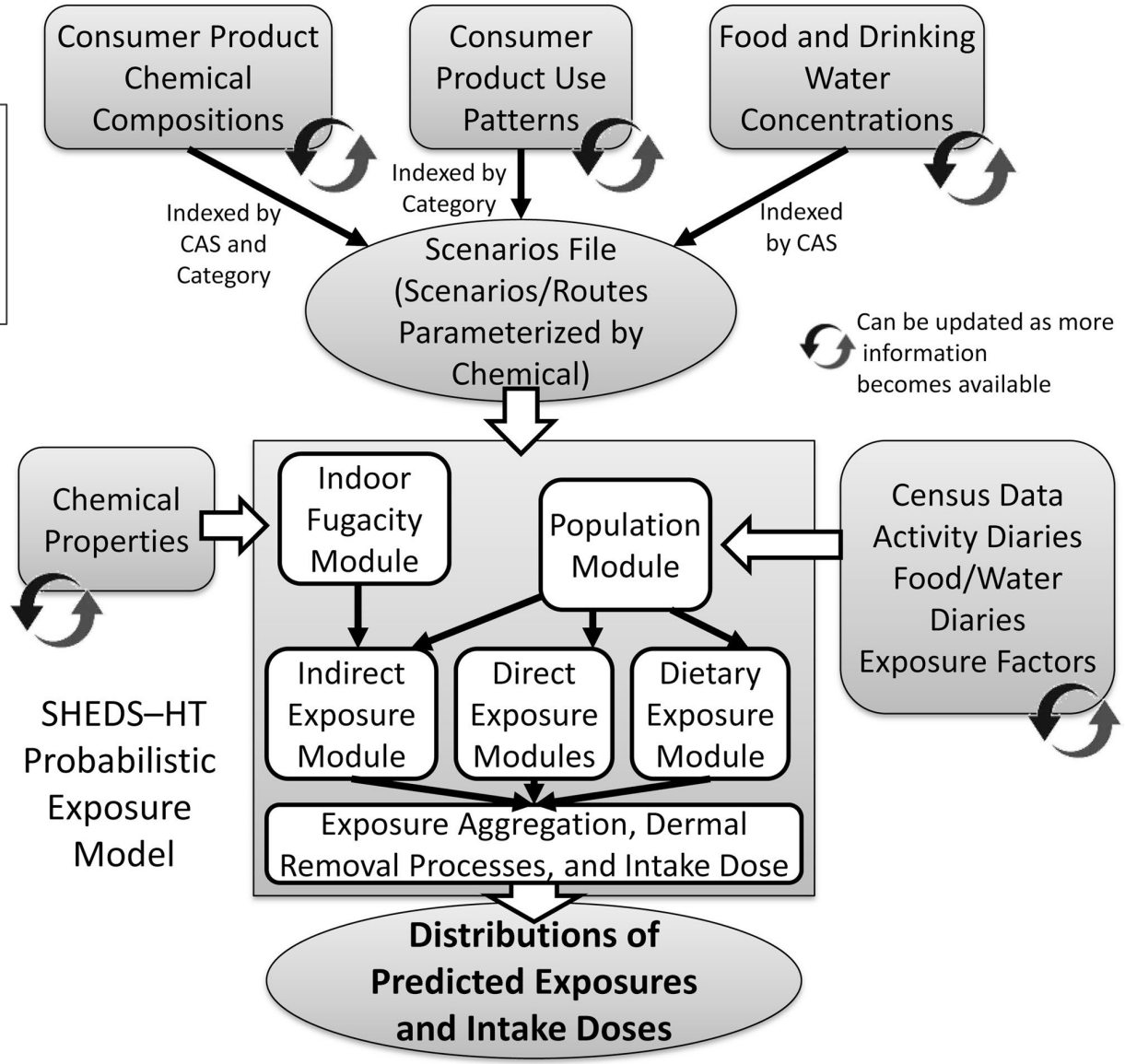
Source to Receptors

- We can trace a chemical's exposure pathways by examining its ***use*** in various commercial sectors
- Commercial sector of use allows us to then define potential pathways associated with a chemical (include potential chemical release, media occurrence, and ultimate receptor exposure)
- Use information (both qualitative and quantitative) are needed to inform models for various pathways



SHEDS-HT

How does use information contribute to exposure modeling?



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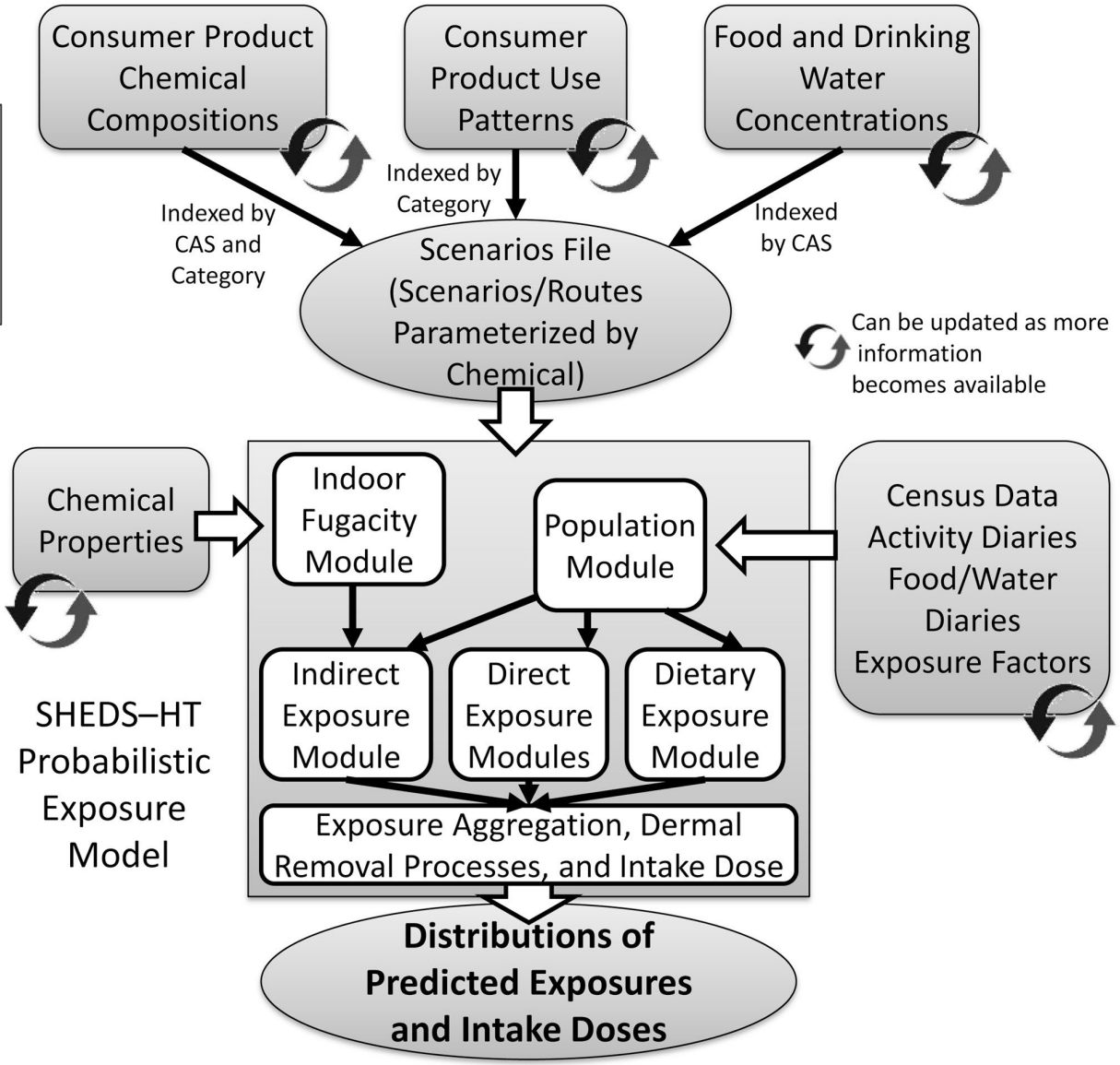
How does use information contribute to exposure modeling?

Models like EPA's SHEDS-HT require information about chemicals and their compositions in products in order to estimate exposures



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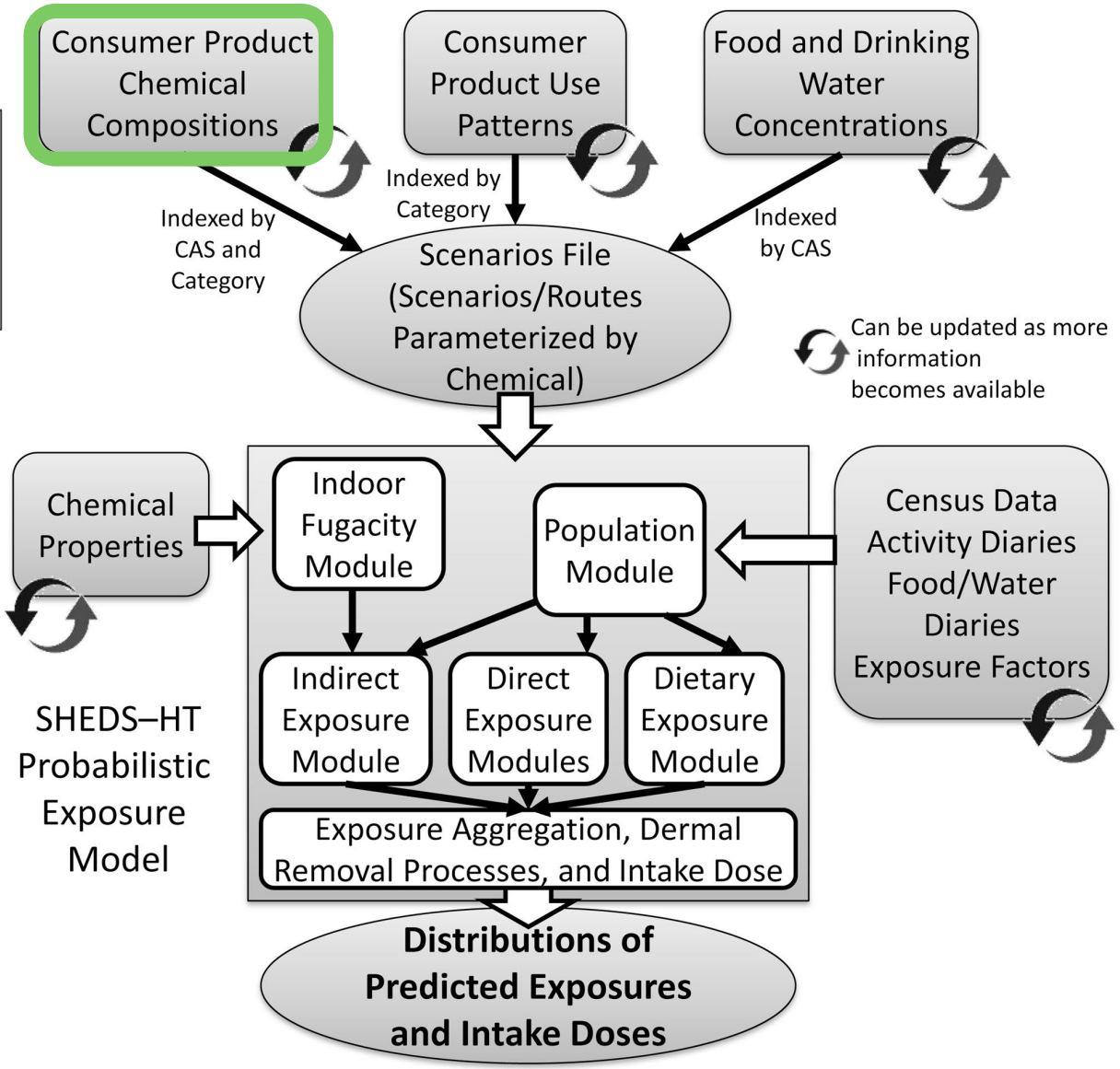
CPDat can provide this information!



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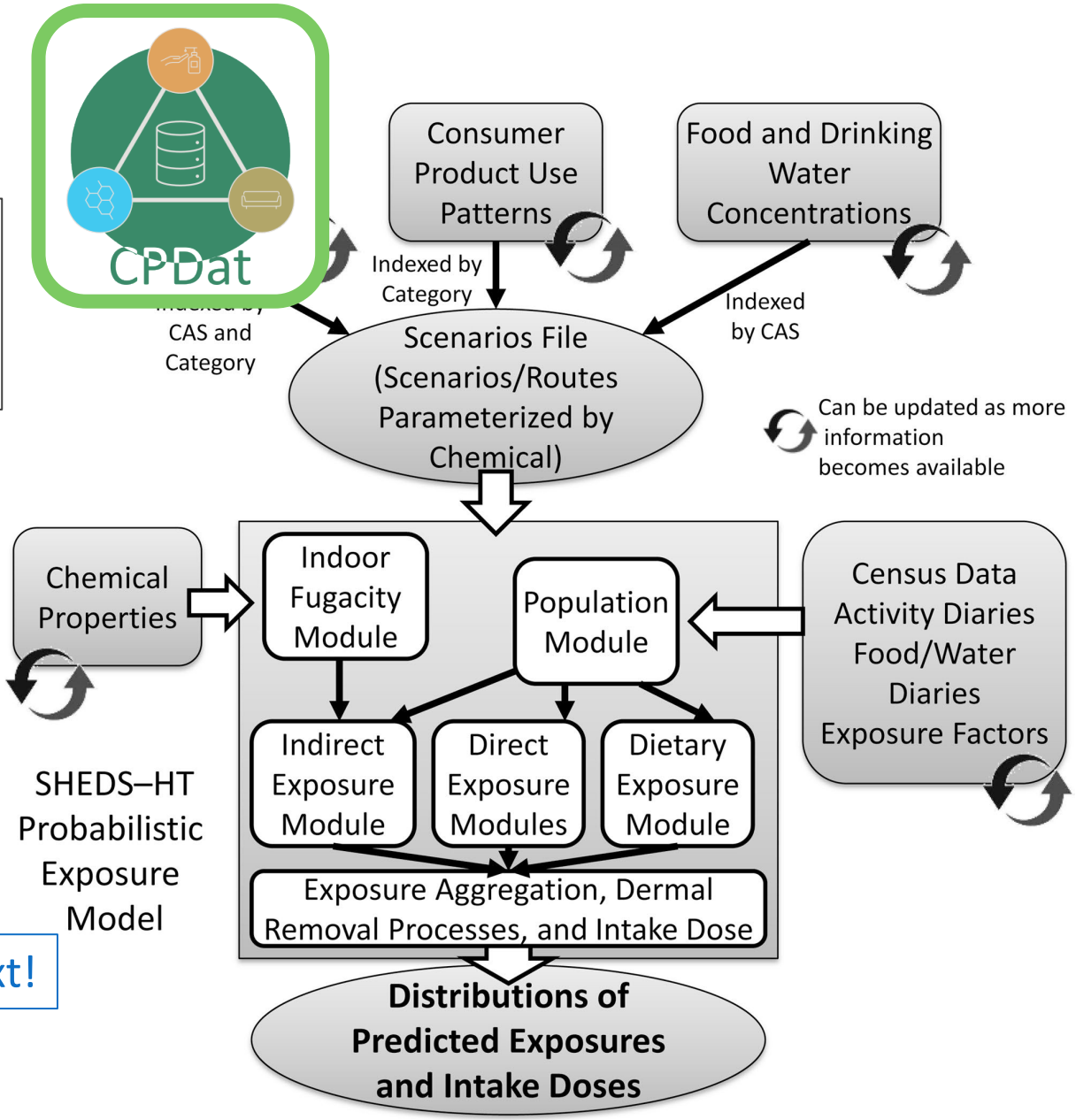
Kristin Isaacs has a demo of SHEDS-HT next!



What Is CPDat?

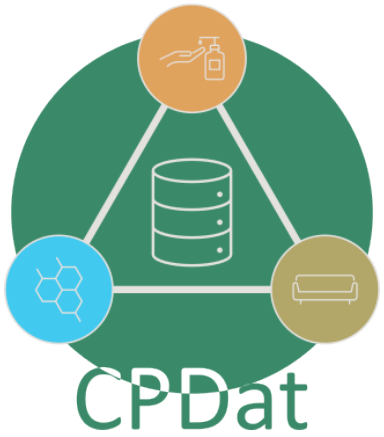
…Factotum?

…ChemExpo?

…how are they all related?

…which should I use?

Chemical and Products Database



nature › scientific data › data descriptors › article

Open Access | Published: 10 July 2018

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

Kathie L. Dionisio, Katherine Phillips, Paul S. Price, Christopher M. Grulke, Antony Williams, Derya Biryol, Tao Hong & Kristin K. Isaacs

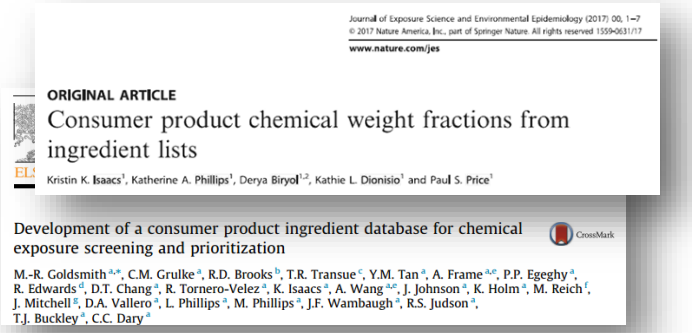
Scientific Data **5**, Article number: 180125 (2018) | Cite this article

30k Accesses | **92** Citations | **21** Altmetric | Metrics

- ORD effort to organize and disseminate information about how **chemicals are used in commerce**, including consumer products, to inform exposure estimation
  - Incorporates previous ORD efforts that collected use information
  - Entire database is currently available for download (set of .xslx files)
  - Summary information from database is available from ORD's **CompTox Chemicals Dashboard** (CCD)
- CCTE is collecting, curating, and storing large amounts of publicly available chemical use information to support the expansion of CPDat
  - **450k+** documents from internet sites, government or industry reports, manufacturer data sheets, and more
  - **3.4 million** chemical records
  - Qualitative and quantitative information
  - Efforts utilize custom internal document management, QA application, and data curation: **Factotum**

CPDat Improvements

CPDat versions 1 – 3



ORIGINAL ARTICLE

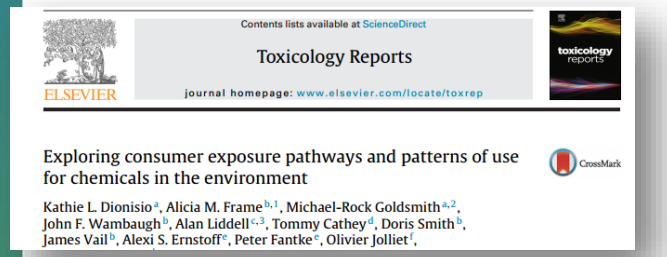
Consumer product chemical weight fractions from ingredient lists

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

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

M.-R. Goldsmith, C.M. Grulke, R.D. Brooks, T.R. Transue, Y.M. Tan, A. Frame, P.P. Egeghy, R. Edwards, D.T. Chang, R. Tornero-Velez, K. Isaacs, A. Wang, J. Johnson, K. Holm, M. Reich, J. Mitchell, D.A. Vallero, L. Phillips, M. Phillips, J.F. Wambaugh, R.S. Judson, T.J. Buckley, C.C. Dary

Ingredient weight fraction data from previous EPA data collection efforts



Contents lists available at ScienceDirect

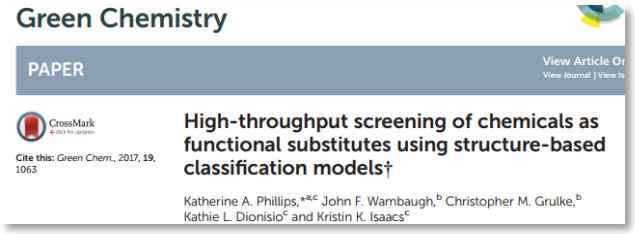
Toxicology Reports

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

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

Kathie L. Dionisio, Alicia M. Frame, Michael-Rock Goldsmith, John F. Wambaugh, Alan Liddell, Tommy Cathey, Doris Smith, James Vail, Alexi S. Ernstoff, Peter Fantke, Olivier Jolliet

General use developed around consumer exposure



Green Chemistry

PAPER

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

Katherine A. Phillips, John F. Wambaugh, Christopher M. Grulke, Kathie L. Dionisio and Kristin K. Isaacs

Functional use terminology and models focused on consumer/personal care products

CPDat version 4

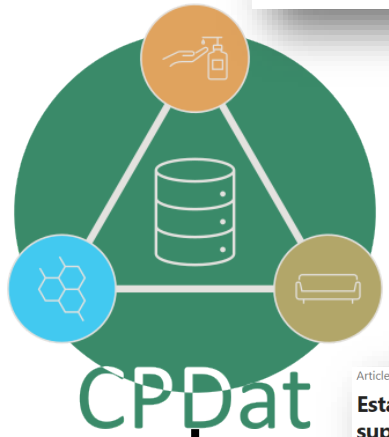
Review Article | Published: 26 November 2022

The chemical landscape of high-throughput new approach methodologies for exposure

Kristin K. Isaacs, Peter Egeghy, Kathie L. Dionisio, Katherine A. Phillips, Angelika Zidek, Caroline Ring, Jon R. Sobus, Elin M. Ulrich, Barbara A. Wetmore, Antony J. Williams & John F. Wambaugh

Journal of Exposure Science & Environmental Epidemiology 32, 820–832 (2022) | Cite this article

Inclusion of industrial products and processes and consumer articles in addition to more consumer formulations



CPDat

Article | Published: 11 November 2019

Establishing a system of consumer product use categories to support rapid modeling of human exposure

Kristin K. Isaacs, Kathie Dionisio, Katherine Phillips, Charles Bevington, Peter Egeghy & Paul S. Price

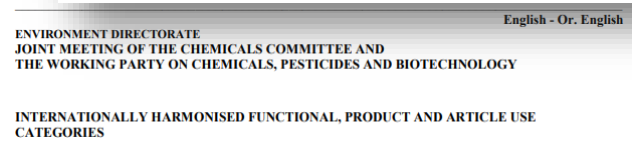
Journal of Exposure Science & Environmental Epidemiology 30, 171–183 (2020) | Cite this article

Article | Publis

Environmental mixtures and breast cancer: identifying co-exposure patterns between understudied vs breast cancer-associated chemicals using chemical inventory informatics

Lauren E. Koval, Kathie L. Dionisio, Katie Paul Friedman, Kristin K. Isaacs & Julia E. Rager

Journal of Exposure Science & Environmental Epidemiology 32, 794–807 (2022) | Cite this article



English - Or. English

ENVIRONMENT DIRECTORATE
JOINT MEETING OF THE CHEMICALS COMMITTEE AND
THE WORKING PARTY ON CHEMICALS, PESTICIDES AND BIOTECHNOLOGY

INTERNATIONALLY HARMONISED FUNCTIONAL, PRODUCT AND ARTICLE USE CATEGORIES

Standardized taxonomy of:

- Product Use Categories (PUCs)
- Function Categories (FCs)
- List Presence Keywords

Chemical Use Definitions

- **Commercial Sector Use**:

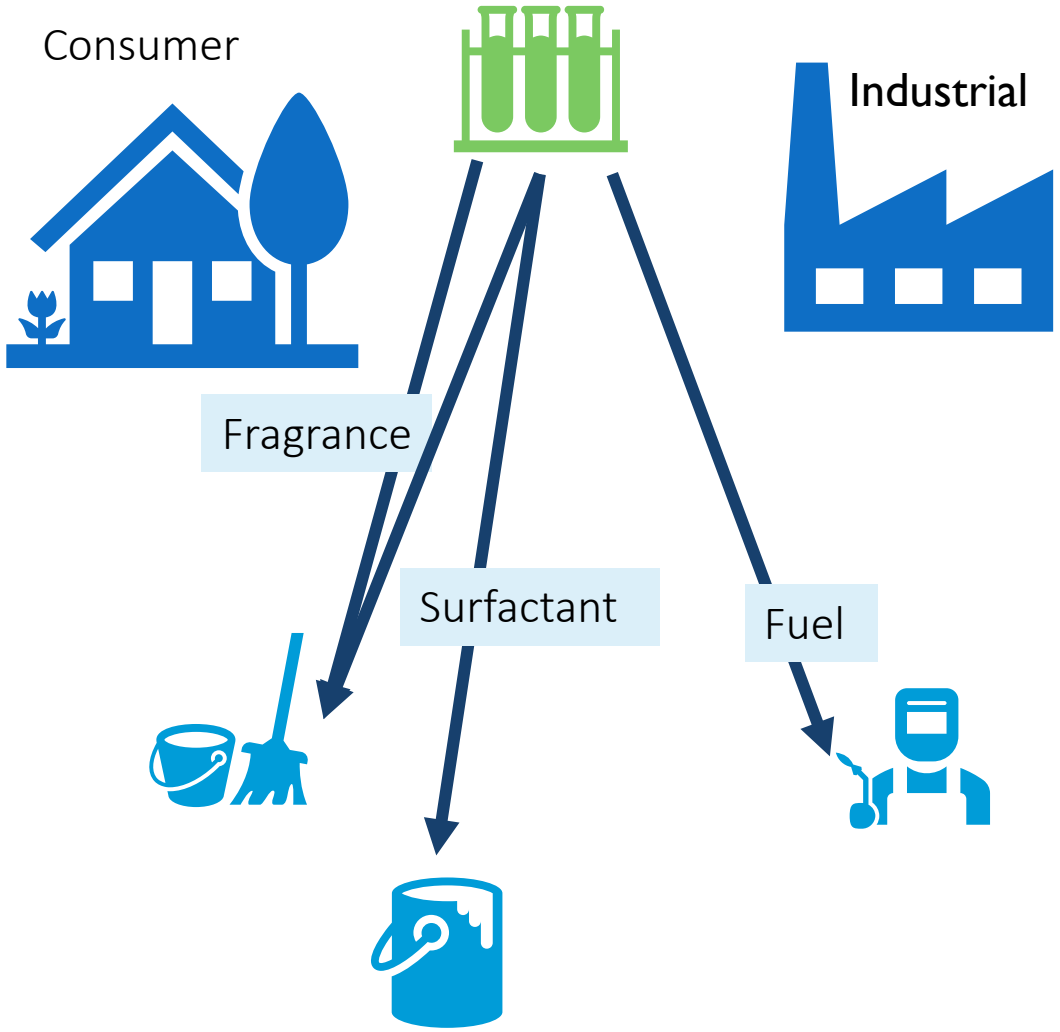
  Which groups use a chemical (i.e., industrial process *versus* consumer product)

- **End-use:**

  The specific commercial sector products or processes in which a chemical is used

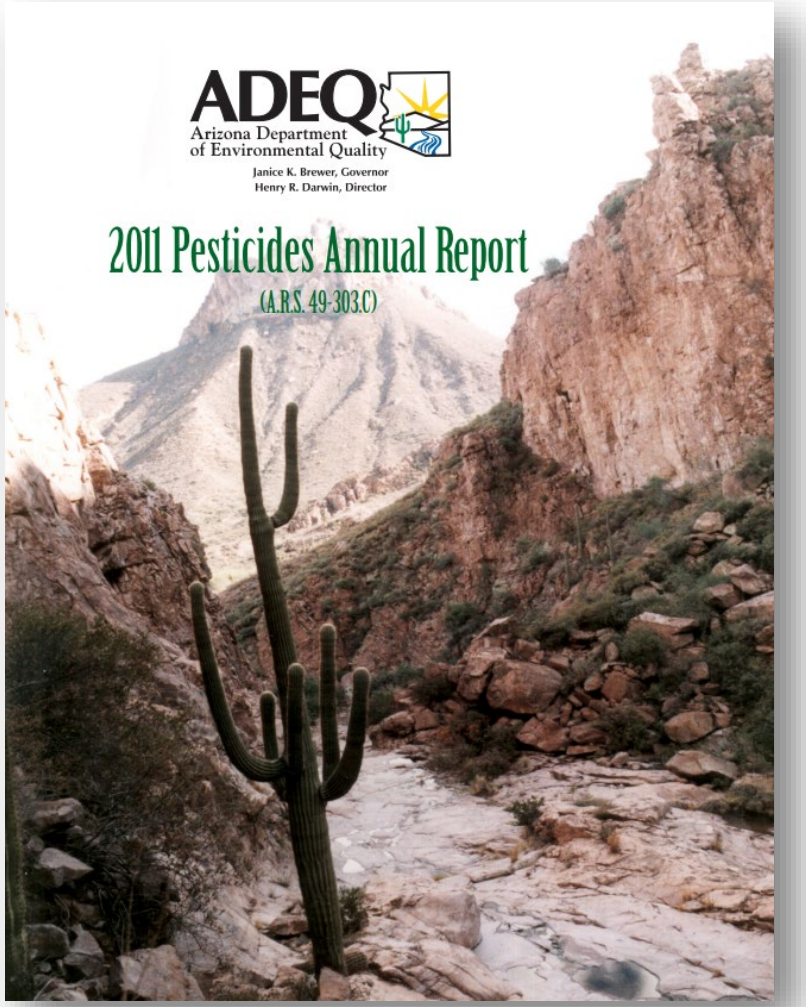
- **Functional Use**:

  Roles a chemical can serve due to its structure and properties



Chemical Use Types in CPDat

- Commercial Sector Use
  - Lists of chemicals used in different commercial or industrial sectors
  - Organized by **Chemical List Presence Keywords**



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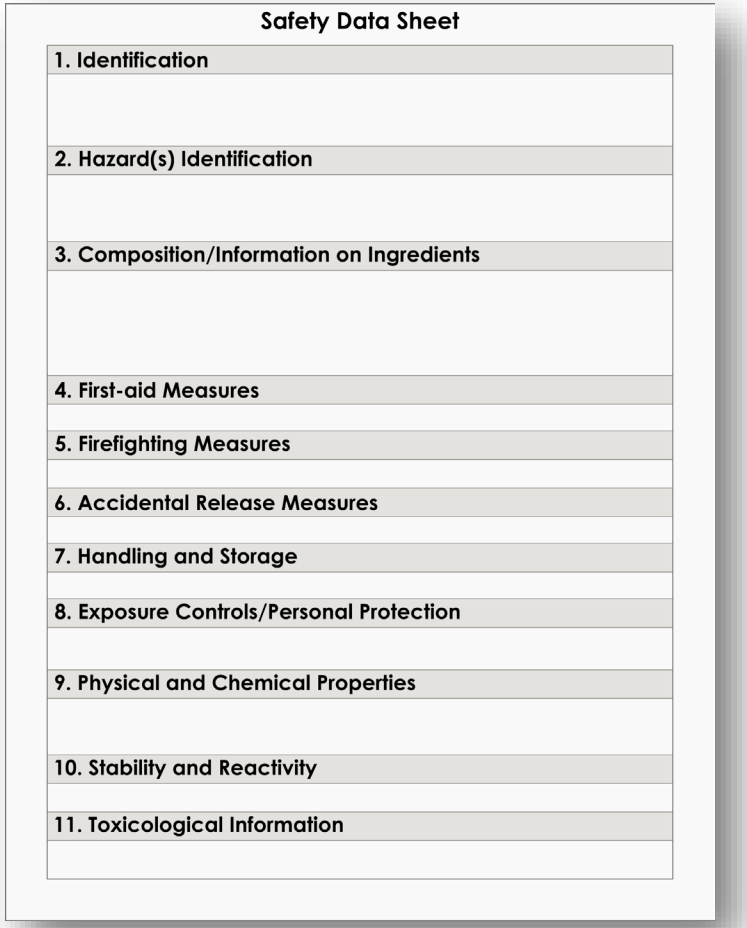

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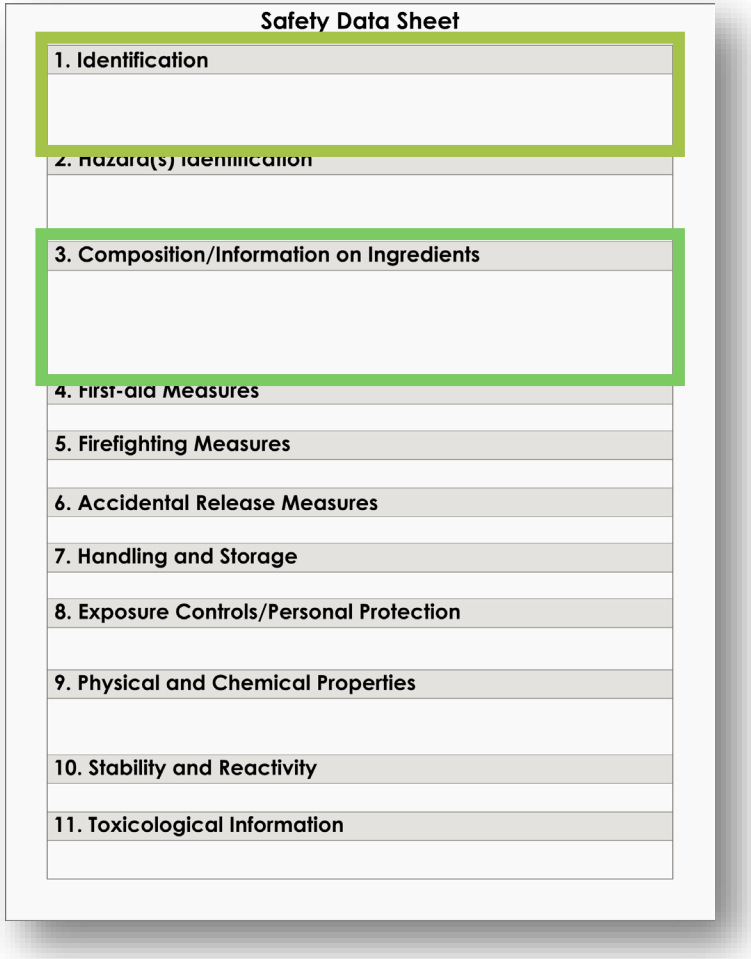

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- Functional use
  - Role the chemical plays in different consumer products or industrial processes
  - Organized by OECD's **Function Categories (FCs)**

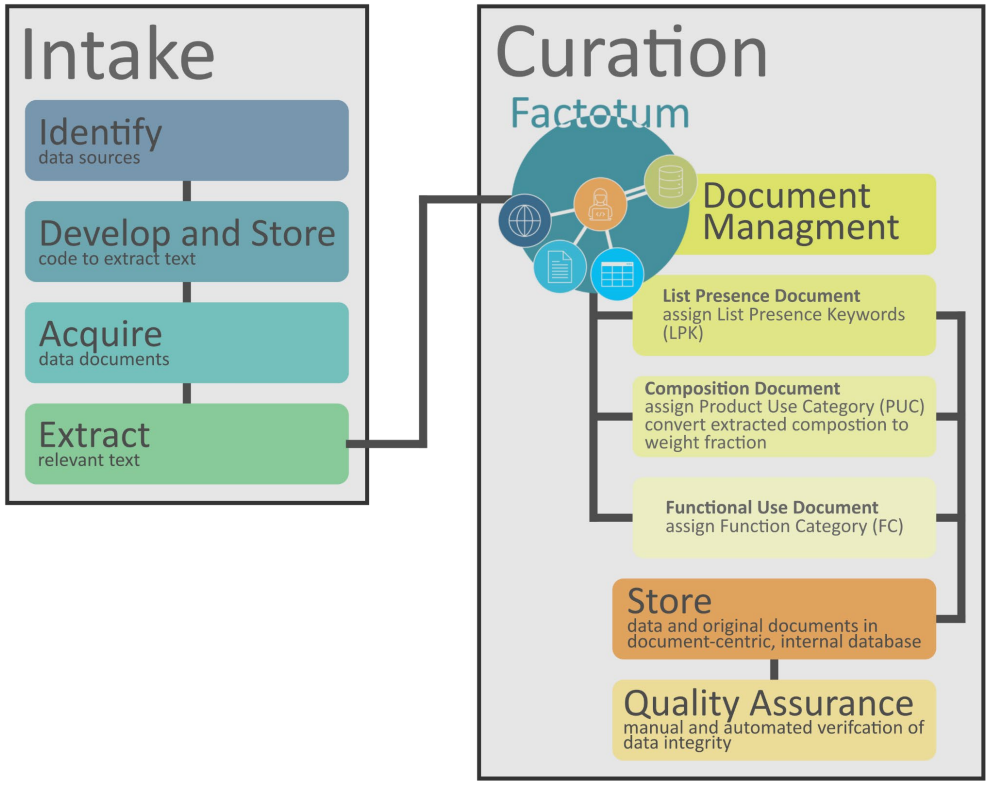
Ingredients		
ingredient	**function**	**CAS #**
water	diluent + solvent	7732-18-5
sodium lauryl sulfate	surfactant (cleaning agent)	68585-47-7
lauramine oxide	surfactant (cleaning agent)	1643-20-5
decyl glucoside	surfactant (cleaning agent)	68515-73-1
lauryl glucoside	surfactant (cleaning agent)	110615-47-9
agrumex	fragrance	88-41-5
benzyl acetate	fragrance	140-11-4
cyclamen aldehyde	fragrance	103-95-7
dihydro myrcenol	fragrance	18479-58-8
dipropylene glycol	fragrance	25265-71-8
hedione	fragrance	24851-98-7
hexyl cinnamic aldehyde	fragrance†	101-86-0
iso e super	fragrance	54464-57-2
linalool	fragrance†	78-70-6
linalyl acetate	fragrance	115-95-7
phenyl ethyl alcohol	fragrance	60-12-8
ethanol	solvent	64-17-5
glycerin	moisturizer	56-81-5
sodium chloride	thickener	7647-14-5
citric acid	pH adjuster	77-92-9
methylchloroisothiazolinone	preservative	26172-55-4
methylisothiazolinone	preservative	2682-20-4
colorant	colorant	CBI

The CPDat Pipeline

We only intake *publicly available* data sources.

Handa et al., *in preparation*

The CPDat Pipeline



Factotum is an ***internal EPA tool*** and not accessible to the public.

Handa et al., *in preparation*

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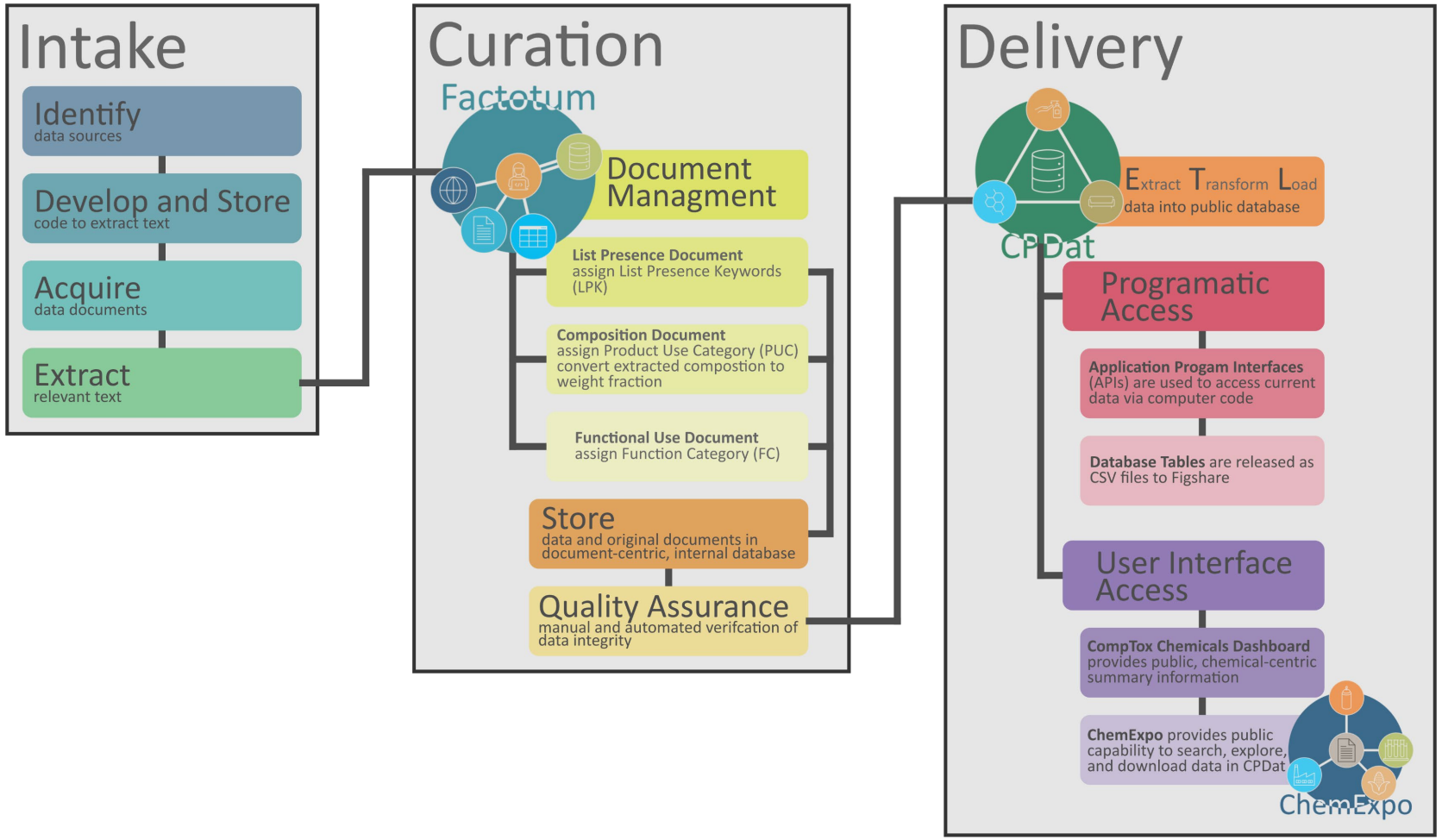


CPDat is a ***versioned, public database*** with the latest Factotum curations.

ChemExpo is a ***public web tool*** to interactively search and download CPDat data.

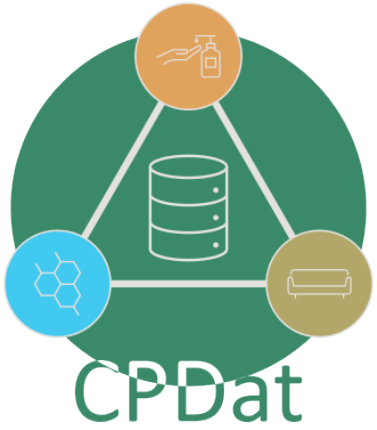
Handa et al., *in preparation*

Bringing it All Together

Private Web Tool

Factotum helps EPA curate data…

Public Database



…that goes into CPDat…

Public Web Tool

…that is then searchable by ChemExpo.

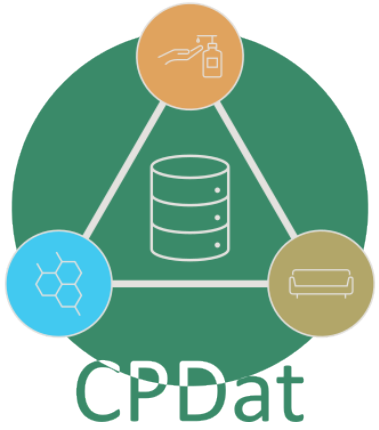
Bringing it All Together

Private Web Tool

Factotum helps EPA curate data…

If you are internal to EPA, then talk to Sakshi, Kristin, or Katherine about how to access and use Factotum!

Public Database



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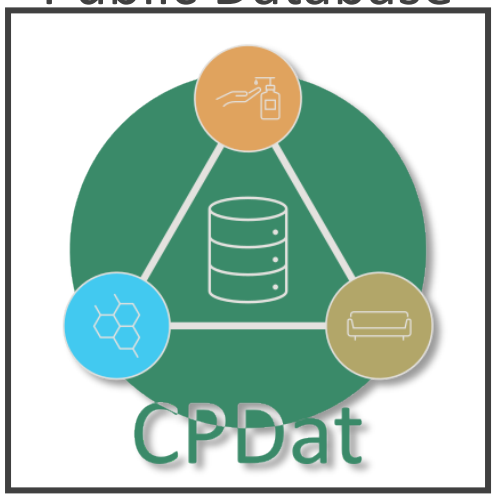

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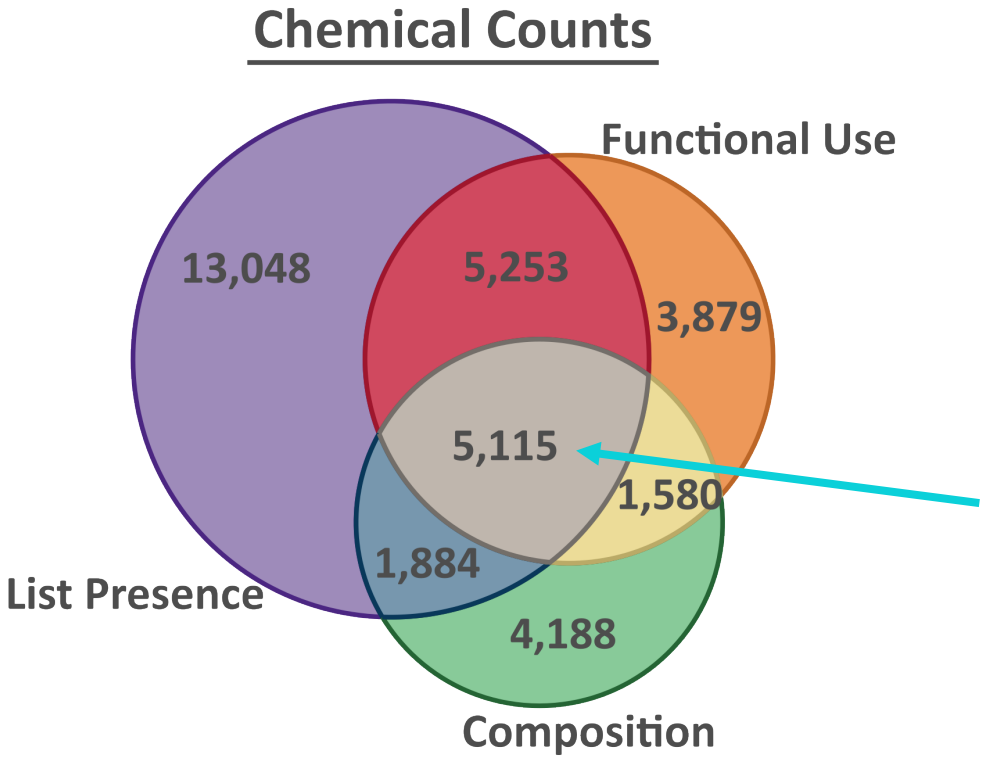
CPDat by the Numbers



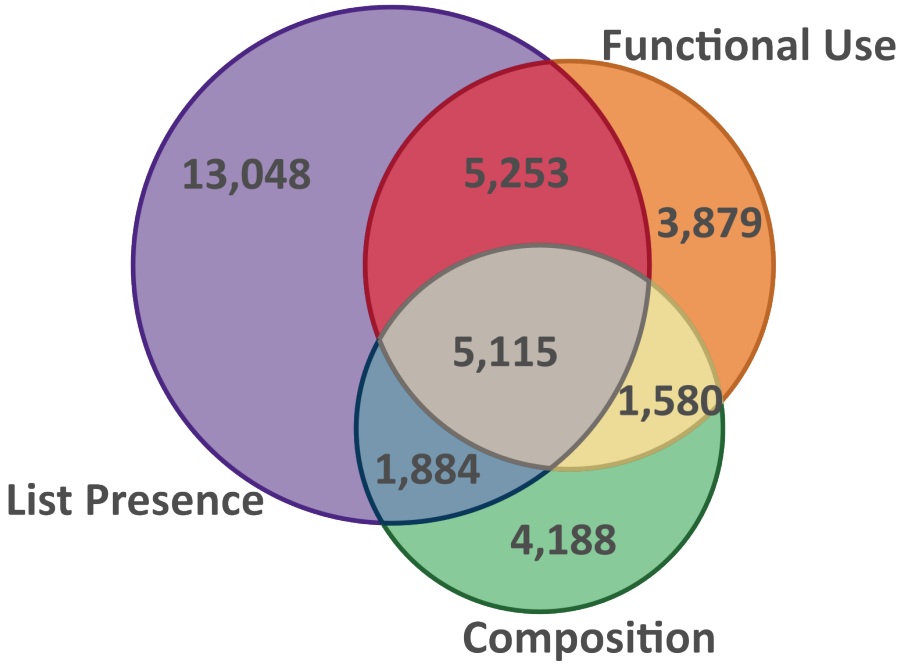
Unique Chemical Substances found across list presence, composition, and functional use type documents.

Note: this doesn't mean there is one document that has all types of information for a chemical.

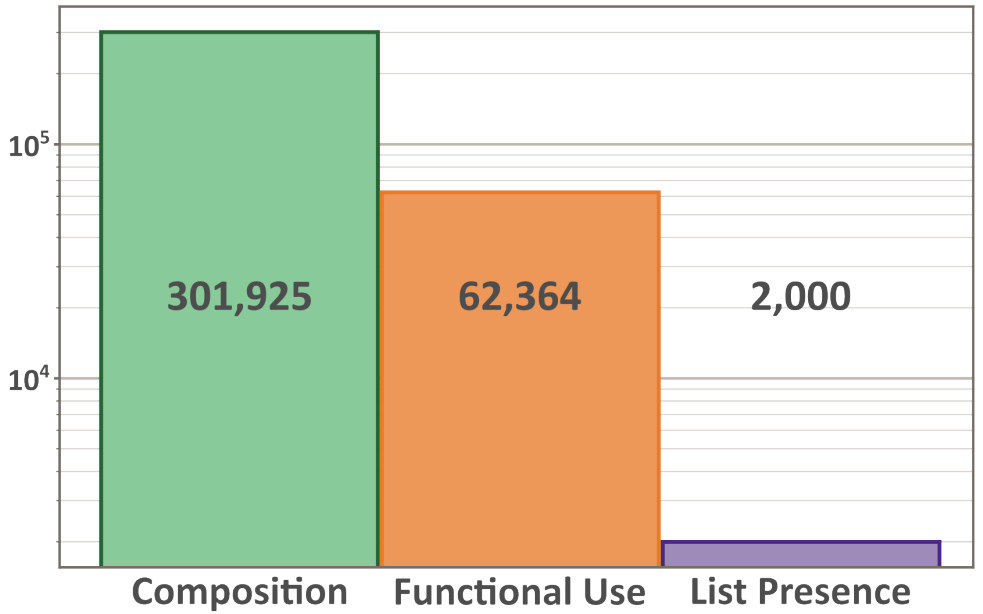
Handa et al., *in preparation*

CPDat by the Numbers

Chemical Counts



Document Counts



Handa et al., *in preparation*

Bringing it All Together

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Factotum helps EPA curate data…

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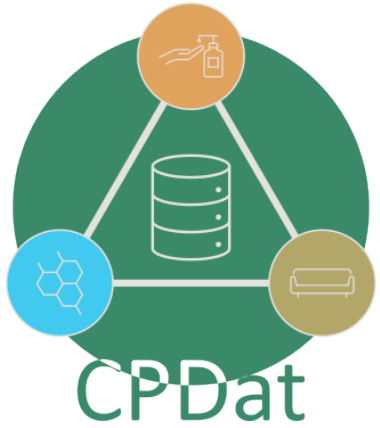

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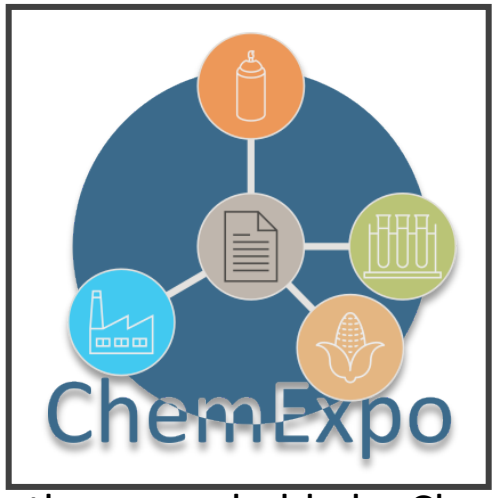
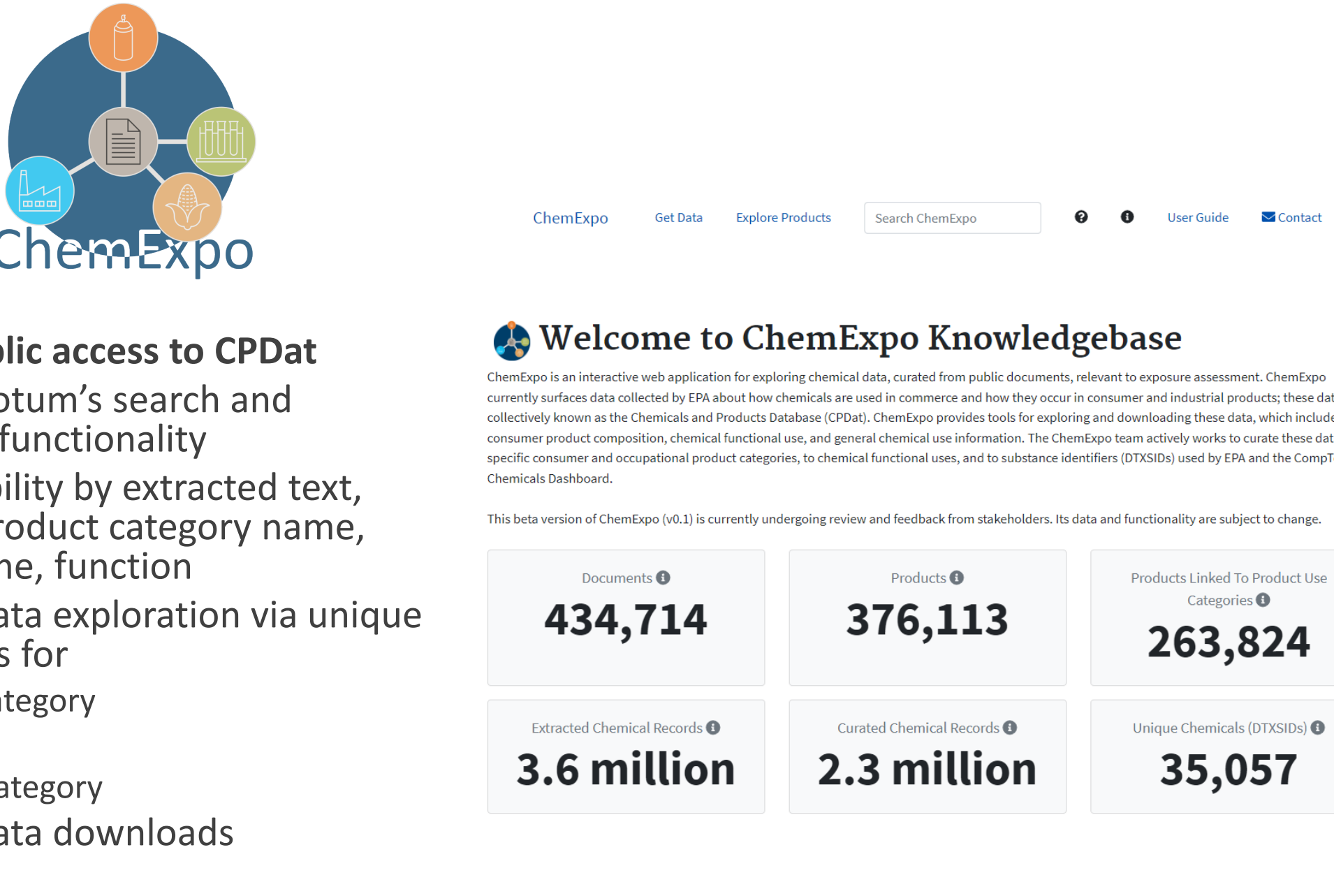


…that is then searchable by ChemExpo.

ChemExpo is currently in its beta release. This means that it is undergoing review and feedback from stakeholders. Its data and functionality are subject to change.

ChemExpo

- **Provides public access to CPDat**
- Built on Factotum's search and visualization functionality
- Search capability by extracted text, product or product category name, chemical name, function
- Interactive data exploration via unique landing pages for
  - product category
  - chemical
  - function category
- Interactive data downloads



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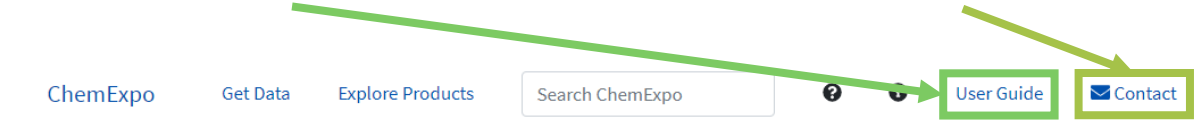
Access our extensive User Guide to learn about of all ChemExpo functionalities.

Contact us directly with questions, ideas, or other feedback.



Welcome to ChemExpo Knowledgebase

ChemExpo is an interactive web application for exploring chemical data, curated from public documents, relevant to exposure assessment. ChemExpo currently surfaces data collected by EPA about how chemicals are used in commerce and how they occur in consumer and industrial products; these data are collectively known as the Chemicals and Products Database (CPDat). ChemExpo provides tools for exploring and downloading these data, which include consumer product composition, chemical functional use, and general chemical use information. The ChemExpo team actively works to curate these data to specific consumer and occupational product categories, to chemical functional uses, and to substance identifiers (DTXSIDs) used by EPA and the CompTox Chemicals Dashboard.

This beta version of ChemExpo (v0.1) is currently undergoing review and feedback from stakeholders. Its data and functionality are subject to change.

Documents	Products	Products Linked To Product Use Categories
434,714	376,113	263,824

Extracted Chemical Records	Curated Chemical Records	Unique Chemicals (DTXSIDs)
3.6 million	2.3 million	35,057

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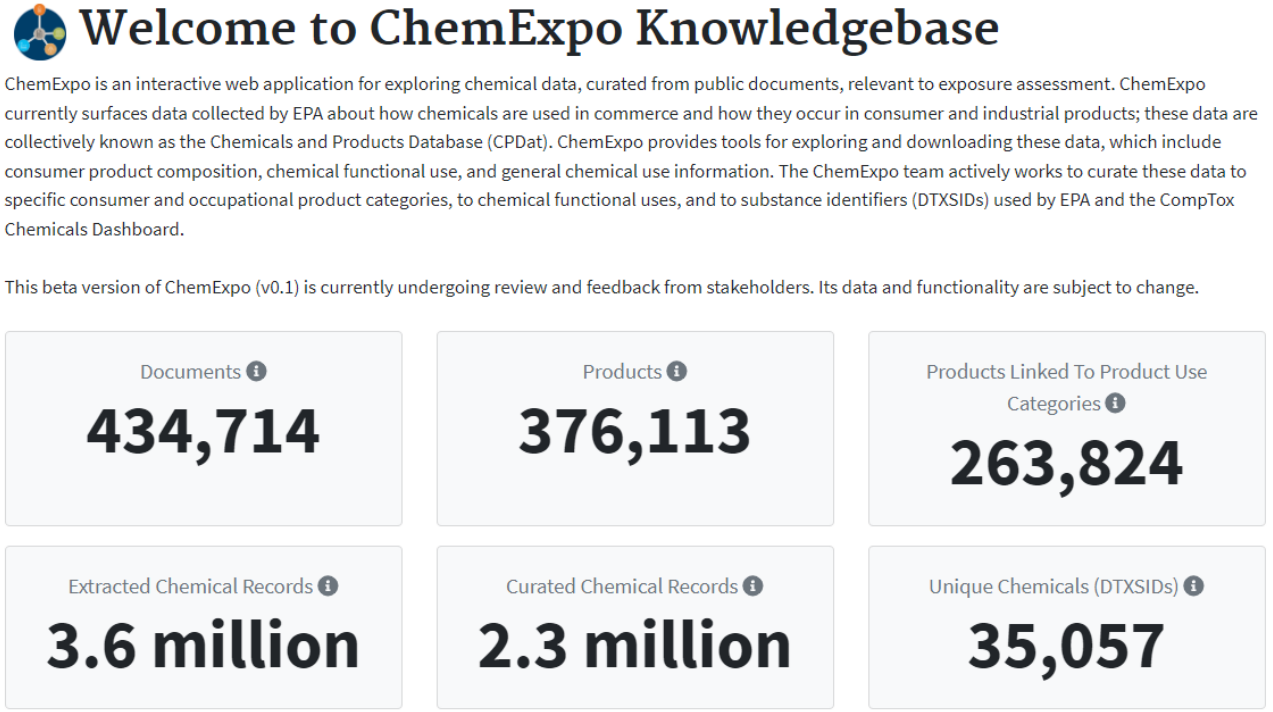
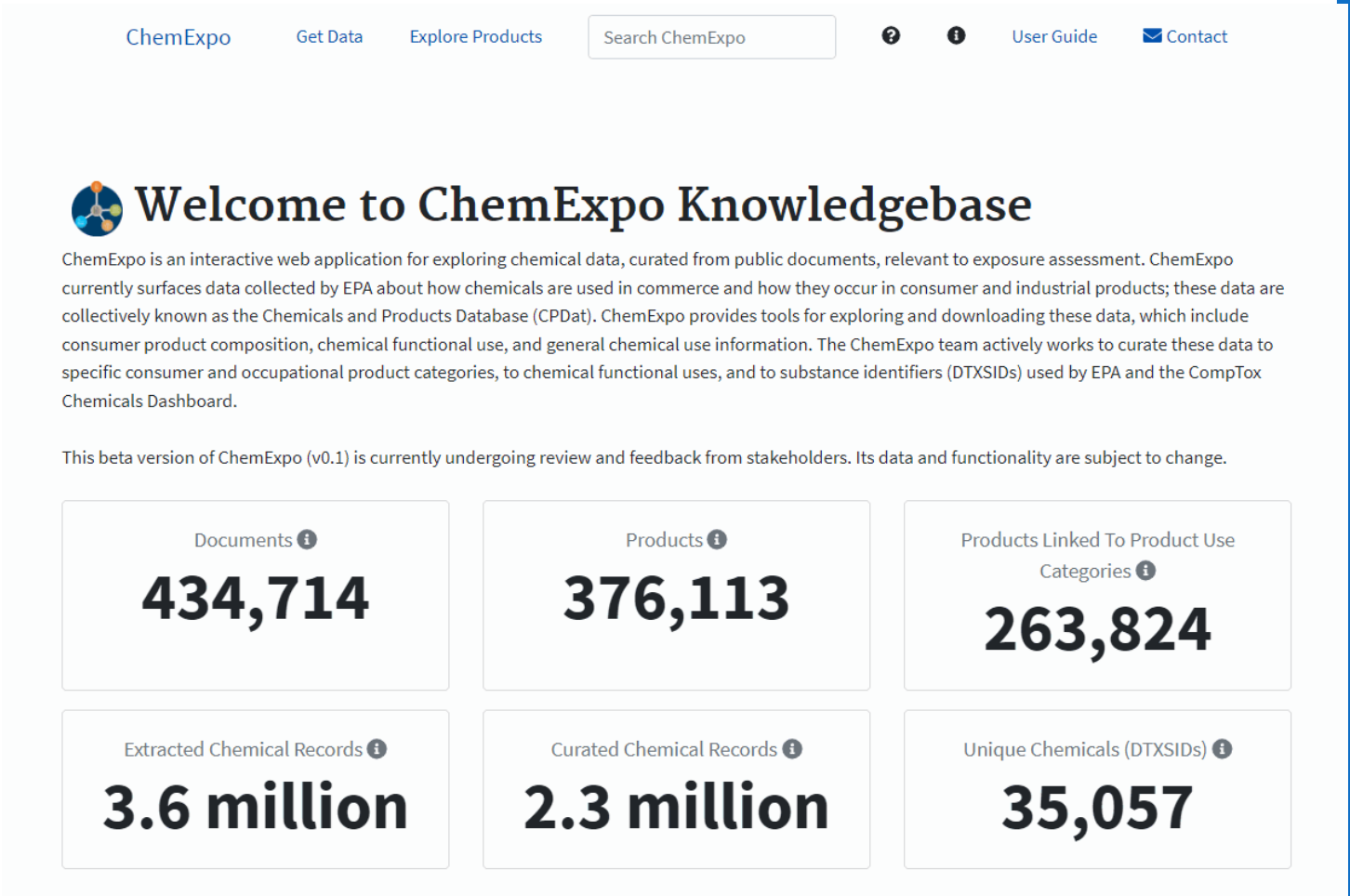
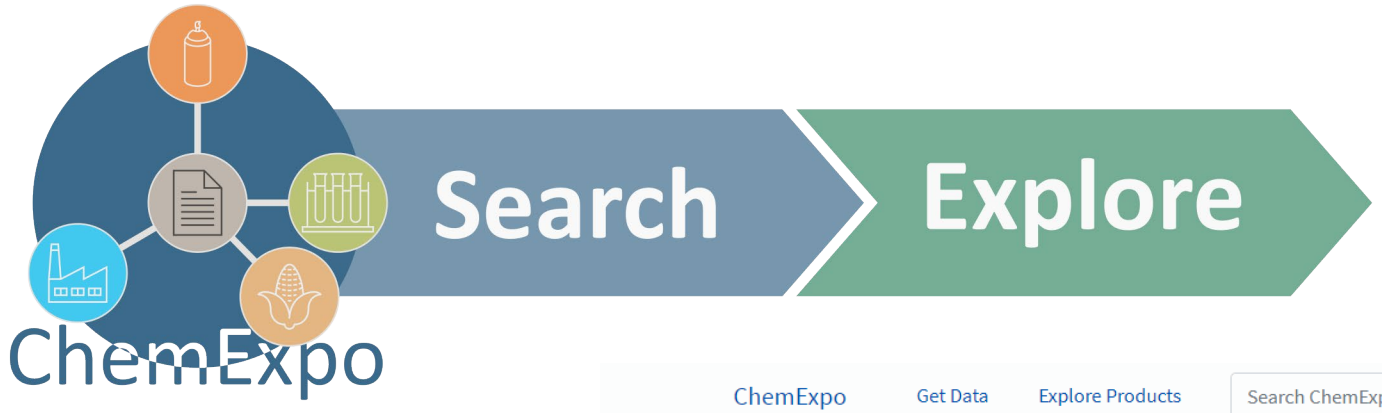


Searching in ChemExpo covers six information domains:

- Chemicals
- Document
- Products
- Product Use Categories
- Function Categories
- Chemical List Presence Keywords

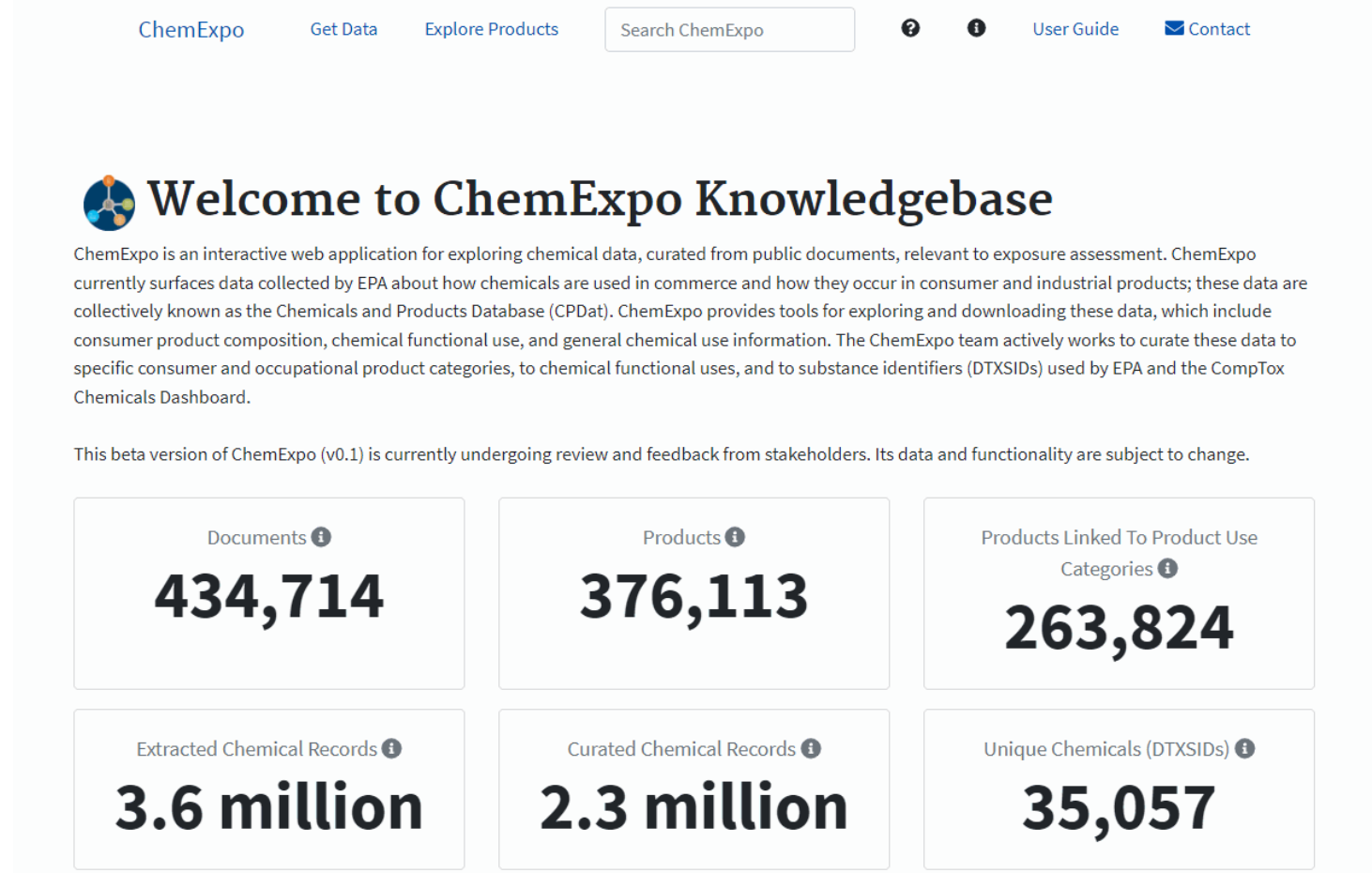
Make sure you're looking at results in the domain you are most interested in (you can always click back to look at others)





ChemExpo uses interactive bubble plots and filterable tables to allow users to explore CPDat data.

Tables from detail pages allow users to filter and explore different products, chemicals, etc.



ChemExpo

Search Explore Download

ChemExpo allows users to download specific tables they come across during their searching and exploration.

In addition, ChemExpo provides bulk download of all three controlled vocabularies and domains of data.

Assumed Attributes

No assumed attributes are associated with this PUC

Allowed Attributes

gel paste

Additional Statistics

Products	1062
Cumulative Products	1062
Documents	1062
Curated Chemicals	794

Products | Documents | Chemicals | **Functions**

Functions Associated with "Personal care - facial cleansing and moisturizing - face scrub"

Show 10 entries Search: Download All Functions Associated with PUC

Classification Method	Document	Chemical Name	CAS	Reported Function	Harmonized Function
Composition	AMOPE PEDI PERFECT EXFOLIATING BRUSH REFILLS	Gadget		Gadget	
Composition	simple facial scrub clear skin oil balancing	Water	7732-18-5	solvent	Solvent
Composition	simple facial scrub clear skin oil	1,2-Propylene glycol	57-55-6	Skin Conditioning	Softener and conditioner

ChemExpo Demo

ChemExpo Homepage

ChemExpo | Get Data | Explore Products | Benzyl Butyl Phthalate | User Guide | Contact

Welcome to ChemExpo Knowledgebase

ChemExpo is an interactive web application for exploring chemical data, curated from public documents, relevant to exposure assessment. ChemExpo currently surfaces data collected by EPA about how chemicals are used in commerce and how they occur in consumer and industrial products; these data are collectively known as the Chemicals and Products Database (CPDat). ChemExpo provides tools for exploring and downloading these data, which include consumer product composition, chemical functional use, and general chemical use information. The ChemExpo team actively works to curate these data to specific consumer and occupational product categories, to chemical functional uses, and to substance identifiers (DTXSIDs) used by EPA and the CompTox Chemicals Dashboard.

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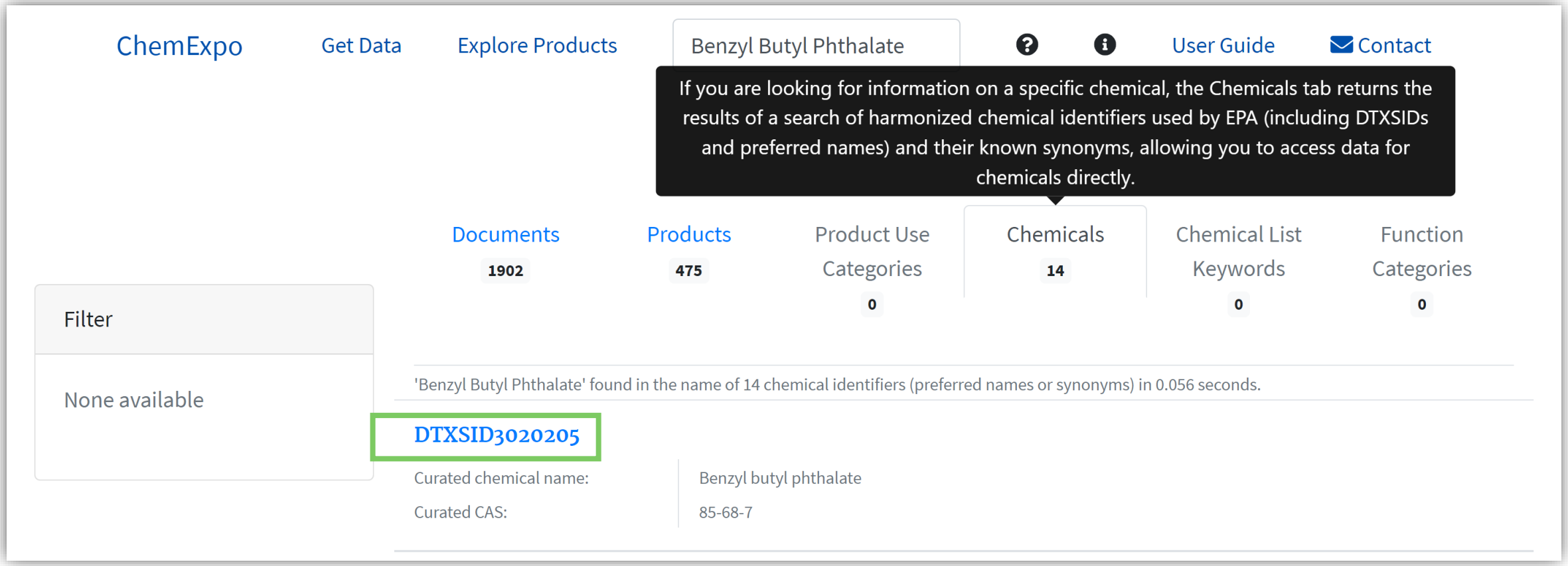
Documents	Products	Products Linked To Product Use Categories
434,714	376,113	263,824

Keyword Search



Chemical Detail Page: Benzyl Butyl Phthalate

Benzyl Butyl Phthalate

DTXSID3020205

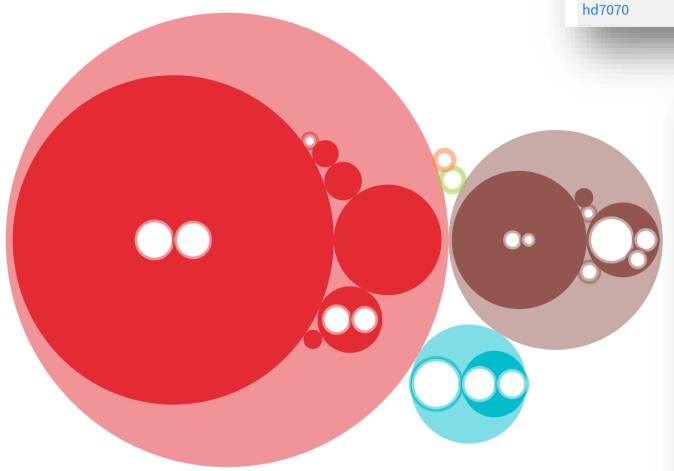
85-68-7

Explore products containing this chemical. Use the filter buttons to filter the tables below to certain Product Use Categories. Click the info
each PUC to access its detailed chemical and product data.
Note: the high-level PUCs link to products that can't be further categorized; drill down to access products with refined PUC categorizations

Formulation PUCs

General Category - Product Family - Product Type

- Arts and crafts/office supplies 10
- Cleaning products and household care 2
- Home maintenance 402
- Personal care 22
- Vehicle 267



Products | Documents | Function

Products Containing "Benzyl butyl phthalate"

Show All Products

Show 10 entries Search:

Download Products and Weight Fractions

Product	Manufacturer	Brand	Document	PUC	PUC Kind	Classification Method
b9014l lucite acrylic lacquer	EI DUPONT/AUTOMOTIVE PRODS DEPT		B9014L LUCITE ACRYLIC LACQUER	Raw materials - paints and primers	Occupation	Manual
acrylic lacquer touch-up paint_ ford-usal81	FORD MOTOR CO		ACRYLIC LACQUER TOUCH-UP PAINT, FORD-USAL81	Vehicle - auto body work - auto paint	Formulation	Manual
hysol hd7070_ hd7070	DEXTER CORP		HYSOL HD7070, HD7070	Specialty occupational products - aviation - aircraft coatings	Occupation	Manual

Products | Documents | Function

Functions Associated with "Benzyl butyl phthalate"

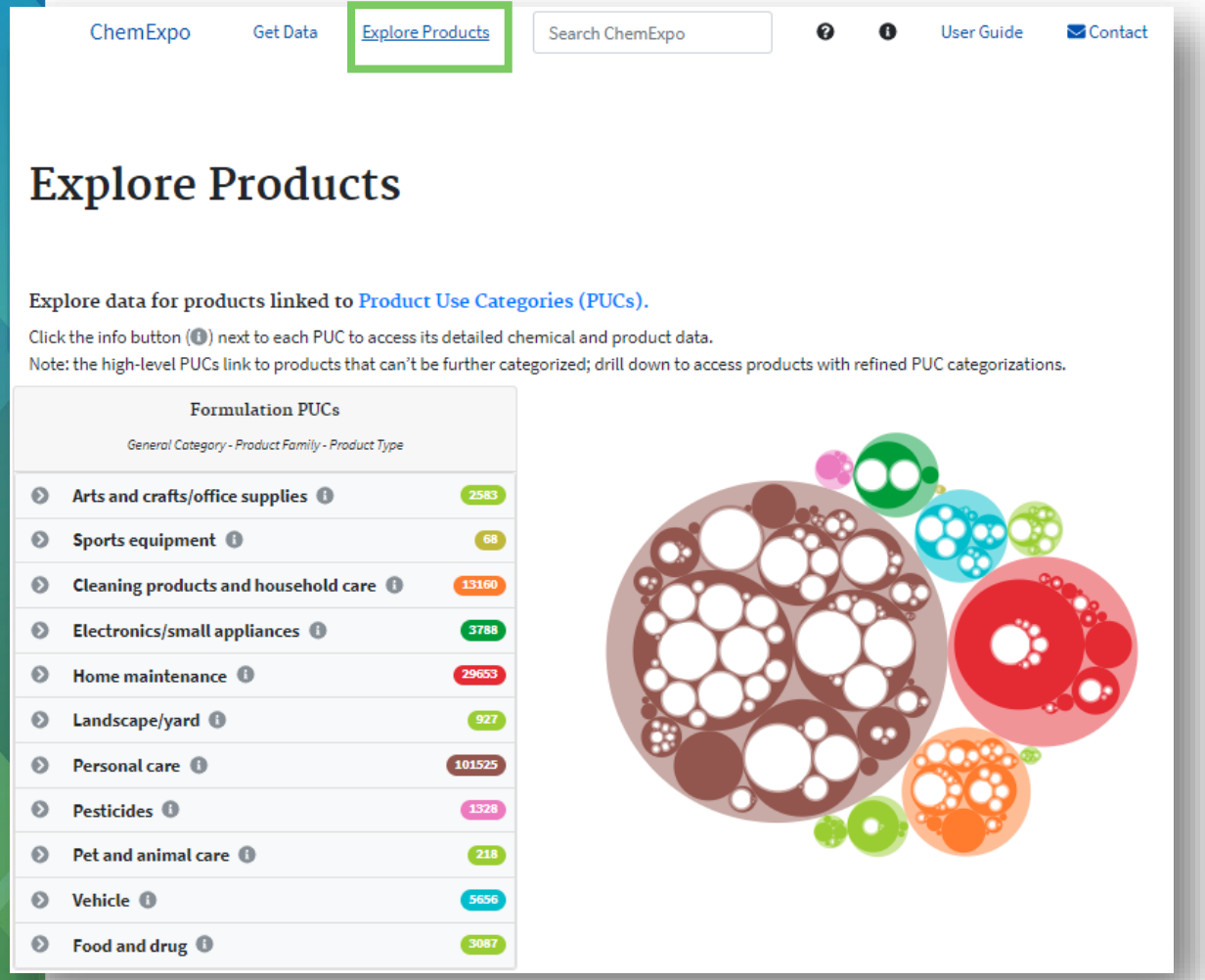
Show All Functions

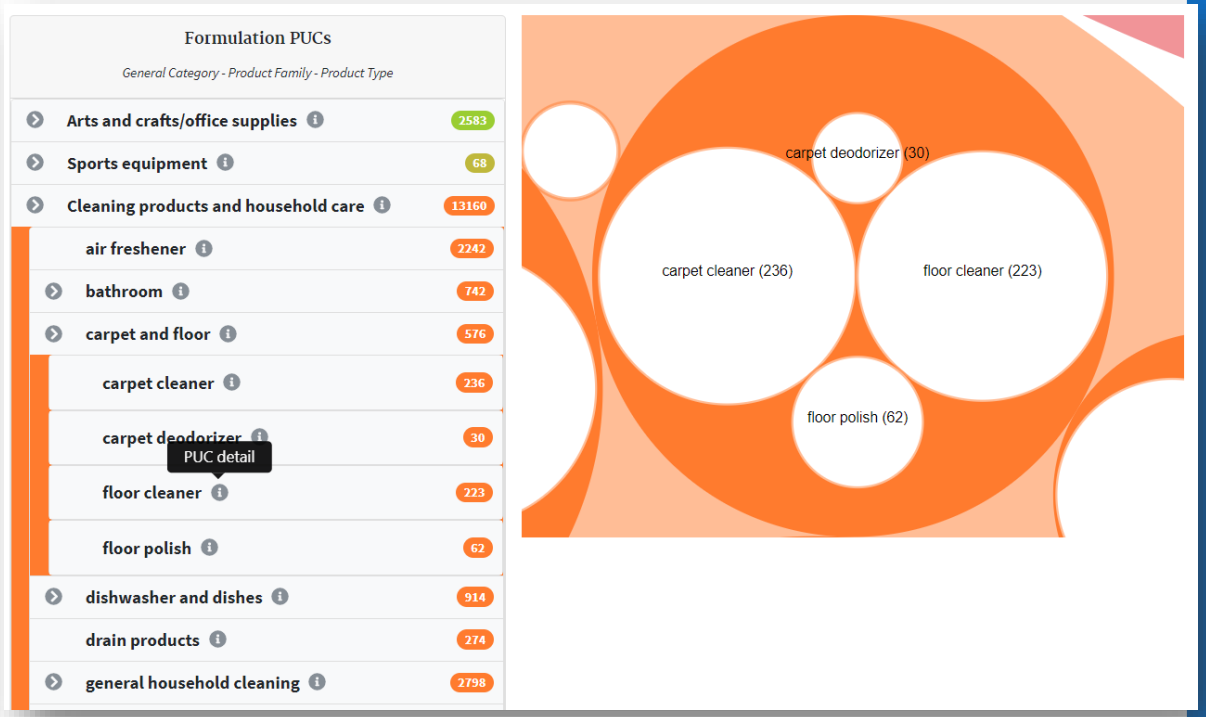
Show 10 entries Search:

Download Functions

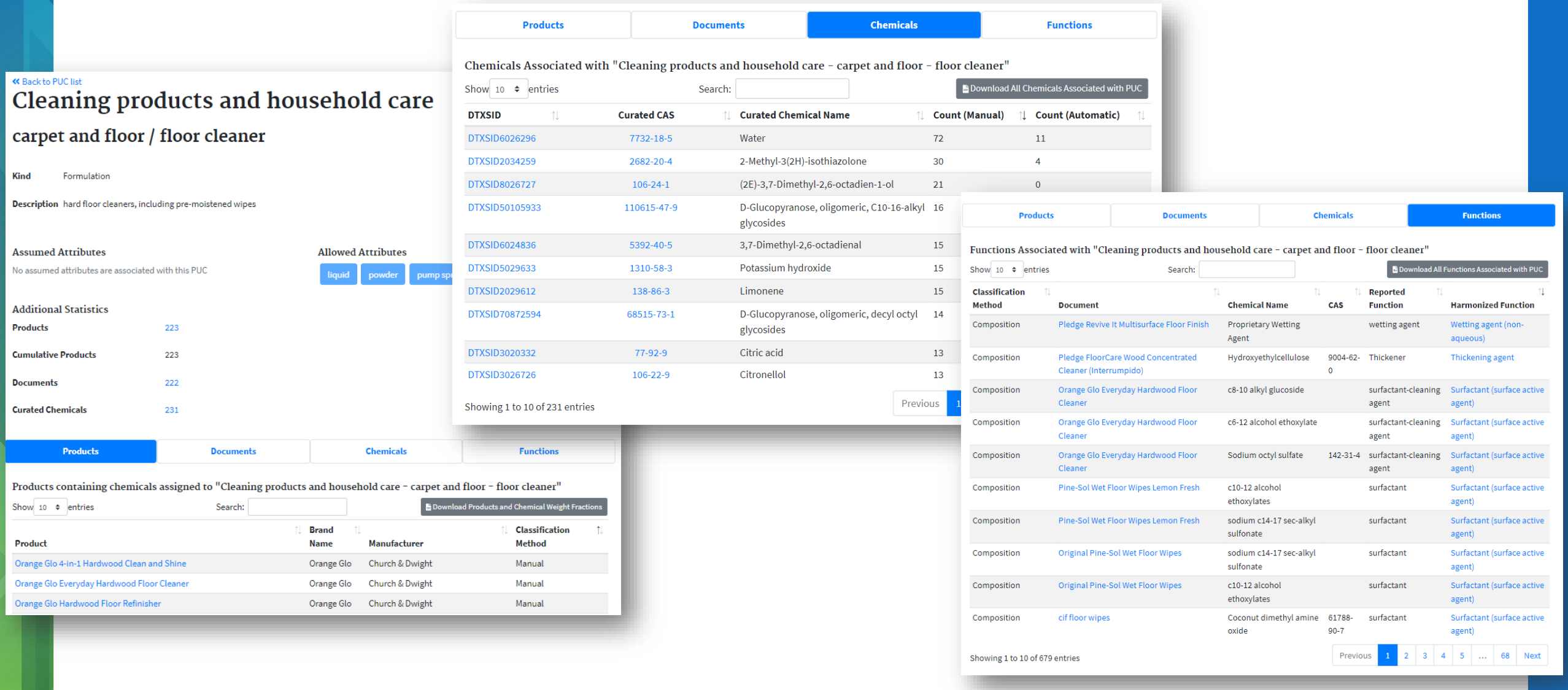
Data Type	Document	Reported Function	Harmonized Function
Function	BBP DLC -A	processing aids	Processing aids not otherwise specified
Composition	air-bloc 33mr	plasticizer	Plasticizer
Composition	dual purpose gray	plastisizer	Plasticizer
Composition	henry 289 white roofing sealant	plasticizer	Plasticizer
Composition	henry air-bloc 32mr	plasticizer	Plasticizer
Composition	stonclad g2-ht4 system	plasticizer	Plasticizer
Composition	stonclad ur with at5	plasticizer	Plasticizer
Composition	stonclad ur-ht4 system	plasticizer	Plasticizer
Composition	vinyl composition tile sample	plasticizer	Plasticizer
Function	butyl benzyl phthalate	plasticiser	Plasticizer

Explore Products

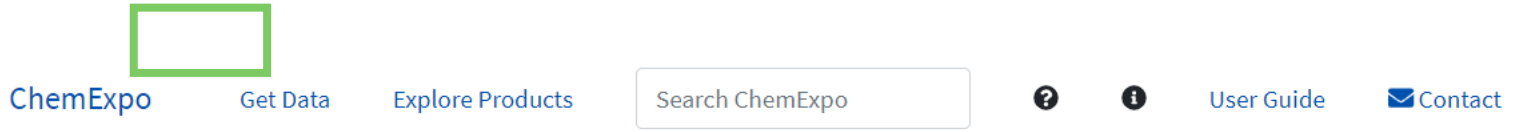


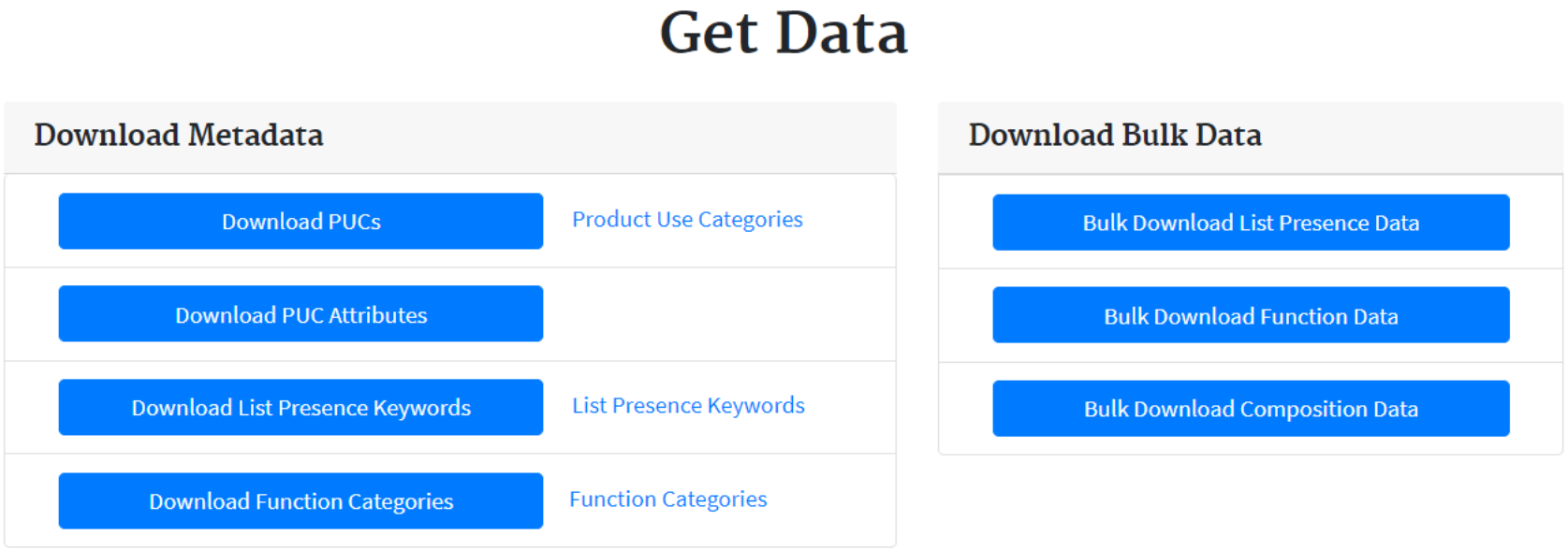


PUC Detail Page: Floor Cleaner



Download Data





Explore Function Categories

Function Categories

Functional Use Categories are harmonized identifiers describing the function a specific chemical serves (for example: fragrance, cleaning agent, filler, etc.). Functional uses reported by source documents are curated to harmonized function categories, In most cases, these are internationally recognized categories and definitions developed by the Organization for Economic Co-operation and Development (OECD). These standardized functional uses contain explicit definitions and exclusions, to reduce ambiguity in category assignment. New function categories will be added as needed to accommodate novel uses. These are indicated as internal to EPA through the use of (EPA) within the category name. Function Categories are harmonized identifiers describing the function a specific chemical serves (for example: fragrance, cleaning agent, filler, etc.). Chemical functions reported by source documents are curated to harmonized function categories, In most cases, these are internationally recognized categories and definitions developed by the Organization for Economic Co-operation and Development (OECD). These standardized functions contain explicit definitions and exclusions, to reduce ambiguity in category assignment. New function categories are added as needed to accommodate novel uses. These are indicated as internal to EPA through the use of (EPA) within the category name. Data on the functions of chemicals in consumer products were originally developed and released as ORD's Functional Use (FuSE) database and are now maintained within CPDat. These data form the basis for ORD's Quantitative Structure Use Relationship (QSUR) models (Phillips et al. (2016)). See User Guide Section 'Explore Chemical Functions' for more information.

Search...

Reset Filters

Function Category	Description	Product ...	Doc...	View Detail
Abrasive	Chemical substance used to abrade, smooth, or polish an object. Used to smooth, scour, scrub, clean, wear down, or polish surfaces by rubbing against the surface and removing imperfections from a surface. May be used in processes such as sputter etching and physical dry etching. Also referred to as a grinding agent; usually in the form of fine powders of hard substances; e.g., sandstones; pumice; quartz; silicates; aluminium oxides; and glass. See closely related: etching agent.	106	567	
Absorbent	Chemical substance used to retain other substances by assimilation. Also referred to as an antisiccative. See closely related: adsorbent.	85	316	
Adhesion/cohesion promoter	Chemical substance, either inorganic or organic, natural or synthetic, used to join opposite surfaces to each other; to promote bonding between other substances; to promote adhesion of surfaces; or to fasten other materials together. Generally applied from a solvent solution and allowed to dry on the two facing surfaces. Also referred to as glue; paste; coupling agent; gum; adhesive cement; bonding agent; inner coating; and anchor coating.	302	1970	
Adsorbent	Chemical substance used to retain other substances by accumulation on their surface; Exhibits a large surface area which can attract dissolved or finely dispersed substances from another medium. See closely related: absorbent; dehydrating agent.	13	13	

flame retardant

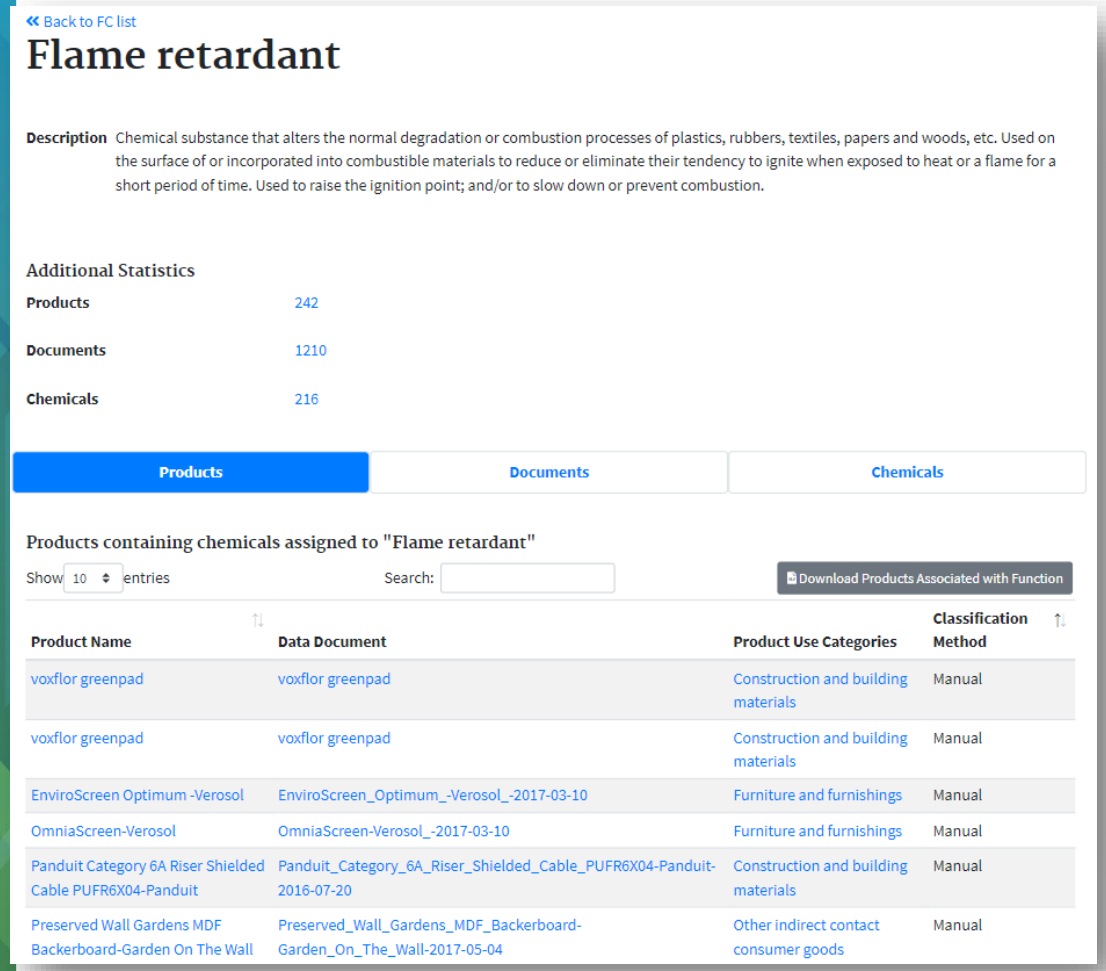
Reset Filters

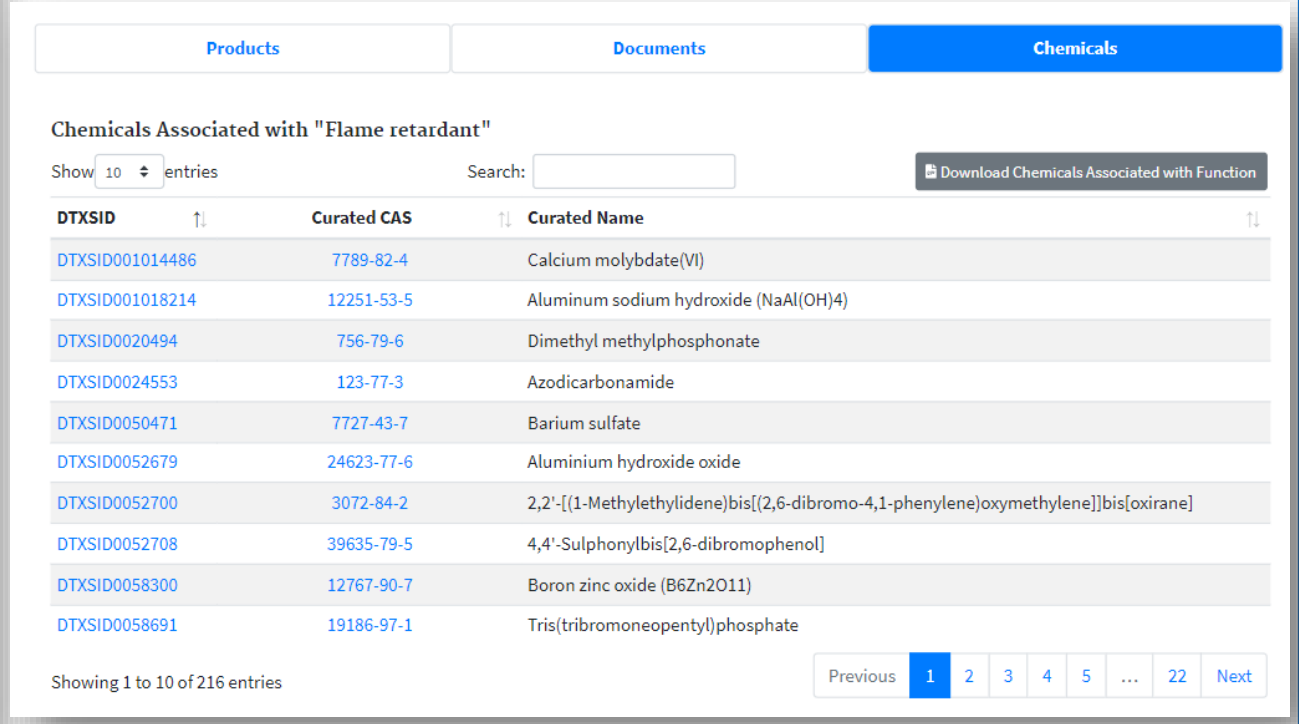
Function Category	Description	Product Count	Document Count	View Detail
Flame retardant	Chemical substance that alters the normal degradation or combustion processes of plastics, rubbers, textiles, papers and woods, etc. Used on the surface of or incorporated into combustible materials to reduce or eliminate their tendency to ignite when exposed to heat or a flame for a short period of time. Used to raise the ignition point; and/or to slow down or prevent combustion.	242	1210	

1 to 1 of 1 Page 1 of 1

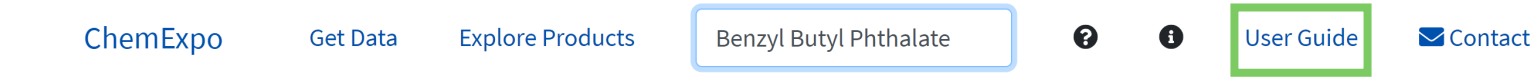
Page Size: 50

Function Detail Page: Flame Retardant





ChemExpo User Guide



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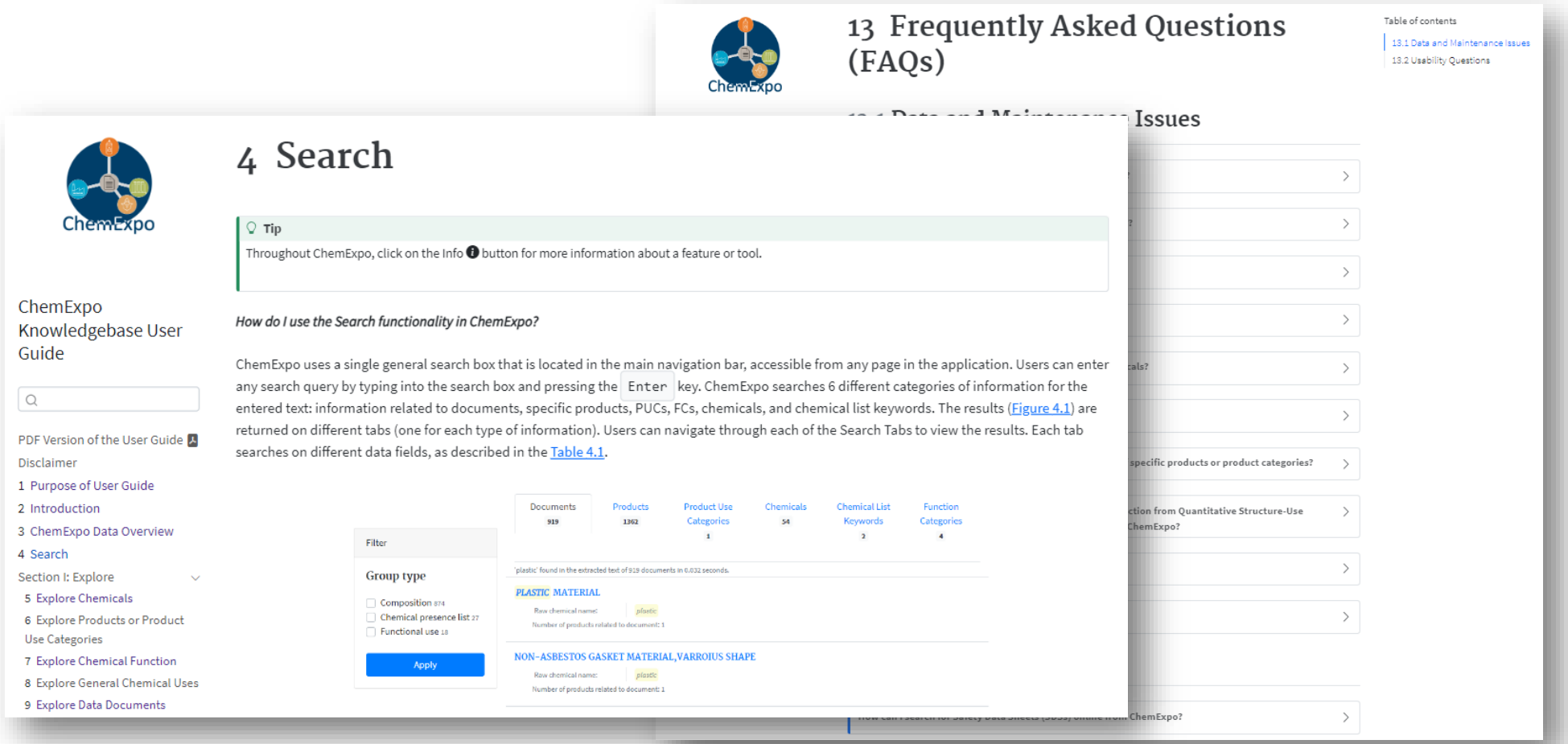
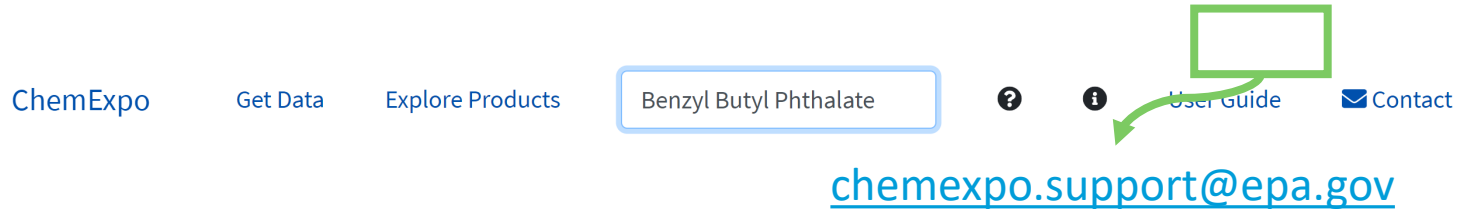


ChemExpo Help



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Interactive Examples

Example 1

You would like to find more information about the chemical **methylparaben**. Search for the chemical, click on the “Chemicals” tab, and navigate to its Chemical Detail Page, which returns all ChemExpo data for this chemical.

- Methylparaben is most commonly found in products associated with which General Category PUC?

Personal Care

- What are the two most common FCs associated with methylparaben?

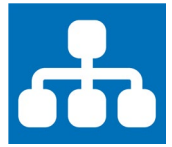
Fragrance and Preservative

- What is the cleaned weight fraction of methylparaben in the product *Germ-X Hand Sanitizer Lotion*?

0.0 - 0.1

If you know a chemical’s DTXSID, you can directly go to it’s Chemical Detail Pages in ChemExpo. Methylparaben’s DTXSID is DTXSID4022529, so the URL for it’s Chemical Detail Page is https://comptox.epa.gov/chemexpo/chemical/DTXSID4022529/

Example 2



Click on the sitemap icon to navigate to this PUC's detail page

You are interested in chemicals used in **commercial dry cleaning**. To determine if there is a PUC related to this industry, go to the Get Data page and then click on Product Use Categories to navigate to the PUC Index page. Search for dry cleaning in the search box above the PUC table.

- Of all the PUCs associated with dry cleaning, which PUC is most likely to have products related to commercial dry cleaning?

Occupation - Specialty Occupational Products - Dry Cleaning Chemicals

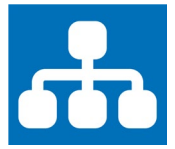
- According to the PUC Detail Page for **Occupation - Specialty Occupational Products - Dry Cleaning Chemicals**, which chemical has the highest count of manually curated products associated with it?

Tetrachloroethylene (manually counted in 70 products)

- For the product *EX-IT Dry Cleaners Textile Deodorant*, what is the FC associated with the chemical pentyl acetate?

Solvent

Example 3



Click on the sitemap icon to navigate to this LPKs detail page

You are interested in the presence of **pharmaceuticals** in groundwater. To explore the general occurrence of pharmaceuticals, go to the Get Data page and click on List Presence Keywords to navigate to the LPK Index page. Search for pharmaceutical in the search box above the LPK table.

- How many documents, in total, have been associated with pharmaceuticals?

91

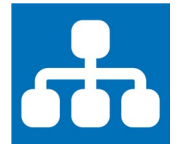
- Which keyword set most likely contains information useful to your interest (i.e., pharmaceuticals in groundwater)?

{MN Chemical Screening, detected, pharmaceutical, ground_water}

- Which document lists pharmaceuticals detected in Minnesota groundwater?

Pharmaceutical Compounds in Shallow Groundwater in Non-Agricultural Areas of Minnesota—Study Design, Methods, and Data, 2013

Example 4



Click on the sitemap icon to navigate to this FCs detail page

You are interested in the chemicals that can serve as **preservatives**. To explore potential preservatives, go to the Get Data page and click on Function Categories to navigate to the FC Index Page. Search for preservative in the search box above the FC table.

- How many documents contain chemicals that are associated with the Functional Category “preservative”?

2627

- How many unique chemicals are associated with the Function Category “preservative”?

274

Wrapping UP

Working with Us

Interested in working with the ChemExpo team to submit data to our knowledgebase?

Send us an email at chemexpo.support@epa.gov to discuss!