




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.



U.S. EPA

Peter Egeghy
Colleen Elonen
Kenta Baron-Furuyama
Terry Brown
Taylor Wall

Michael Metcalf*
Christian Lutz*

GDIT

Lionel Girardin
Karen Hausman
Alison Larger

*Trainees



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



Chemical Exposure

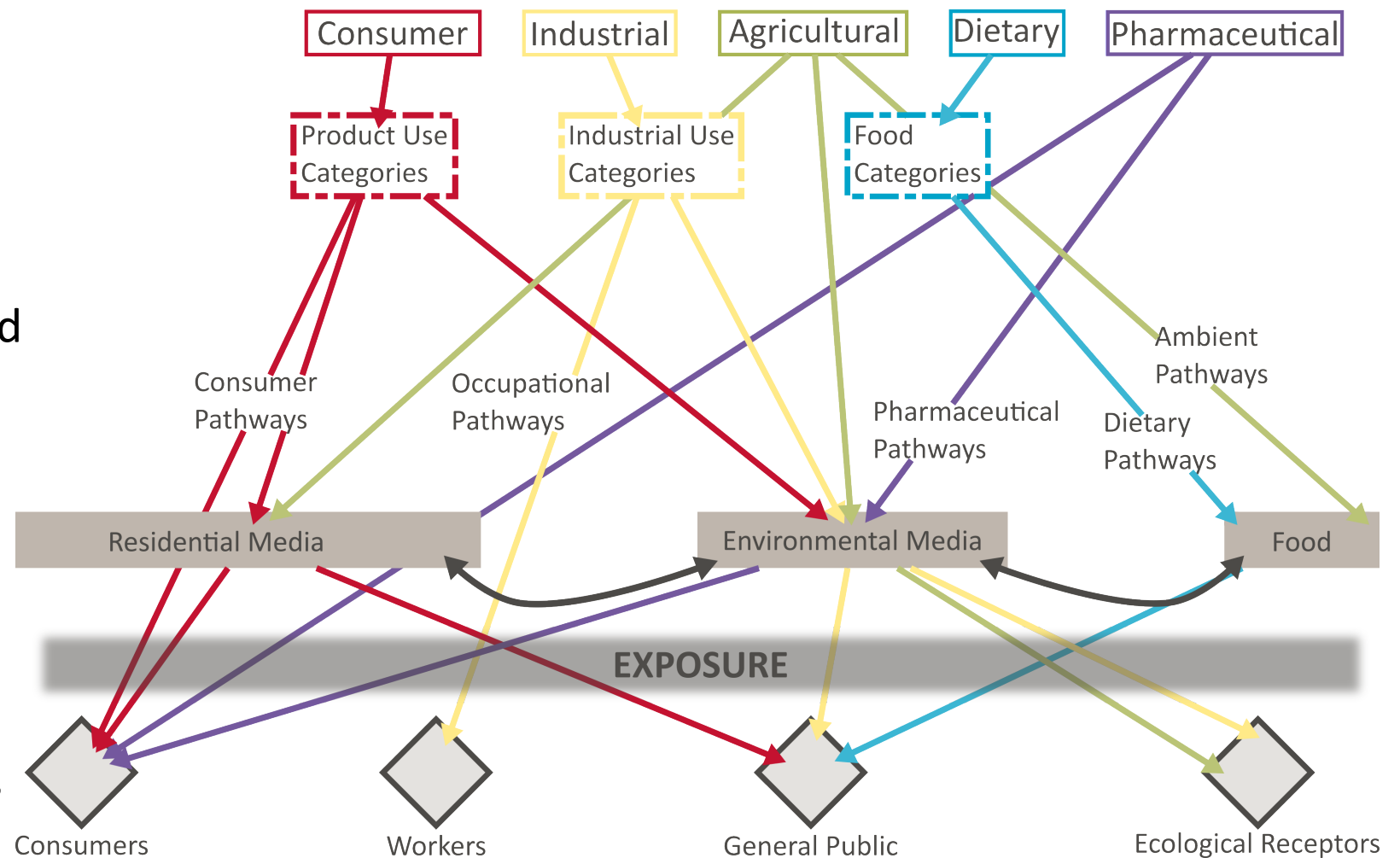
- Humans interact with thousands of chemicals on a regular basis
- We often don't know precisely...
 - ...which chemicals we contact in our everyday lives
 - ...the quantities of those chemicals
 - ...the ultimate fate of those chemicals in our bodies
- Tools developed for Computational Exposure Science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



Exposure Pathways:

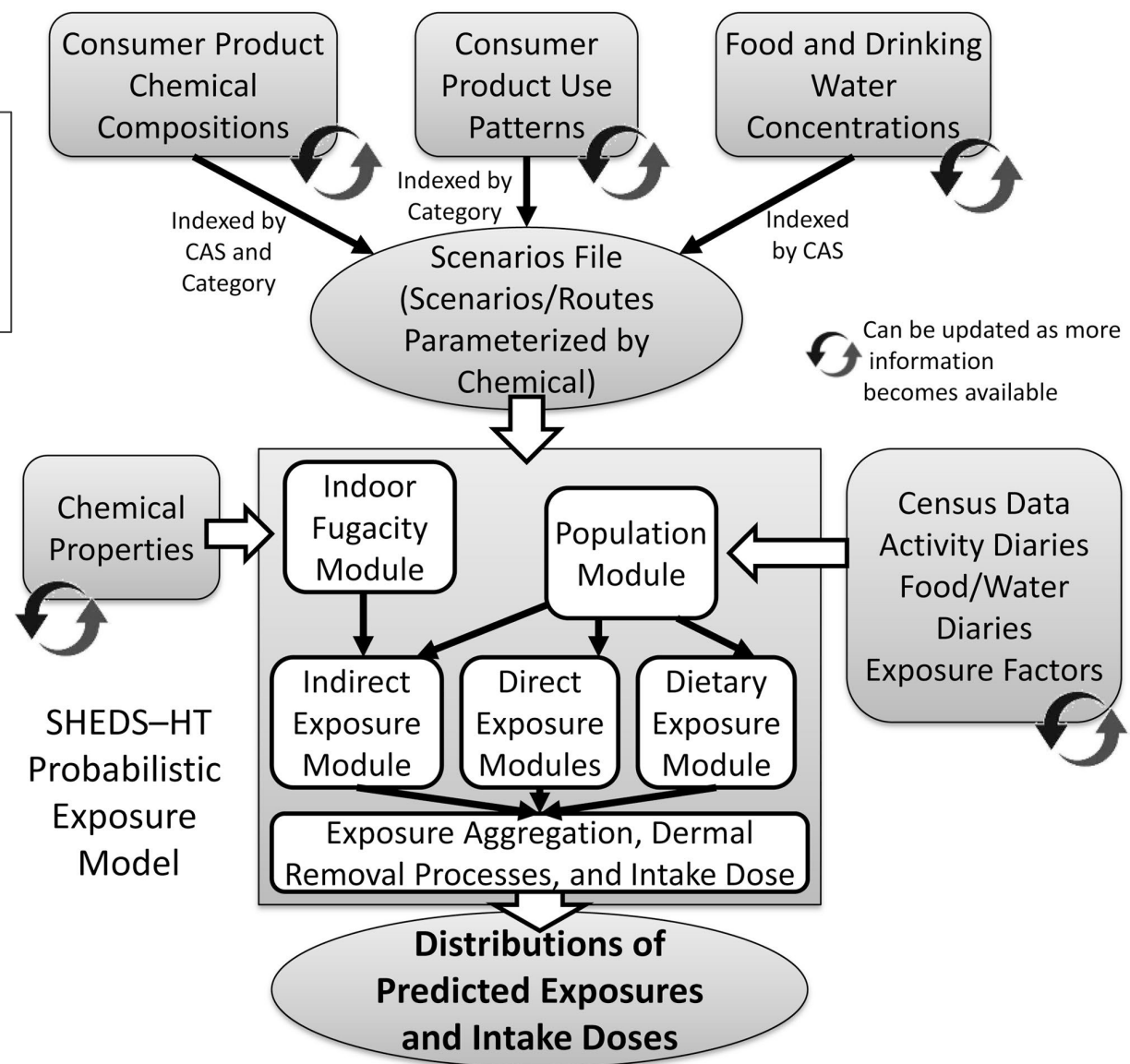
Source to Receptors

- 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

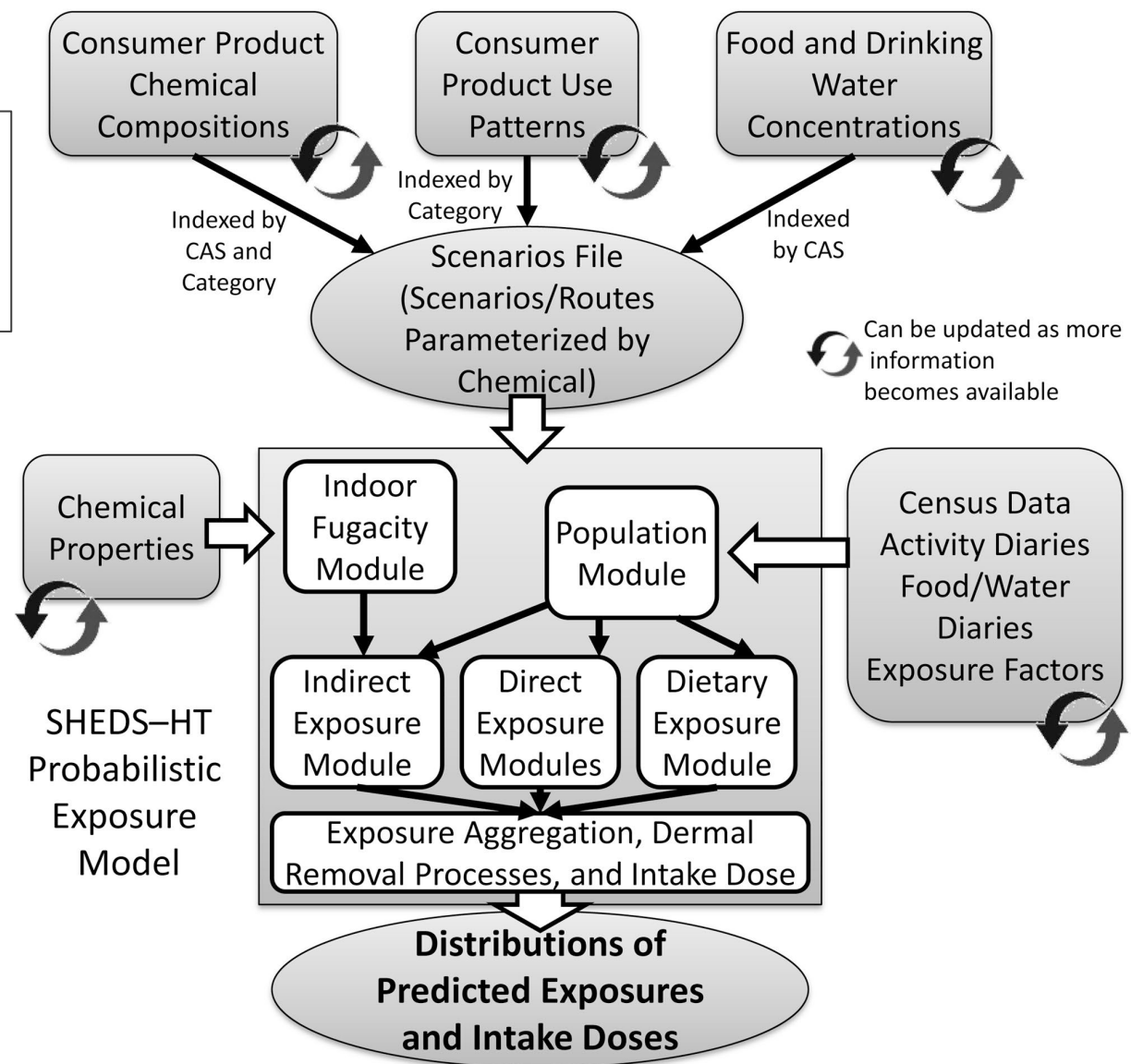
How does use information contribute to exposure modeling?



SHEDS-HT

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

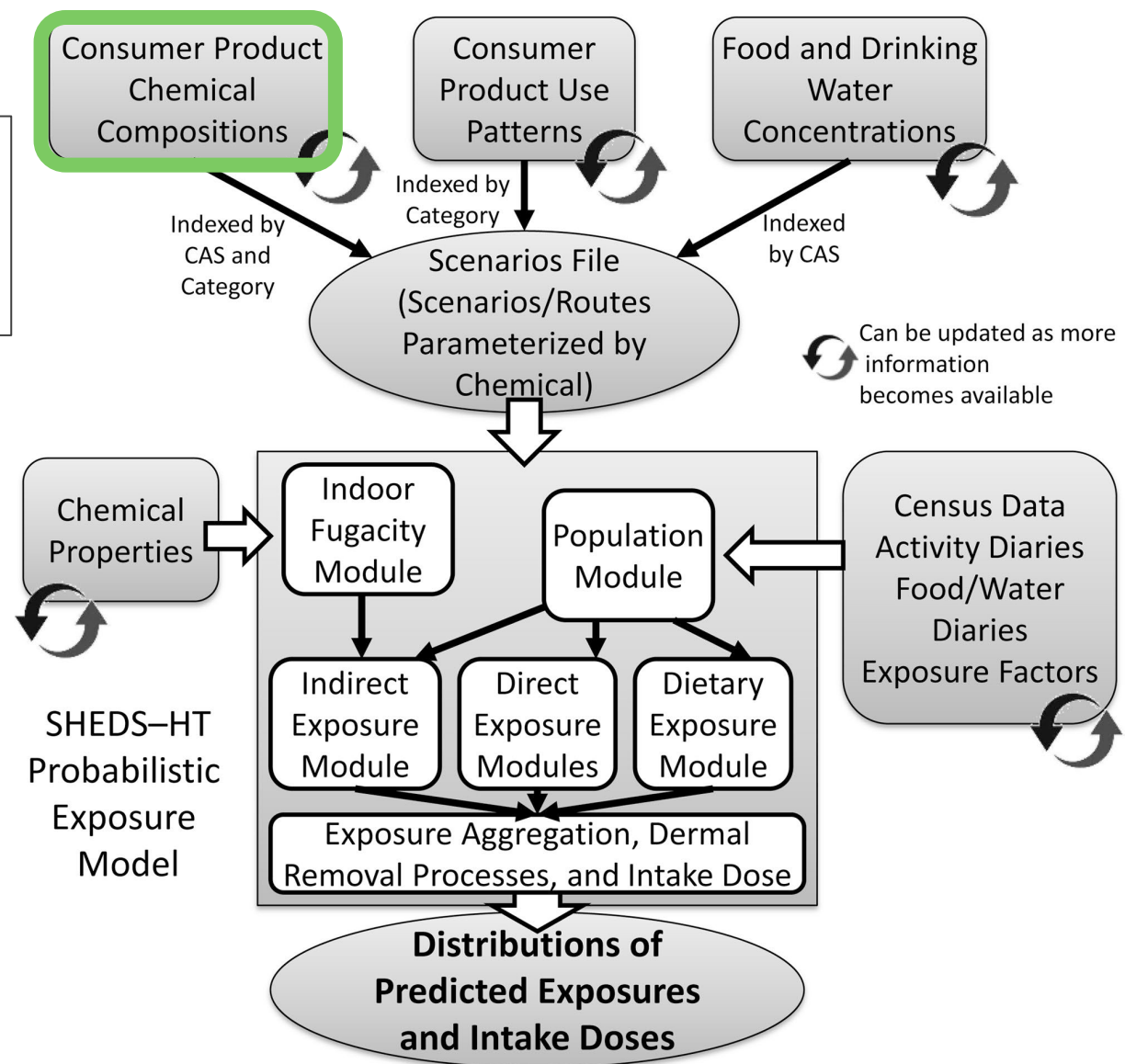


SHEDS-HT

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

CPDat can provide this information!



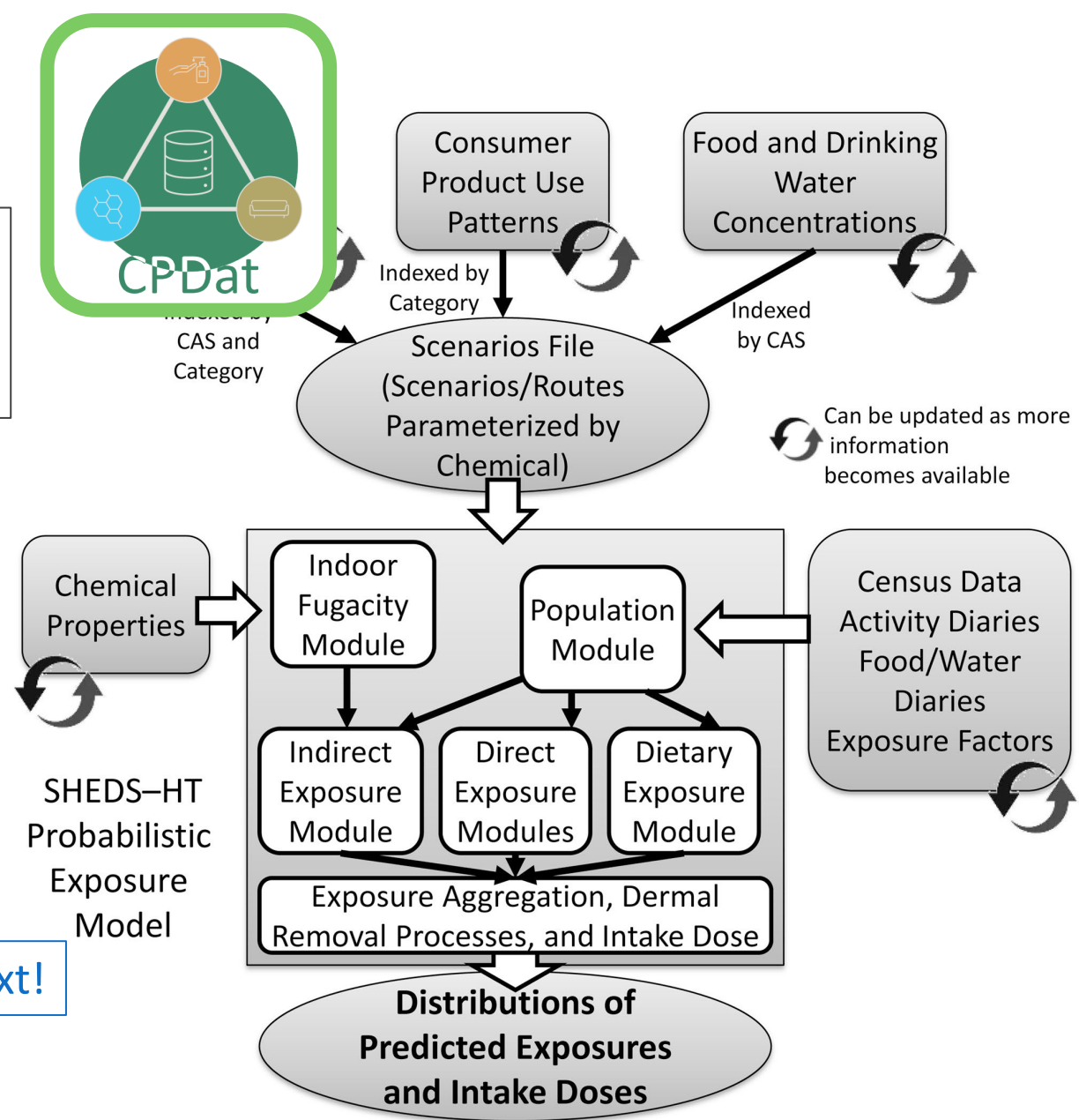
SHEDS-HT

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

CPDat can provide this information!

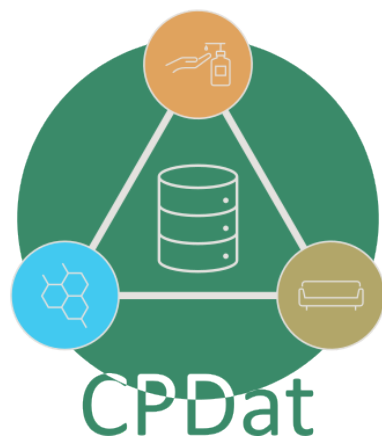
Kristin Isaacs has a demo of SHEDS-HT next!



What Is CPDat?

- ...Factotum?
- ...ChemExpo?
- ...how are they all related?
- ...which should I use?

Chemical and Products Database



- 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 .xlsx files)
 - Summary information from database is available from ORD's **CompTox Chemicals Dashboard (CCD)**
- CTE 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**

[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](#)

CPDat Improvements

CPDat versions 1 – 3

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^a, Katherine A. Phillips^a, Derya Biryol^{1,2}, Kathie L. Dionisio³ and Paul S. Price³

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

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

Ingredient weight fraction data from previous EPA data collection efforts

Contents lists available at ScienceDirect

Toxicology Reports

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

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

Kathie L. Dionisio^a, Alicia M. Frame^{b,1}, Michael-Rock Goldsmith^{a,2}, John F. Wambaugh^b, Alan Liddell^{a,3}, Tommy Cathey^a, Doris Smith^b, James Vail^a, Alexi S. Ernstoff^a, Peter Fantke^a, Olivier Jolliet^c

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^{a,b,c}, John F. Wambaugh^b, Christopher M. Grulke^b, Kathie L. Dionisio^c and Kristin K. Isaacs^c

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

CPDat version 4

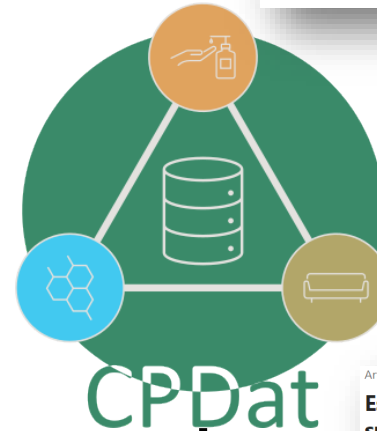
Review Article | Published: 26 November 2022

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

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

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



Article | Published: 11 November 2019

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

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

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

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

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

Organisa
Organisa [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:

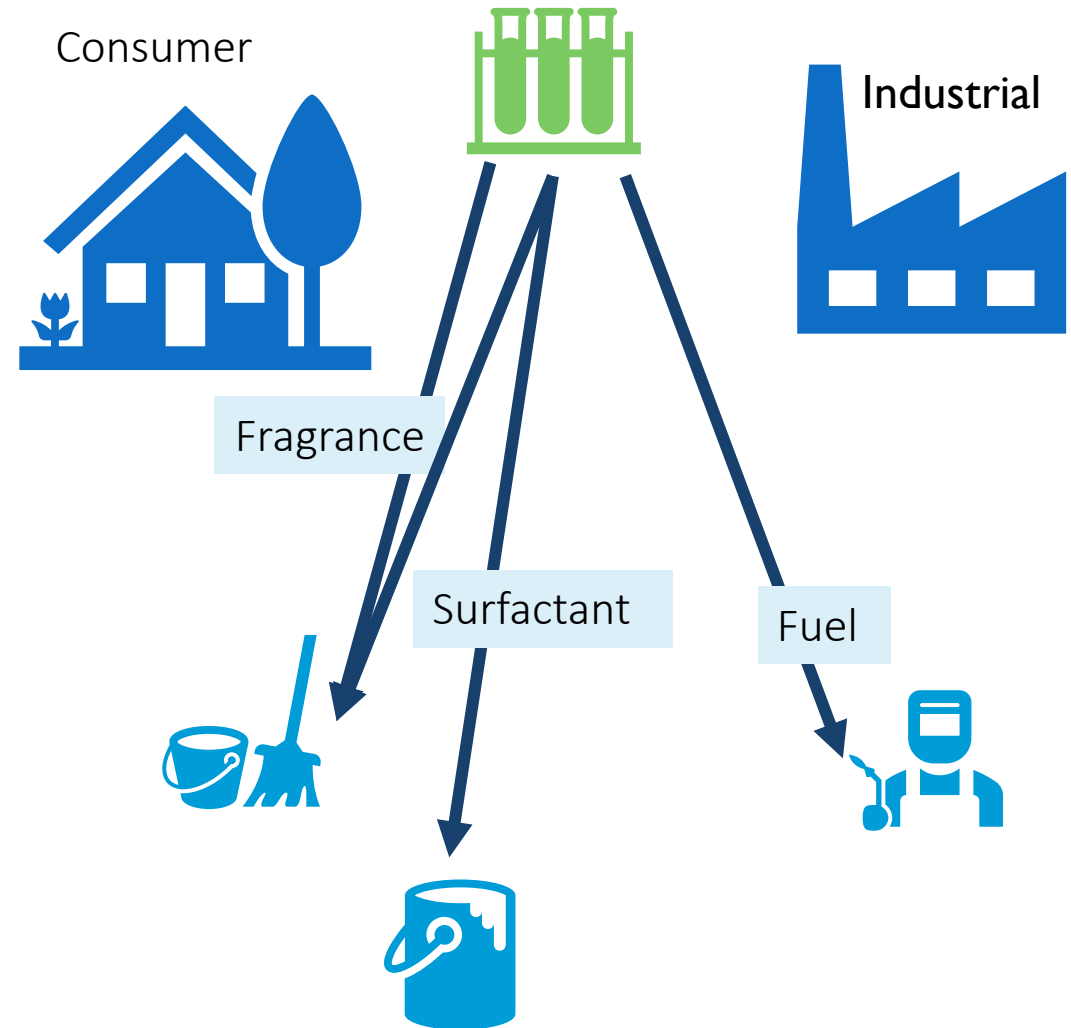
Which groups use a chemical (i.e., industrial process *versus* consumer product)

- End-use:

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

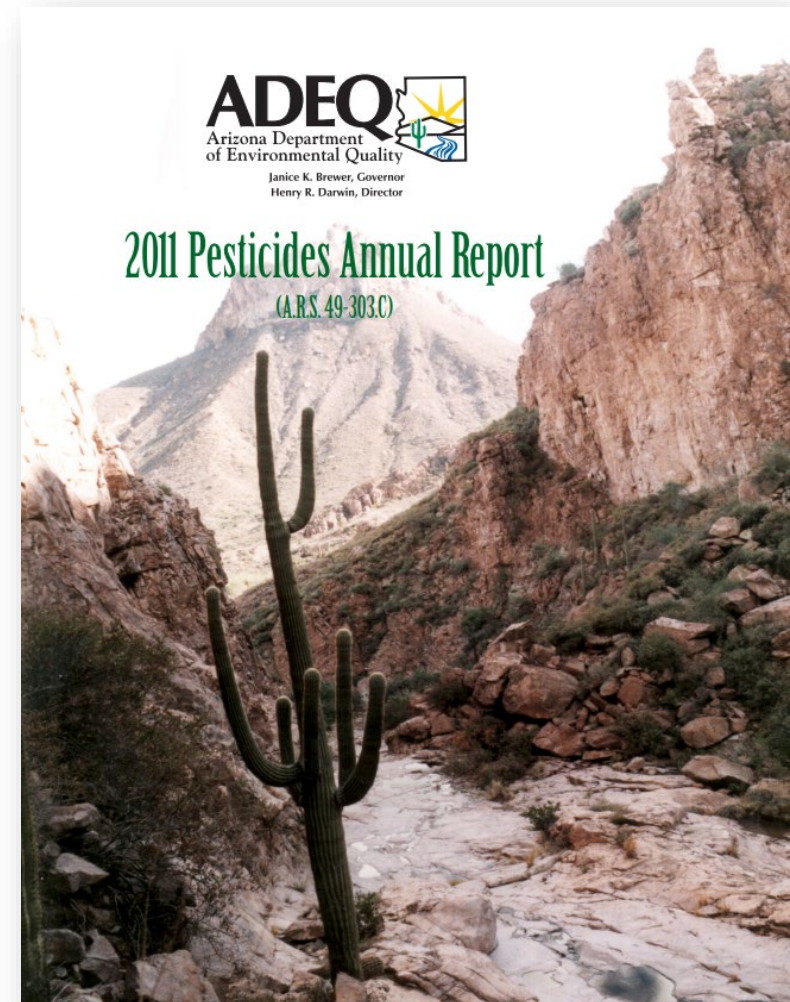
- Functional Use:

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**



Chemical Use Types in CPDat

- Commercial Sector Use
 - Lists of chemicals used in different commercial or industrial sectors
 - Organized by **Chemical List Presence Keywords**
- End-Use
 - Use in particular products or product types
 - Organized by **Product Use Categories (PUCs)**

Safety Data Sheet	
1. Identification	
2. Hazard(s) Identification	
3. Composition/Information on Ingredients	
4. First-aid Measures	
5. Firefighting Measures	
6. Accidental Release Measures	
7. Handling and Storage	
8. Exposure Controls/Personal Protection	
9. Physical and Chemical Properties	
10. Stability and Reactivity	
11. Toxicological Information	

Chemical Use Types in CPDat

- Commercial Sector Use
 - Lists of chemicals used in different commercial or industrial sectors
 - Organized by **Chemical List Presence Keywords**
- End-Use
 - Use in particular products or product types
 - Organized by **Product Use Categories (PUCs)**

Safety Data Sheet	
1. Identification	
2. Hazard(s) Identification	
3. Composition/Information on Ingredients	
4. First-aid Measures	
5. Firefighting Measures	
6. Accidental Release Measures	
7. Handling and Storage	
8. Exposure Controls/Personal Protection	
9. Physical and Chemical Properties	
10. Stability and Reactivity	
11. Toxicological Information	

Chemical Use Types in CPDat

- Commercial Sector Use
 - Lists of chemicals used in different commercial or industrial sectors
 - Organized by **Chemical List Presence Keywords**
- End-Use
 - Use in particular products or product types
 - Organized by **Product Use Categories (PUCs)**
- Functional use
 - Role the chemical plays in different consumer products or industrial processes
 - Organized by OECD's **Function Categories (FCs)**

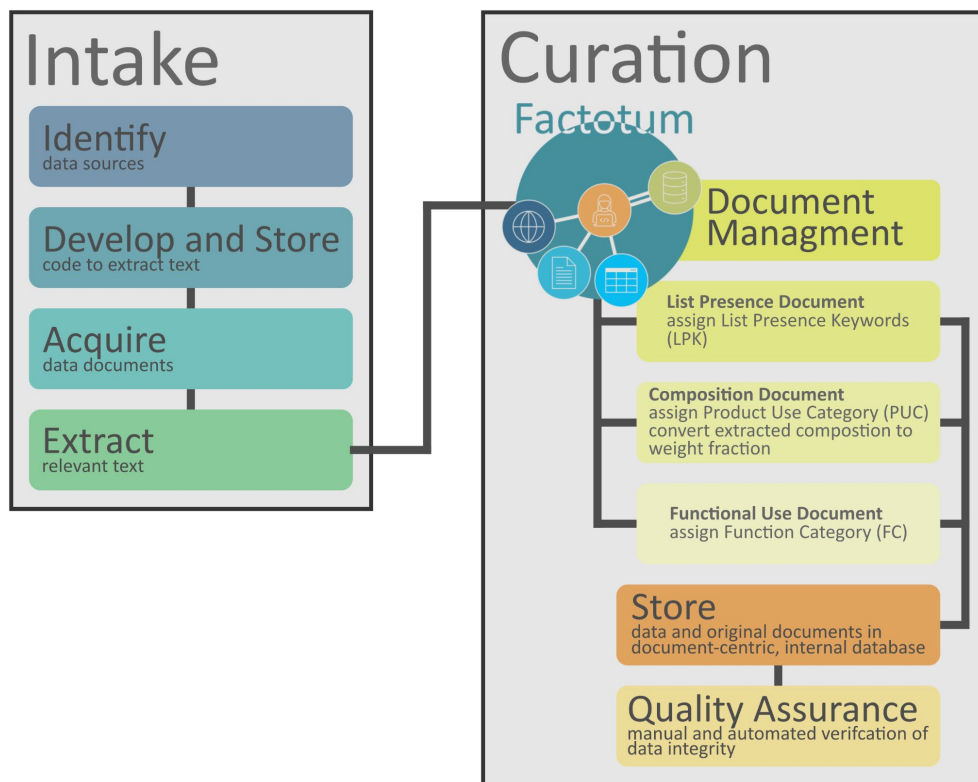
Ingredients		
ingredient	function	CAS #
water	diluent + solvent	7732-18-5
sodium lauryl sulfate	surfactant (cleaning agent)	68585-47-7
lauramine oxide	surfactant (cleaning agent)	1643-20-5
decyl glucoside	surfactant (cleaning agent)	68515-73-1
lauryl glucoside	surfactant (cleaning agent)	110615-47-9
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.

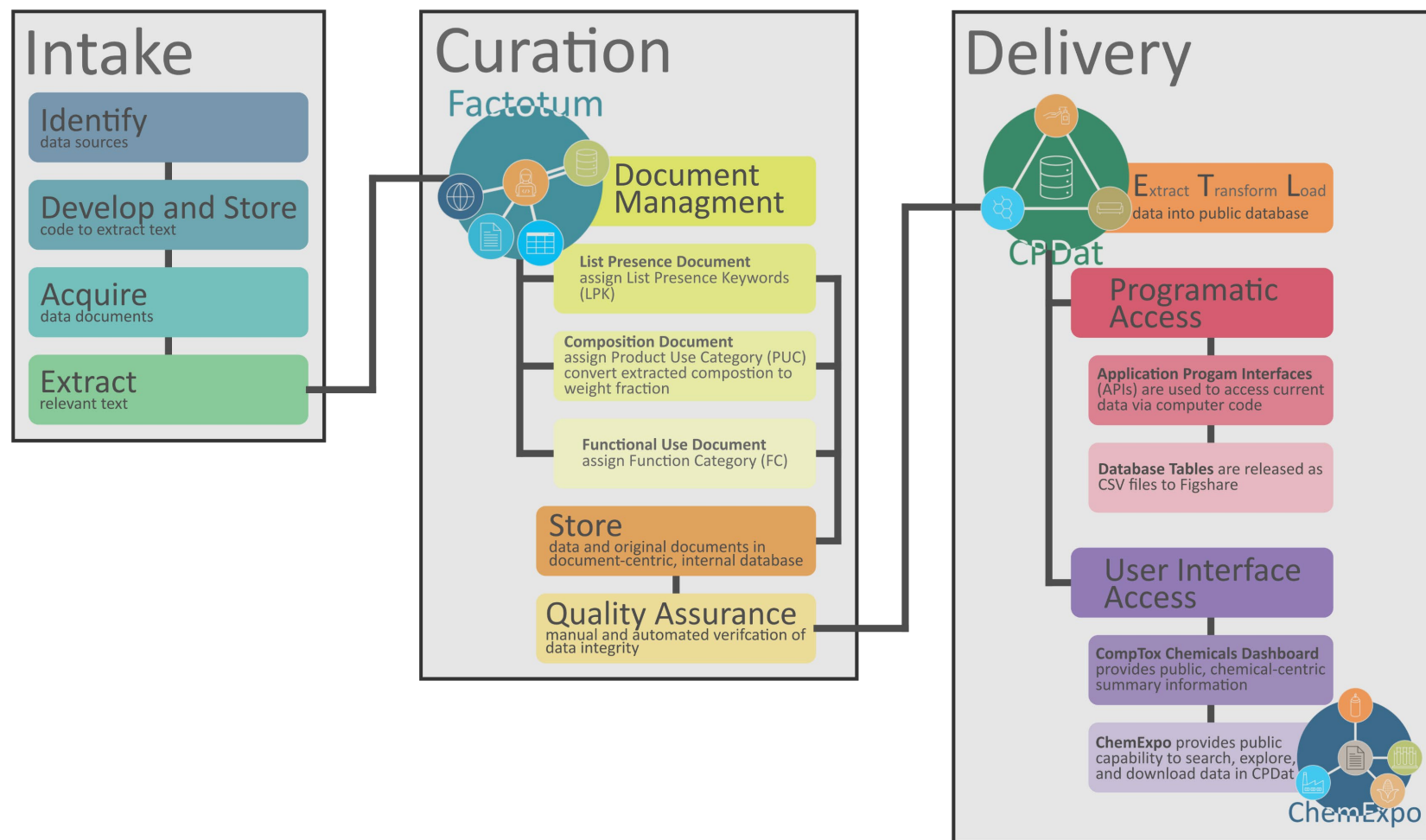


The CPDat Pipeline



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

The CPDat Pipeline



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

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

Bringing it All Together

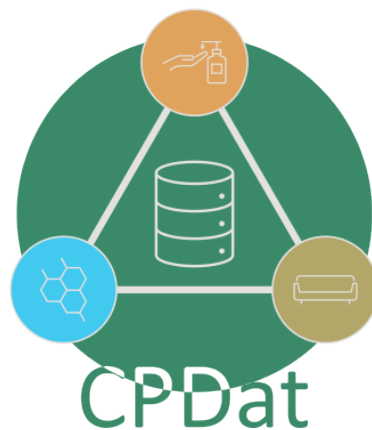
Private Web Tool

Factotum



Factotum helps EPA curate data...

Public Database



...that goes into CPDat...

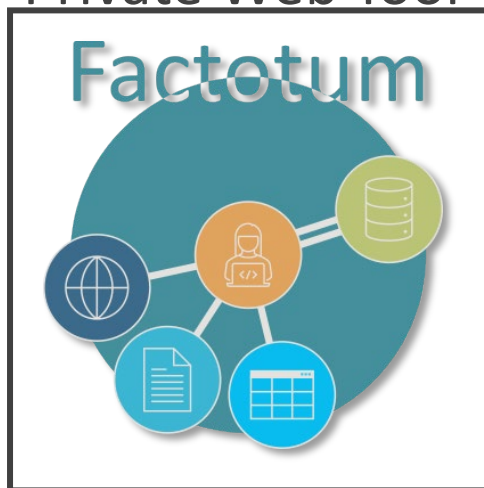
Public Web Tool



...that is then searchable by ChemExpo.

Bringing it All Together

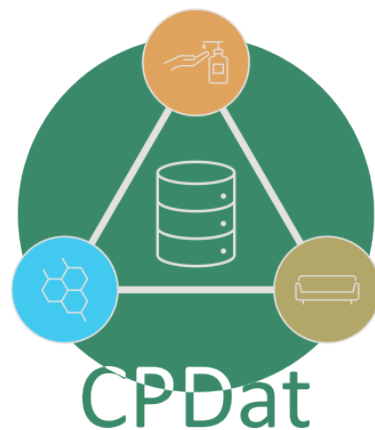
Private Web Tool



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



...that goes into CPDat...

Public Web Tool



...that is then searchable by ChemExpo.

Bringing it All Together

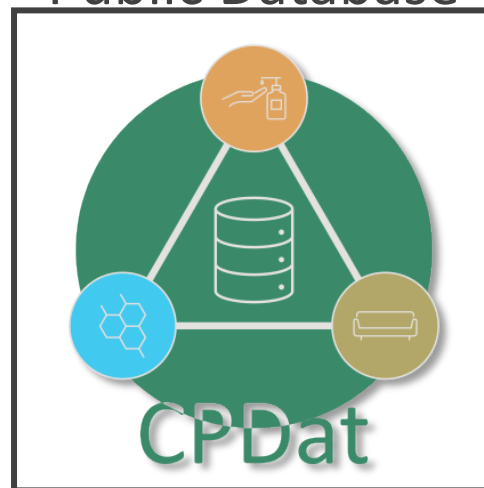
Private Web Tool

Factotum



Factotum helps EPA curate data...

Public Database



...that goes into CPDat...

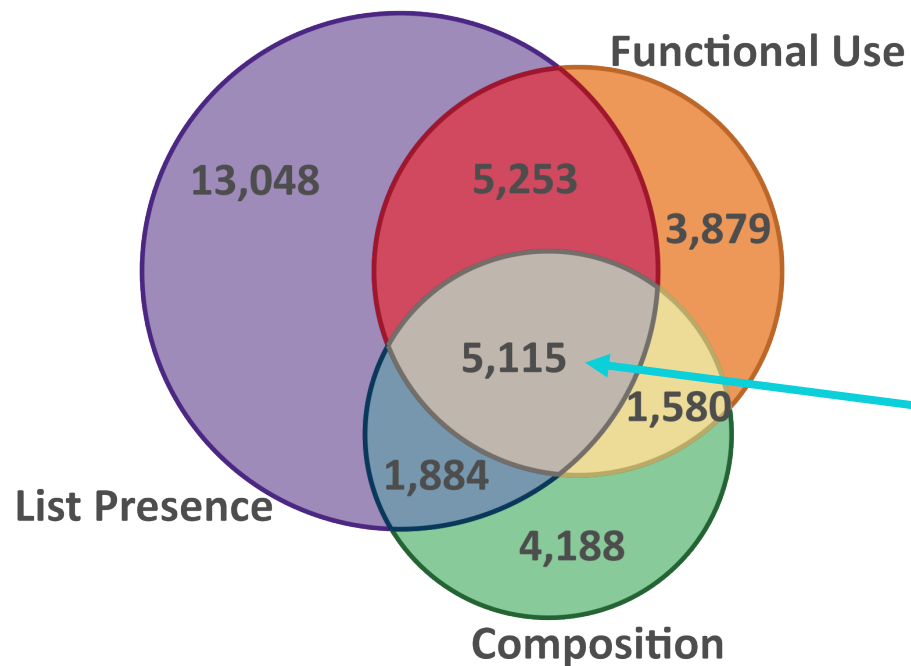
Public Web Tool



...that is then searchable by ChemExpo.

CPDat by the Numbers

Chemical Counts

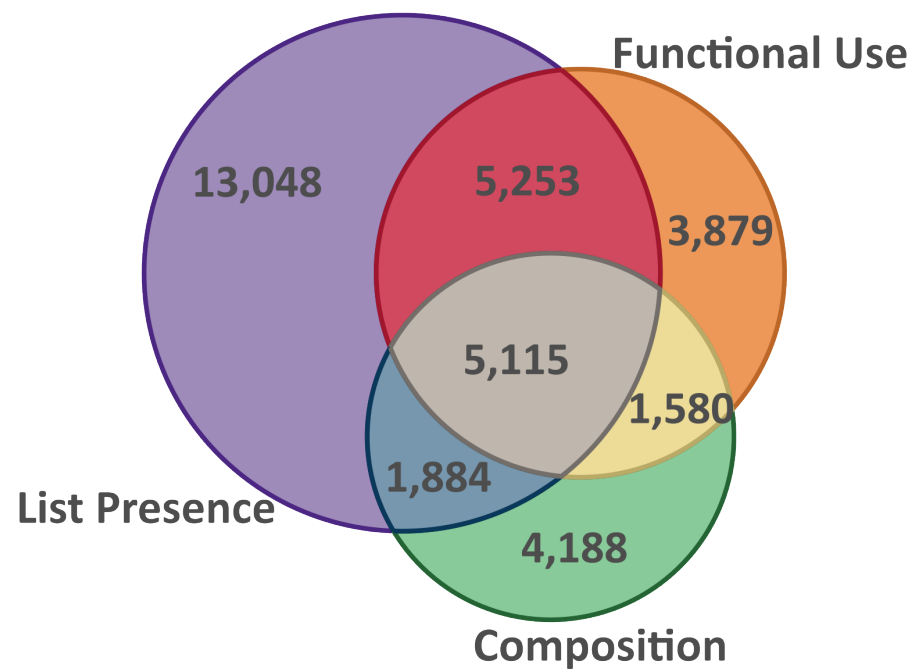


Unique Chemical Substances found across list presence, composition, and functional use type documents.

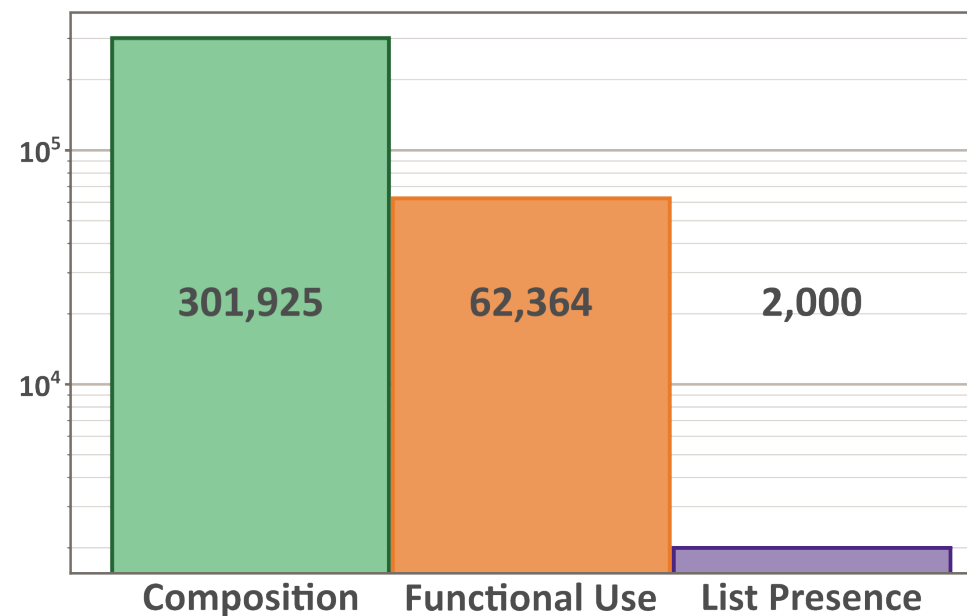
Note: this doesn't mean there is one document that has all types of information for a chemical.

CPDat by the Numbers

Chemical Counts



Document Counts



Bringing it All Together

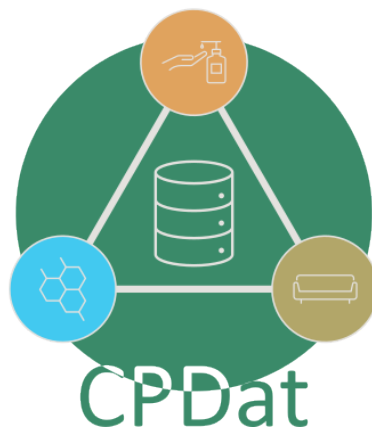
Private Web Tool

Factotum



Factotum helps EPA curate data...

Public Database



CPDat

...that goes into CPDat...

Public Web Tool



...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.



- 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

ChemExpo

Get Data

Explore Products

Search ChemExpo




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.


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

Documents 


434,714

Products 


376,113

Products Linked To Product Use
Categories 

263,824

Extracted Chemical Records 

3.6 million

Curated Chemical Records 

2.3 million

Unique Chemicals (DTXSIDs) 

35,057



- 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

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 ⓘ

434,714

Products ⓘ

376,113

Products Linked To Product Use
Categories ⓘ

263,824

Extracted Chemical Records ⓘ

3.6 million

Curated Chemical Records ⓘ

2.3 million

Unique Chemicals (DTXSIDs) ⓘ

35,057



- 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

Search ChemExpo

ChemExpo

Get Data

Explore Products

Search ChemExpo



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.

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

Documents ⓘ

434,714

Products ⓘ

376,113

Products Linked To Product Use
Categories ⓘ

263,824

Extracted Chemical Records ⓘ

3.6 million

Curated Chemical Records ⓘ

2.3 million

Unique Chemicals (DTXSIDs) ⓘ

35,057



ChemExpo

Get Data

Explore Products

Search ChemExpo



User Guide

Contact

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)

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 ⓘ

434,714

Products ⓘ

376,113

Products Linked To Product Use
Categories ⓘ

263,824

Extracted Chemical Records ⓘ

3.6 million

Curated Chemical Records ⓘ

2.3 million

Unique Chemicals (DTXSIDs) ⓘ

35,057



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.

The screenshot shows the ChemExpo Knowledgebase homepage. At the top, there is a navigation bar with links for 'ChemExpo', 'Get Data', 'Explore Products', a search box labeled 'Search ChemExpo', and utility links for 'User Guide' and 'Contact'. The main heading is 'Welcome to ChemExpo Knowledgebase', accompanied by a molecular structure icon. Below the heading is a paragraph describing the application's purpose and data sources. A disclaimer states that the beta version (v0.1) is under review. The bottom section features six data cards in a 2x3 grid, each with an information icon and a large numerical value.

ChemExpo

Get Data Explore Products Search ChemExpo 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.

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

Documents ⓘ 434,714	Products ⓘ 376,113	Products Linked To Product Use Categories ⓘ 263,824
Extracted Chemical Records ⓘ 3.6 million	Curated Chemical Records ⓘ 2.3 million	Unique Chemicals (DTXSIDs) ⓘ 35,057



Search

Explore

Download

ChemExpo

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.

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

Documents

434,714

Products

376,113

Products Linked To Product Use
Categories

263,824

Keyword Search

ChemExpo

Get Data

Explore Products

Benzyl Butyl Phthalate



User Guide

Contact

If you are looking for information on a specific chemical, the Chemicals tab returns the results of a search of harmonized chemical identifiers used by EPA (including DTXSIDs and preferred names) and their known synonyms, allowing you to access data for chemicals directly.

Documents

1902

Products

475

Product Use
Categories

0

Chemicals

14

Chemical List
Keywords

0

Function
Categories

0

Filter

None available

'Benzyl Butyl Phthalate' found in the name of 14 chemical identifiers (preferred names or synonyms) in 0.056 seconds.

DTXSID3020205

Curated chemical name:

Benzyl butyl phthalate

Curated CAS:

85-68-7

Chemical Detail Page: Benzyl Butyl Phthalate

Benzyl Butyl Phthalate

DTXSID3020205

85-68-7

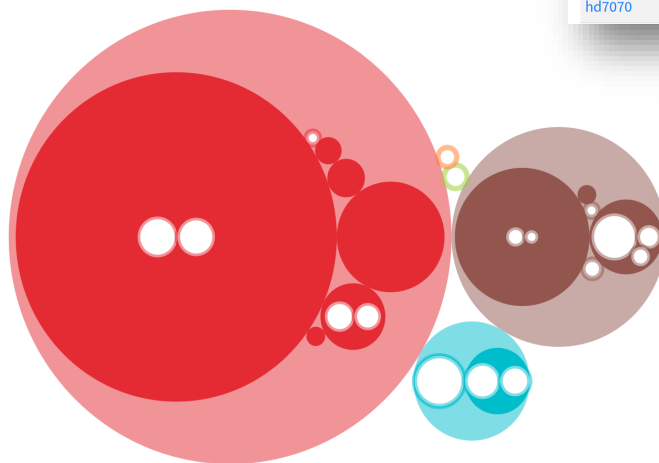
Explore products containing this chemical. Use the filter buttons to filter the tables below to certain Product Use Categories. Click the info icon for each PUC to access its detailed chemical and product data.

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	i ⌵	10
➤	Cleaning products and household care	i ⌵	2
➤	Home maintenance	i ⌵	402
➤	Personal care	i ⌵	22
➤	Vehicle	i ⌵	267



Products		Documents	Function			
Products Containing "Benzyl butyl phthalate"						
Show 10 entries		Search: <input type="text"/>	Show All Products			
Download Products and Weight Fractions						
Product	Manufacturer	Brand	Document	PUC	PUC Kind	Classification Method
b9014luciteacryliclacquer	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 10 entries		Search: <input type="text"/>	Show All Functions
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	plasticizer	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

ChemExpo Get Data **Explore Products** Search ChemExpo ? ⓘ User Guide Contact

Explore Products

Explore data for products linked to [Product Use Categories \(PUCs\)](#).

Click the info button (ⓘ) next to 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	
<i>General Category - Product Family - Product Type</i>	
▶ Arts and crafts/office supplies ⓘ	2583
▶ Sports equipment ⓘ	68
▶ Cleaning products and household care ⓘ	13160
▶ Electronics/small appliances ⓘ	3788
▶ Home maintenance ⓘ	29653
▶ Landscape/yard ⓘ	927
▶ Personal care ⓘ	101525
▶ Pesticides ⓘ	1328
▶ Pet and animal care ⓘ	218
▶ Vehicle ⓘ	5656
▶ Food and drug ⓘ	3087

Formulation PUCs	
<i>General Category - Product Family - Product Type</i>	
▶ Arts and crafts/office supplies ⓘ	2583
▶ Sports equipment ⓘ	68
▶ Cleaning products and household care ⓘ	13160
▶ air freshener ⓘ	2242
▶ bathroom ⓘ	742
▶ carpet and floor ⓘ	576
▶ carpet cleaner ⓘ	236
▶ carpet deodorizer ⓘ	30
▶ floor cleaner ⓘ	223
▶ floor polish ⓘ	62
▶ dishwasher and dishes ⓘ	914
▶ drain products ⓘ	274
▶ general household cleaning ⓘ	2798



PUC Detail Page: Floor Cleaner

[← Back to PUC list](#)

Cleaning products and household care

carpet and floor / floor cleaner

Kind Formulation

Description hard floor cleaners, including pre-moistened wipes

Assumed Attributes

No assumed attributes are associated with this PUC

Allowed Attributes

liquid powder pump spr

Additional Statistics

Products 223
Cumulative Products 223
Documents 222
Curated Chemicals 231

Products	Documents	Chemicals	Functions
Chemicals Associated with "Cleaning products and household care - carpet and floor - floor cleaner"			
Show 10 entries		Search:	Download All Chemicals Associated with PUC
DTXSID	Curated CAS	Curated Chemical Name	Count (Manual) Count (Automatic)
DTXSID6026296	7732-18-5	Water	72 11
DTXSID2034259	2682-20-4	2-Methyl-3(2H)-isothiazolone	30 4
DTXSID8026727	106-24-1	(2E)-3,7-Dimethyl-2,6-octadien-1-ol	21 0
DTXSID50105933	110615-47-9	D-Glucopyranose, oligomeric, C10-16-alkyl glycosides	16
DTXSID6024836	5392-40-5	3,7-Dimethyl-2,6-octadienal	15
DTXSID5029633	1310-58-3	Potassium hydroxide	15
DTXSID2029612	138-86-3	Limonene	15
DTXSID70872594	68515-73-1	D-Glucopyranose, oligomeric, decyl octyl glycosides	14
DTXSID3020332	77-92-9	Citric acid	13
DTXSID3026726	106-22-9	Citronellol	13
Showing 1 to 10 of 231 entries			Previous 1

Products	Documents	Chemicals	Functions		
Functions Associated with "Cleaning products and household care - carpet and floor - floor cleaner"					
Show 10 entries		Search:	Download All Functions Associated with PUC		
Classification Method	Document	Chemical Name	CAS	Reported Function	Harmonized Function
Composition	Pledge Revive It Multisurface Floor Finish	Proprietary Wetting Agent		wetting agent	Wetting agent (non-aqueous)
Composition	Pledge FloorCare Wood Concentrated Cleaner (Interrumpido)	Hydroxyethylcellulose	9004-62-0	Thickener	Thickening agent
Composition	Orange Glo Everyday Hardwood Floor Cleaner	c8-10 alkyl glucoside		surfactant-cleaning agent	Surfactant (surface active agent)
Composition	Orange Glo Everyday Hardwood Floor Cleaner	c6-12 alcohol ethoxylate		surfactant-cleaning agent	Surfactant (surface active agent)
Composition	Orange Glo Everyday Hardwood Floor Cleaner	Sodium octyl sulfate	142-31-4	surfactant-cleaning agent	Surfactant (surface active agent)
Composition	Pine-Sol Wet Floor Wipes Lemon Fresh	c10-12 alcohol ethoxylates		surfactant	Surfactant (surface active agent)
Composition	Pine-Sol Wet Floor Wipes Lemon Fresh	sodium c14-17 sec-alkyl sulfonate		surfactant	Surfactant (surface active agent)
Composition	Original Pine-Sol Wet Floor Wipes	sodium c14-17 sec-alkyl sulfonate		surfactant	Surfactant (surface active agent)
Composition	Original Pine-Sol Wet Floor Wipes	c10-12 alcohol ethoxylates		surfactant	Surfactant (surface active agent)
Composition	cif floor wipes	Coconut dimethyl amine oxide	61788-90-7	surfactant	Surfactant (surface active agent)
Showing 1 to 10 of 679 entries			Previous 1 2 3 4 5 ... 68 Next		

Products	Documents	Chemicals	Functions
Products containing chemicals assigned to "Cleaning products and household care - carpet and floor - floor cleaner"			
Show 10 entries		Search:	Download Products and Chemical Weight Fractions
Product	Brand Name	Manufacturer	Classification Method
Orange Glo 4-in-1 Hardwood Clean and Shine	Orange Glo	Church & Dwight	Manual
Orange Glo Everyday Hardwood Floor Cleaner	Orange Glo	Church & Dwight	Manual
Orange Glo Hardwood Floor Refinisher	Orange Glo	Church & Dwight	Manual

Download Data

ChemExpo Get Data Explore Products ? i User Guide Contact

Get Data

Download Metadata

Download PUCs	Product Use Categories
Download PUC Attributes	
Download List Presence Keywords	List Presence Keywords
Download Function Categories	Function Categories

Download Bulk Data

Bulk Download List Presence Data
Bulk Download Function Data
Bulk Download Composition 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.

[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 antiscavative. 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	

[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 Size:

Function Detail Page: Flame Retardant

[← Back to FC list](#)

Flame retardant

Description 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.

Additional Statistics

Products	242
Documents	1210
Chemicals	216

Products

Documents

Chemicals

Products containing chemicals assigned to "Flame retardant"

Show 10 entries

Search:

Download Products Associated with Function

Product Name	Data Document	Product Use Categories	Classification Method
voxflor greenpad	voxflor greenpad	Construction and building materials	Manual
voxflor greenpad	voxflor greenpad	Construction and building materials	Manual
EnviroScreen Optimum -Verosol	EnviroScreen_Optimum_-Verosol_-2017-03-10	Furniture and furnishings	Manual
OmniaScreen-Verosol	OmniaScreen-Verosol_-2017-03-10	Furniture and furnishings	Manual
Panduit Category 6A Riser Shielded Cable PUF6X04-Panduit	Panduit_Category_6A_Riser_Shielded_Cable_PUF6X04-Panduit-2016-07-20	Construction and building materials	Manual
Preserved Wall Gardens MDF Backerboard-Garden On The Wall	Preserved_Wall_Gardens_MDF_Backerboard-Garden_On_The_Wall-2017-05-04	Other indirect contact consumer goods	Manual

Products

Documents

Chemicals

Chemicals Associated with "Flame retardant"

Show 10 entries

Search:

Download Chemicals Associated with Function

DTXSID	Curated CAS	Curated Name
DTXSID001014486	7789-82-4	Calcium molybdate(VI)
DTXSID001018214	12251-53-5	Aluminum sodium hydroxide (NaAl(OH)4)
DTXSID0020494	756-79-6	Dimethyl methylphosphonate
DTXSID0024553	123-77-3	Azodicarbonamide
DTXSID0050471	7727-43-7	Barium sulfate
DTXSID0052679	24623-77-6	Aluminium hydroxide oxide
DTXSID0052700	3072-84-2	2,2'-[(1-Methylethylidene)bis[(2,6-dibromo-4,1-phenylene)oxymethylene]]bis[oxirane]
DTXSID0052708	39635-79-5	4,4'-Sulphonylbis[2,6-dibromophenol]
DTXSID0058300	12767-90-7	Boron zinc oxide (B6Zn2O11)
DTXSID0058691	19186-97-1	Tris(tribromoneopentyl)phosphate

Showing 1 to 10 of 216 entries

Previous 1 2 3 4 5 ... 22 Next

ChemExpo User Guide

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.


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

Documents 

434,714

Products 

376,113

Products Linked To Product Use
Categories 

263,824

ChemExpo User Guide

The screenshot displays the ChemExpo Knowledgebase User Guide interface. The main content area is titled "4 Search". A tip box states: "Throughout ChemExpo, click on the Info button for more information about a feature or tool." Below this, the text asks "How do I use the Search functionality in ChemExpo?" and explains that ChemExpo uses a single general search box accessible from any page. It searches 6 categories: documents, products, PUCs, FCs, chemicals, and chemical list keywords. Results are returned on different tabs, and users can navigate through Search Tabs. A table shows the number of results for each category: Documents (919), Products (1362), Product Use Categories (1), Chemicals (54), Chemical List Keywords (2), and Function Categories (4). The search results for "plastic" are shown, including "PLASTIC MATERIAL" and "NON-ASBESTOS GASKET MATERIAL,VARROUIS SHAPE".

4 Search

Tip
Throughout ChemExpo, click on the Info button for more information about a feature or tool.

How do I use the Search functionality in ChemExpo?

ChemExpo uses a single general search box that is located in the main navigation bar, accessible from any page in the application. Users can enter any search query by typing into the search box and pressing the Enter key. ChemExpo searches 6 different categories of information for the entered text: information related to documents, specific products, PUCs, FCs, chemicals, and chemical list keywords. The results (Figure 4.1) are returned on different tabs (one for each type of information). Users can navigate through each of the Search Tabs to view the results. Each tab searches on different data fields, as described in the Table 4.1.

Documents	Products	Product Use Categories	Chemicals	Chemical List Keywords	Function Categories
919	1362	1	54	2	4

Filter

Group type

- Composition 874
- Chemical presence list 27
- Functional use 18

Apply

Documents: 919, Products: 1362, Product Use Categories: 1, Chemicals: 54, Chemical List Keywords: 2, Function Categories: 4

'plastic' found in the extracted text of 919 documents in 0.032 seconds.

PLASTIC MATERIAL
Raw chemical name: plastic
Number of products related to document: 1

NON-ASBESTOS GASKET MATERIAL,VARROUIS SHAPE
Raw chemical name: plastic
Number of products related to document: 1

13 Frequently Asked Questions (FAQs)

Table of contents

- 13.1 Data and Maintenance Issues
- 13.2 Usability Questions

ChemExpo Help

ChemExpo

Get Data

Explore Products

Benzyl Butyl Phthalate



User Guide

Contact

chemexpo.support@epa.gov



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 (DTXIDs) 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

434,714

Products

376,113

Products Linked To Product Use
Categories

263,824



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?

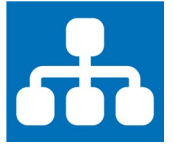
Fragrance and Preservative

- 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 its Chemical Detail Pages in ChemExpo. Methylparaben’s DTXSID is DTXSID4022529, so the URL for its 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

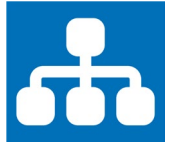
- According to the PUC Detail Page for **Occupation - Specialty Occupational Products - Dry Cleaning Chemicals**, which chemical has the highest count of manually curated products associated with it?

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 Functional 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!

