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INTRODUCING EPA'S CHEMICAL EXPOSURE KNOWLEDGEBASE

Sakshi Handa, Katherine Phillips, Kristin Isaacs

U.S. EPA, Office of Research and Development,

Center for Computational Toxicology and Exposure

EPA CompTox Communities of Practice Sep. 28, 2023

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BACKGROUND

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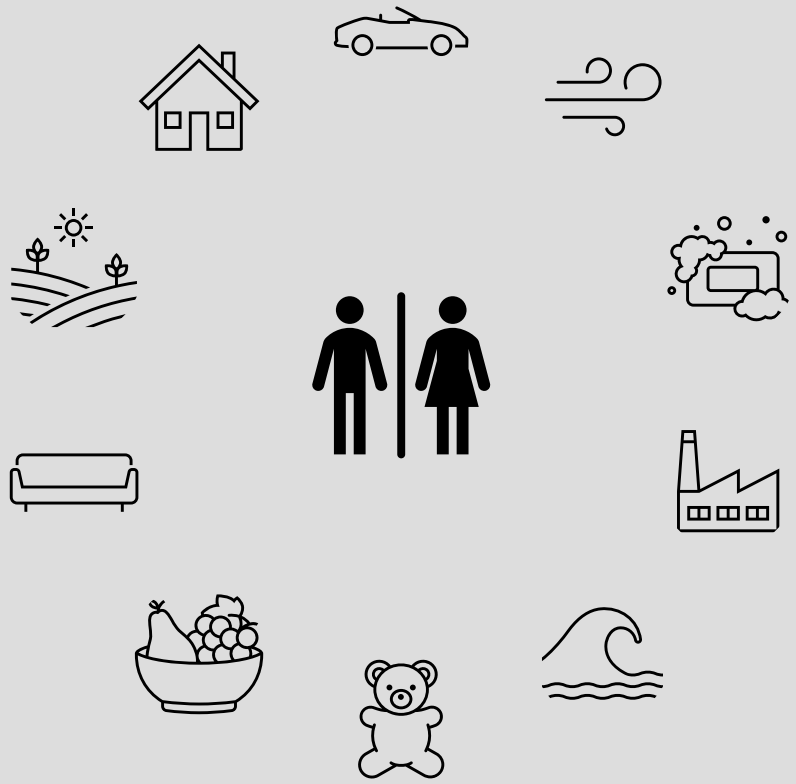
CHEMICAL EXPOSURE

- 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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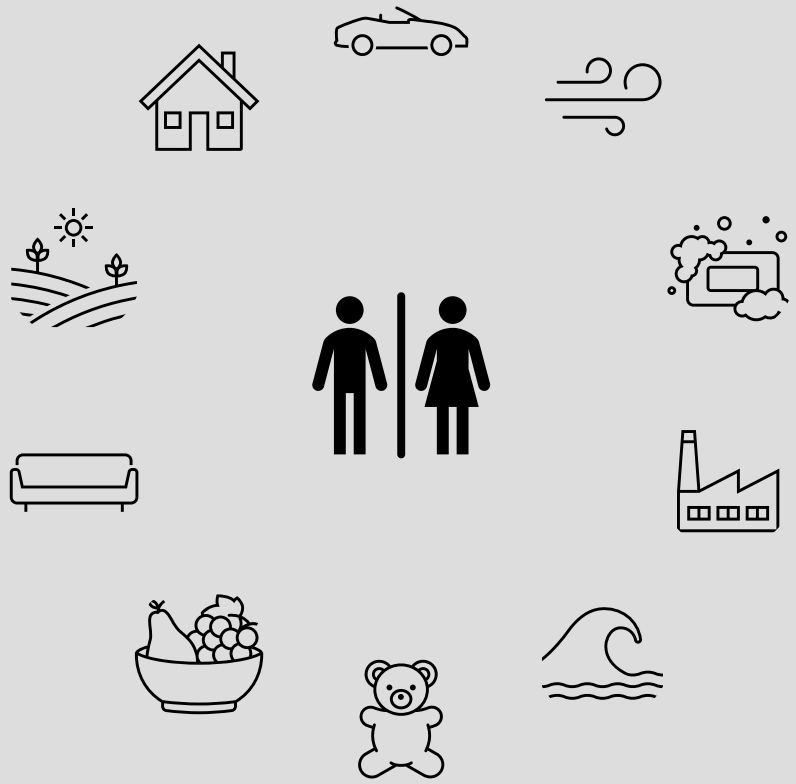

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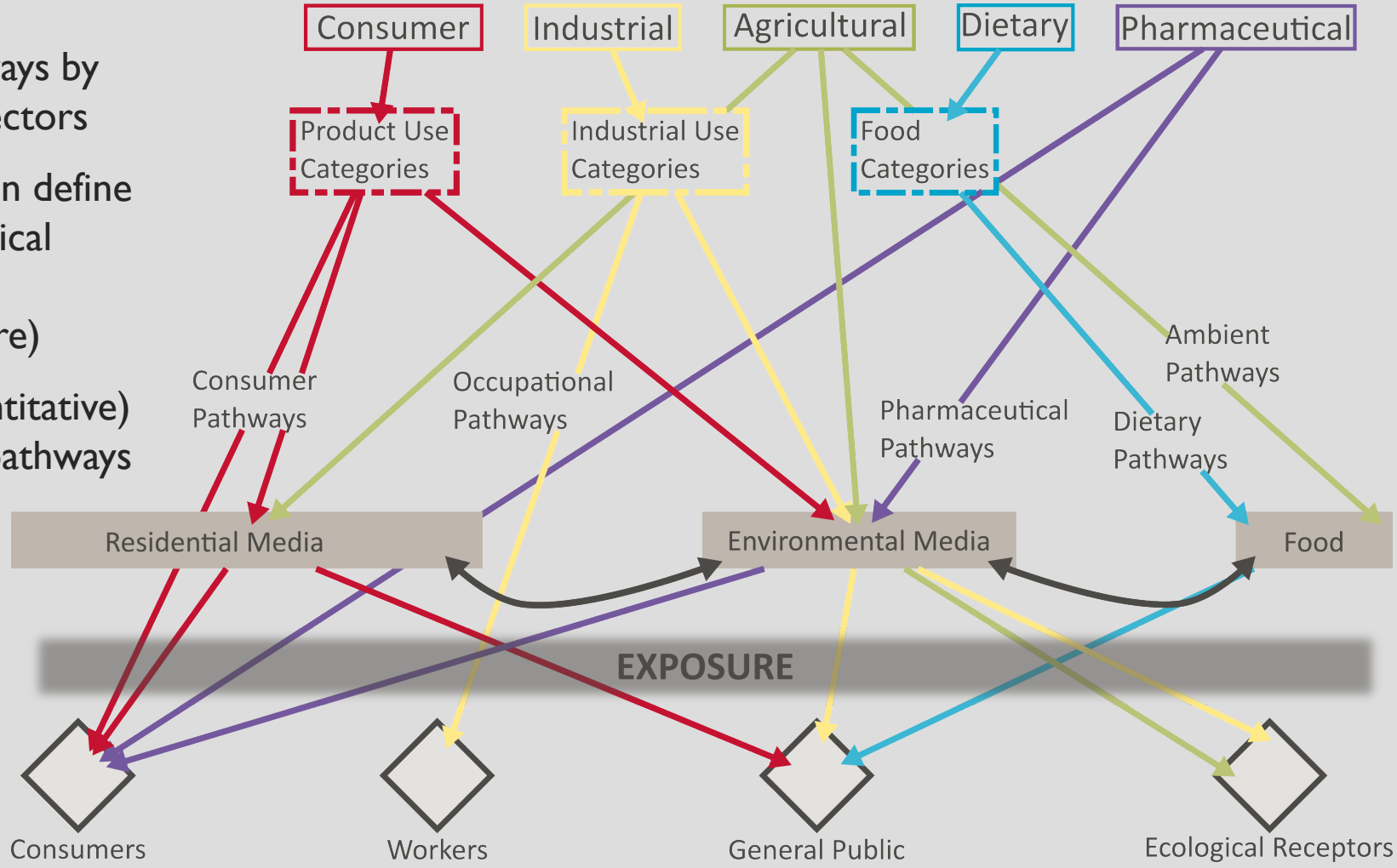
EXPOSURE PATHWAYS:
SOURCE TO RECEPTORS

- 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



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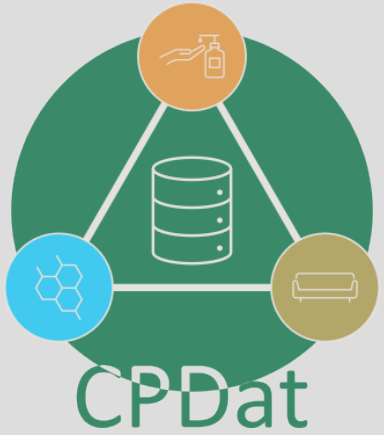
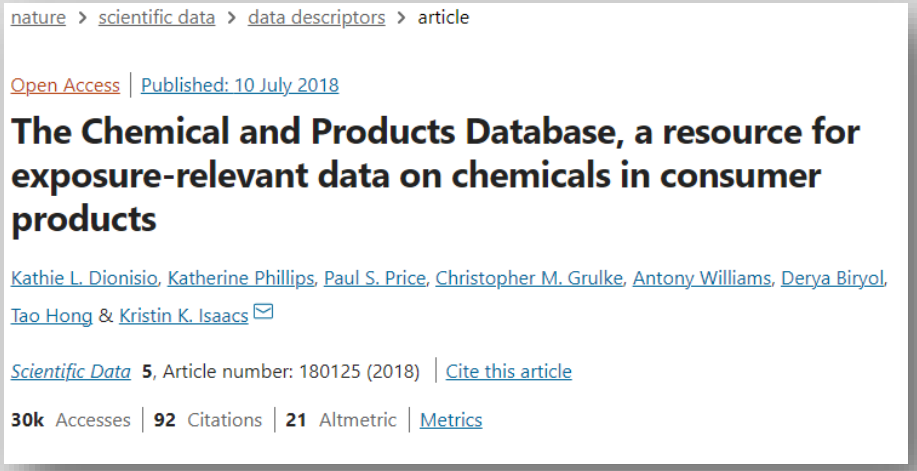
CHEMICAL AND PRODUCTS DATABASE





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

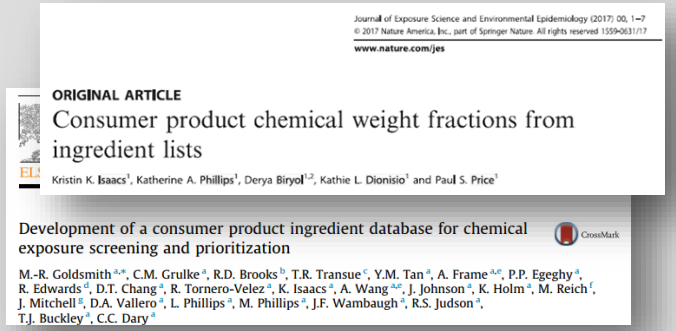
Scientific Data **5**, Article number: 180125 (2018) | Cite this article

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


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]

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]

Ingredient weight fraction data from previous EPA data collection efforts

Contents lists available at ScienceDirect

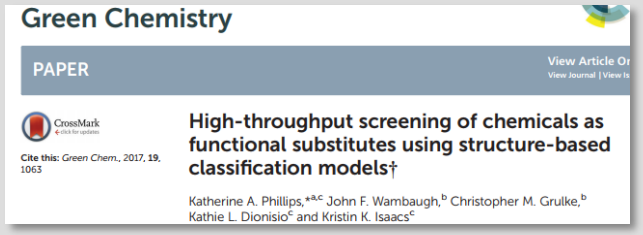
Toxicology Reports

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

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

Kathie L. Dionisio[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],

General use developed around consumer exposure


Green Chemistry

PAPER

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

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

Katherine A. Phillips,*[a,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

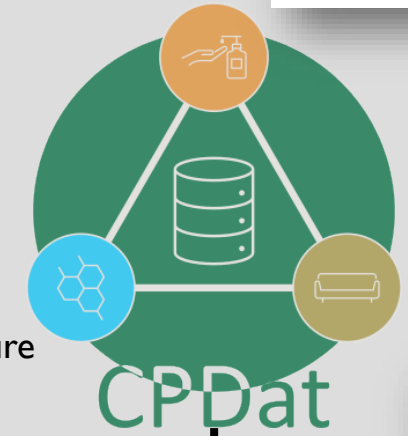
Review Article | Published: 26 November 2022

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

Kristin K. Isaacs, 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



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 | Publish...

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

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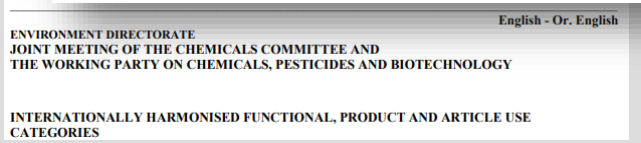
Journal of Exposure Science & Environmental Epidemiology 32, 794–807 (2022) | Cite this article


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**:

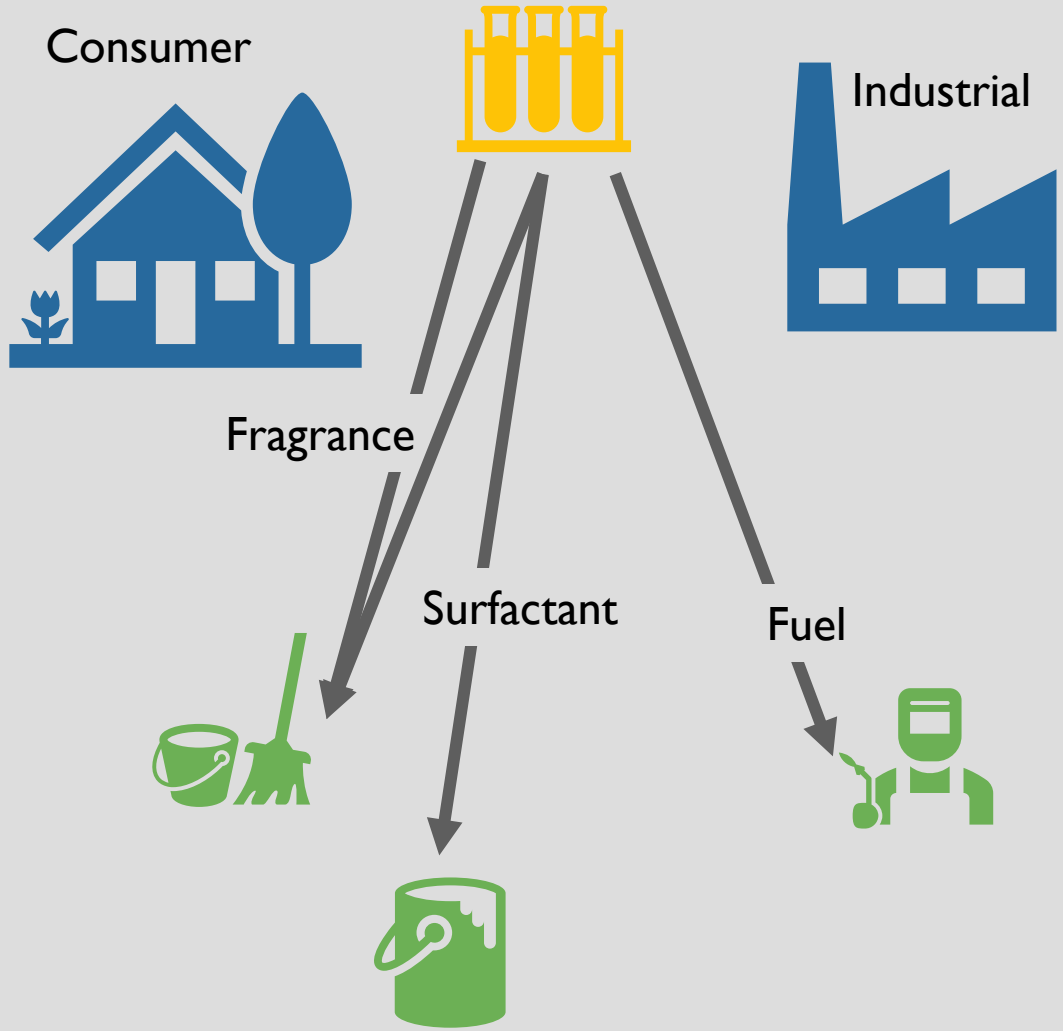
  Which groups use a chemical (i.e., industrial process *versus* consumer product)

- **End-use:**

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

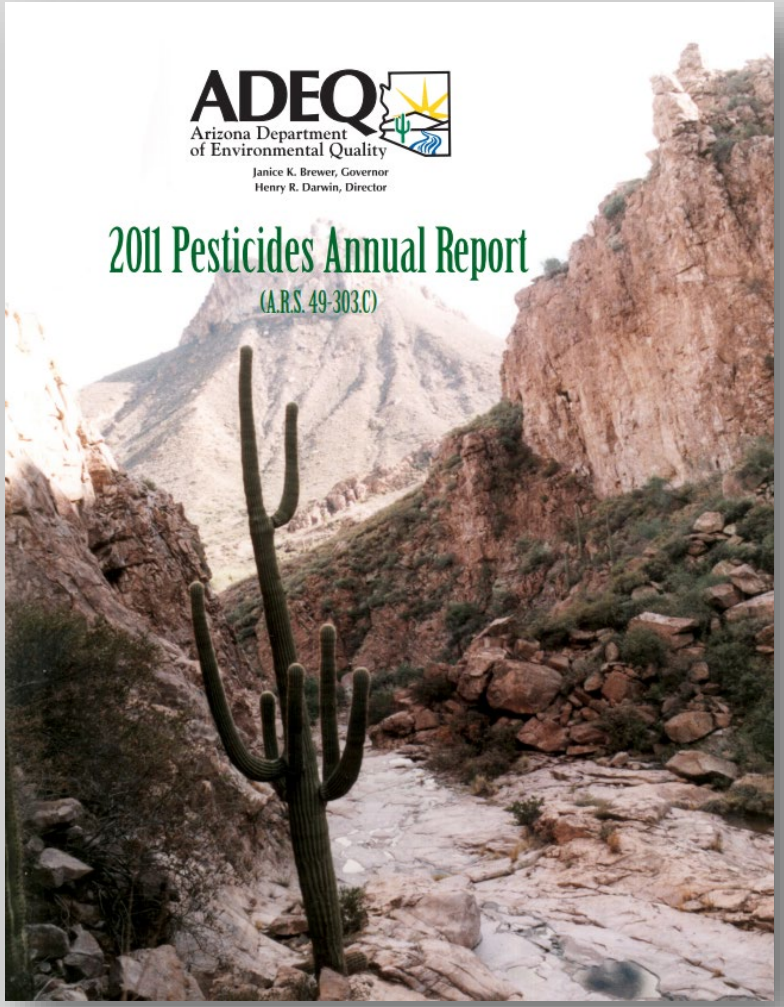
- **Functional Use**:

  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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CHEMICAL USE TYPES IN CPDAT

- Commercial Sector Use
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  - Use in particular products or product types
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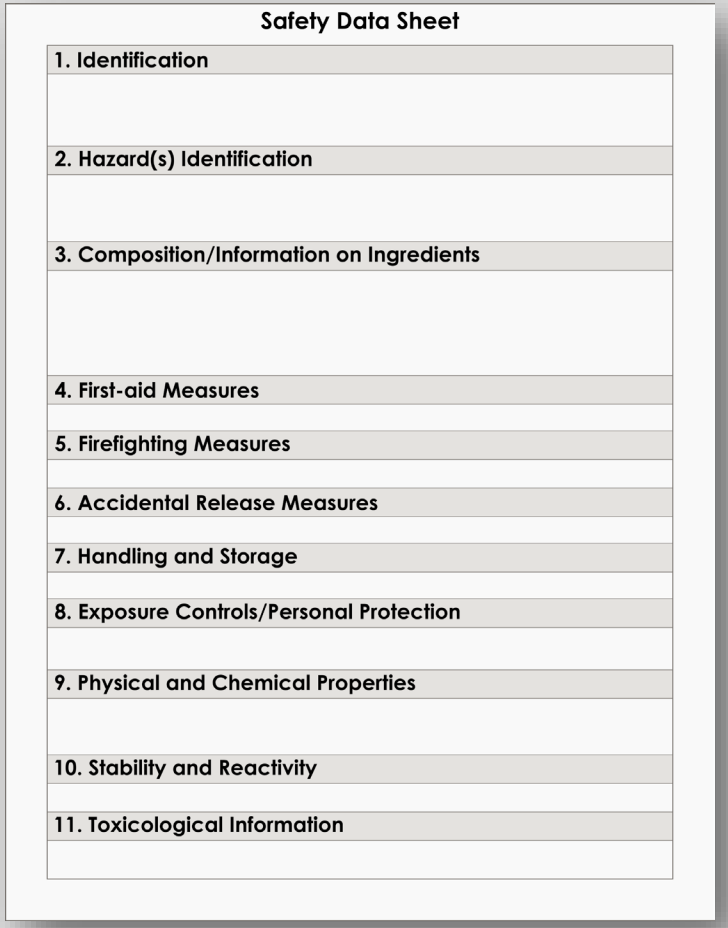
Safety Data Sheet

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

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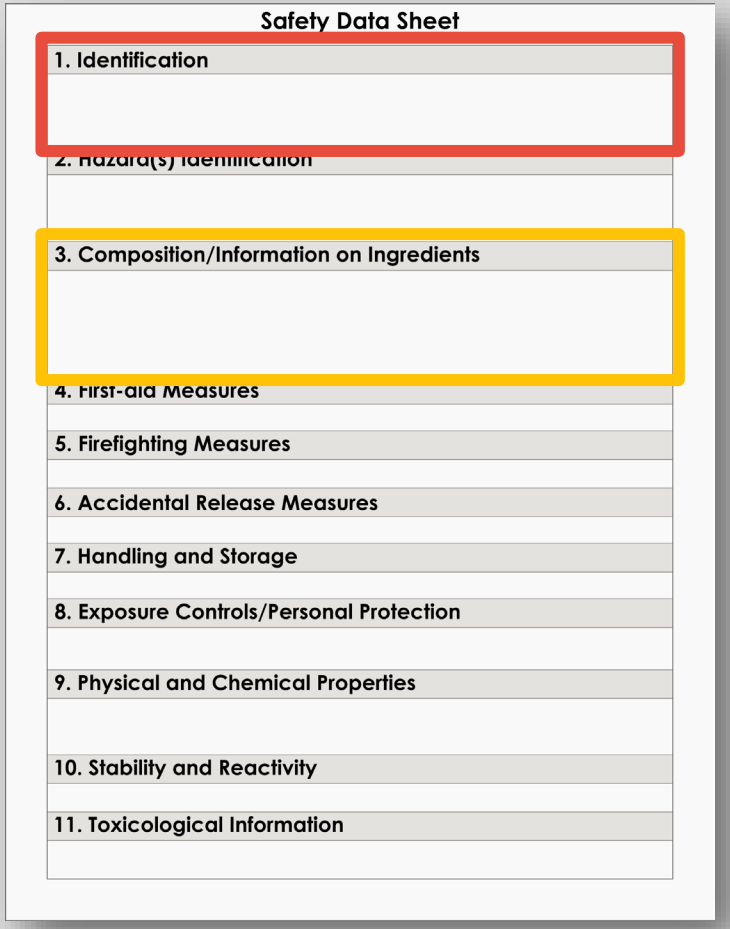

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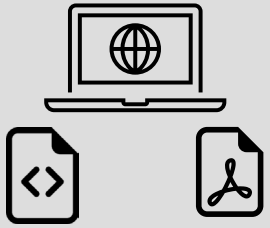
  - Use in particular products or product types
  - Organized by **Product Use Categories (PUCs)**
- Functional use
  - Role the chemical plays in different consumer products or industrial processes
  - Organized by OECD's **Function Categories (FCs)**

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

OVERVIEW OF CPDAT PIPELINE

Document Sources



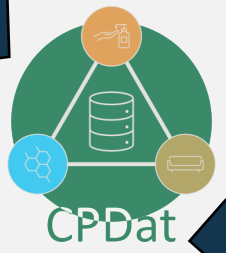
Publicly available data sources that have been identified for intake

Factotum

Internal EPA tool for curating exposure data and ensuring data provenance

- Document Management
- Data Curation
  - Composition Documents
  - List Presence Documents
  - Functional Use Documents
- Quality Assurance
- Data Delivery

Public Data Delivery



CPDat

Versioned, public database with latest Factotum curations

ChemExpo

Public web application for searching, exploring, and downloading latest version of CPDat

CompTox Chemicals Dashboard (CCD)
(Summary Data)

Public web application that surfaces only summary CPDat information

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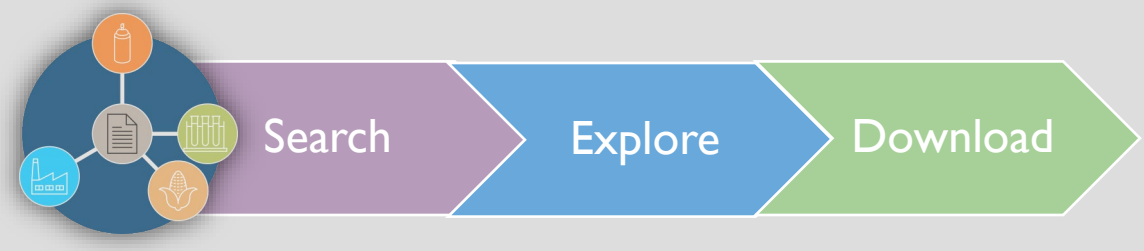
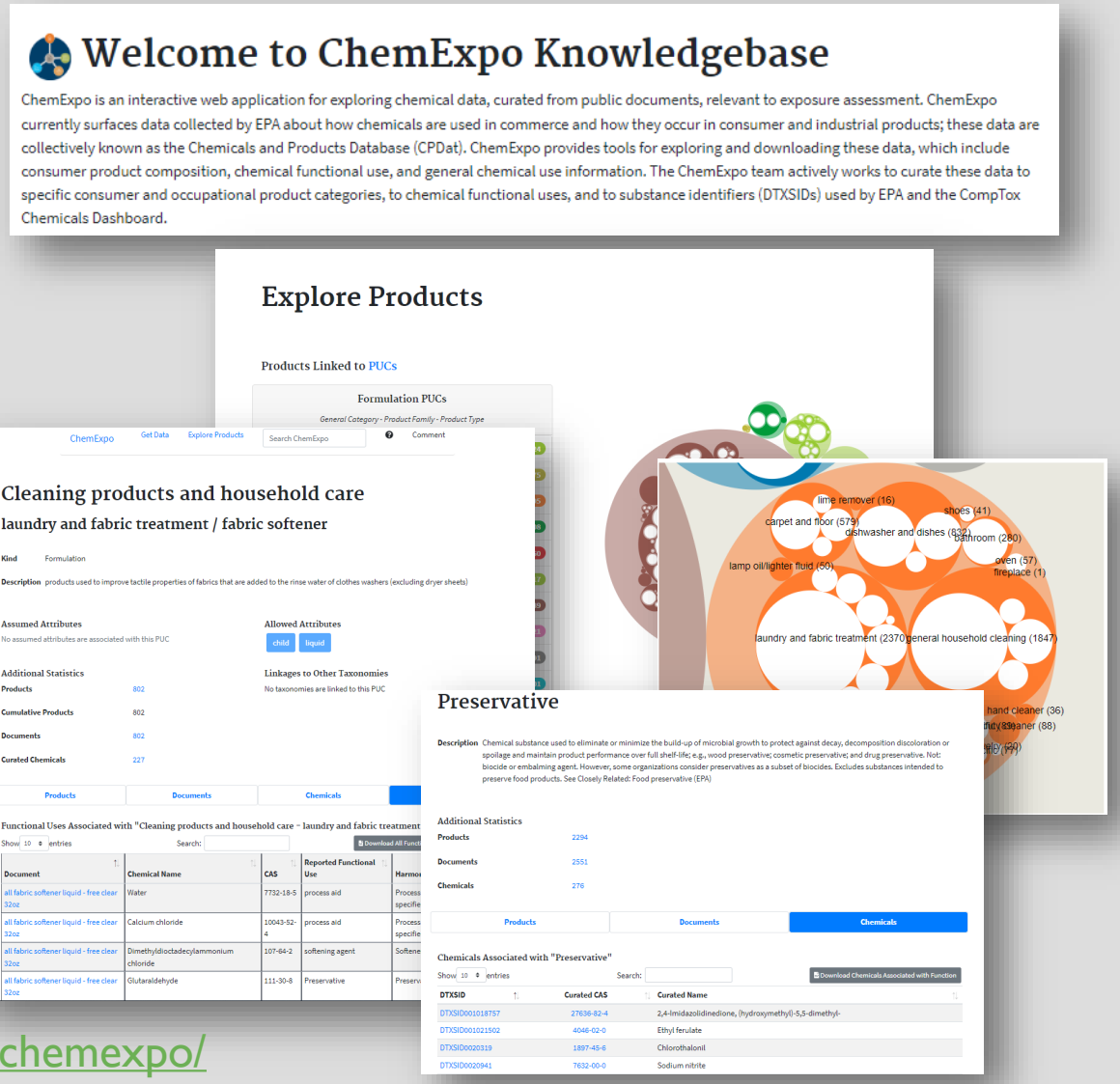
Center for Computational Toxicology and Exposure

CHEMEXPO KNOWLEDGEBASE

- **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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https://comptox.epa.gov/chemexpo/

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CHEMEXPO DEMO

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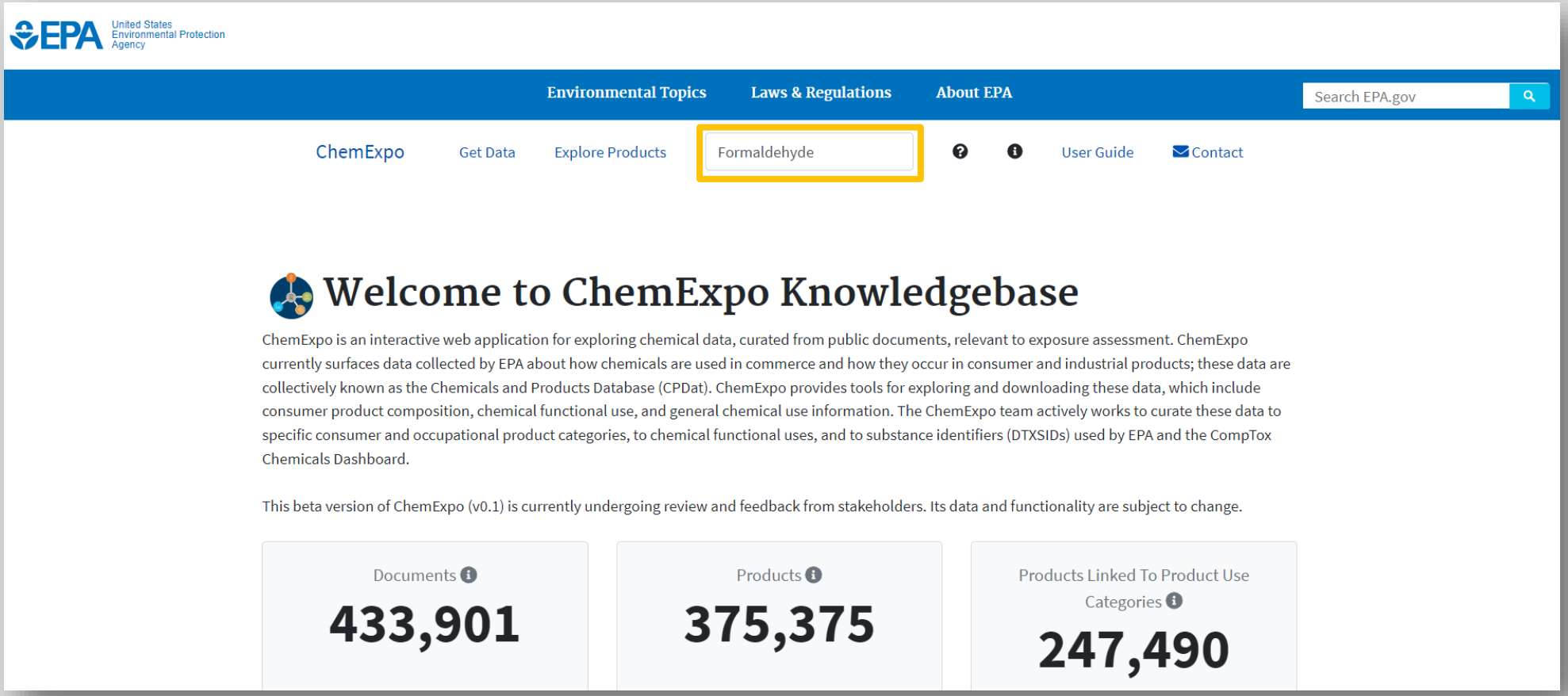
CHEMEXPO HOMEPAGE



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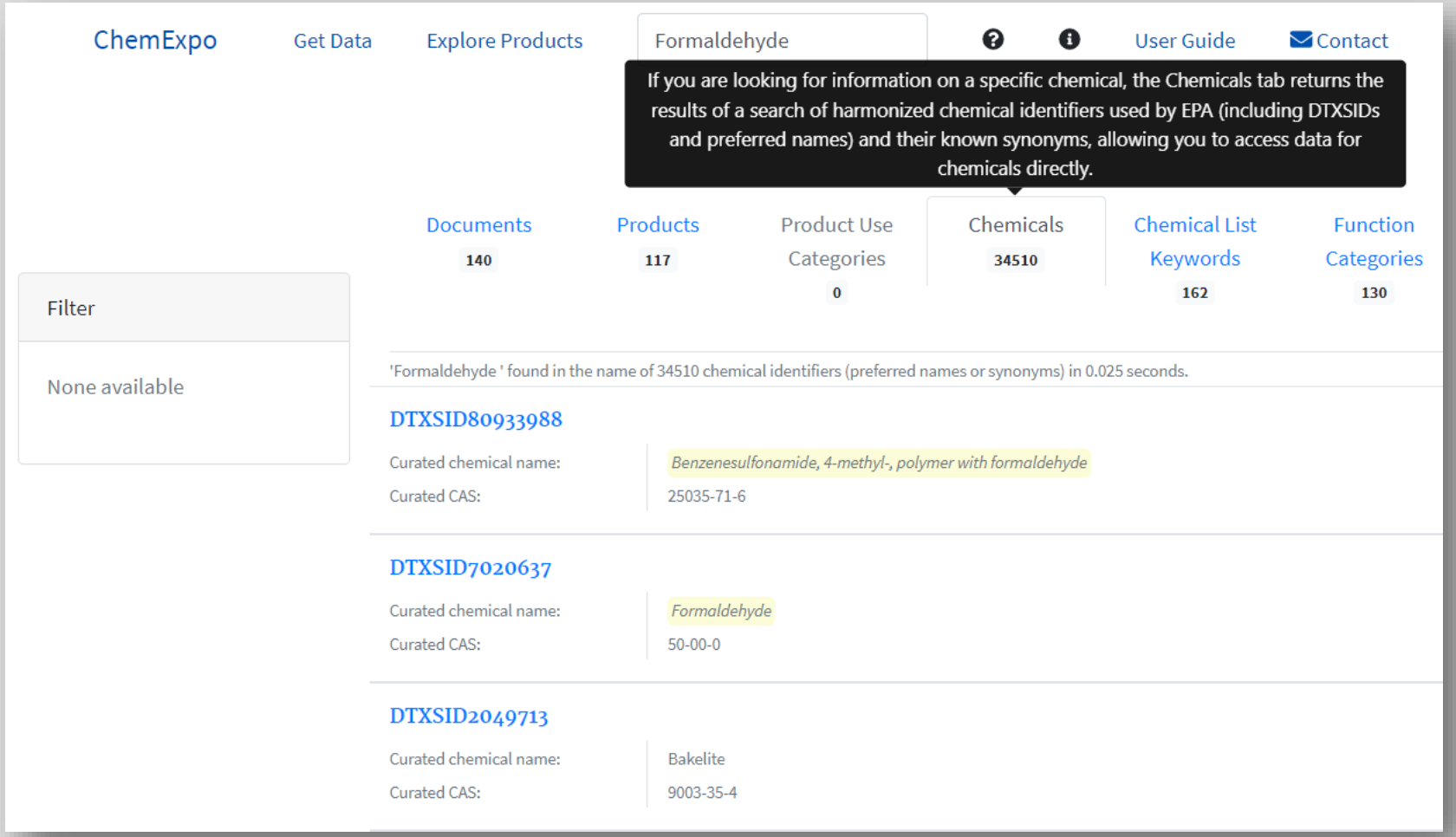
KEYWORD SEARCH



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CHEMICAL DETAIL PAGE: FORMALDEHYDE

Formaldehyde

DTXSID7020637

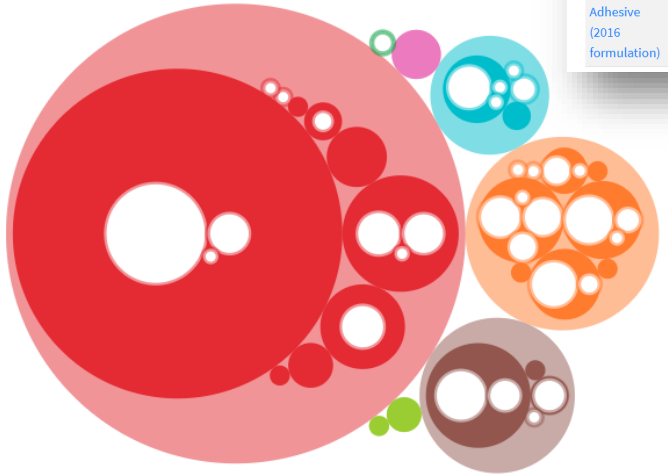
50-00-0

Explore products containing this chemical. Use the filter buttons to filter the tables below to certain Product Use Categories. Click the info b
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 1
- Cleaning products and household care 72
- Electronics/small appliances 2
- Food and drug 3
- Home maintenance 376
- Personal care 38
- Pesticides 6
- Vehicle 29



Products | Documents | Function

Products Containing "Formaldehyde"

Show All Products

Show 10 entries Search: Download Products and Weight Fractions

Product	Manufacturer	Brand	Document	PUC	PUC Kind	Classification Method
Ardell Starter Kit, 105 Black (2014 formulation)	American International Industries	Ardell	Ardell Starter Kit, 105 Black (2014 formulation)	Personal care - makeup and related - eye makeup	Formulation	Bulk Assignment
Salon Perfect Strip Eyelash Adhesive (old formulation)			Salon Perfect Strip Eyelash Adhesive (old formulation)	Personal care - makeup and related - eye makeup	Formulation	Bulk Assignment
Duo Striplash Adhesive (2016 formulation)		Duo	Duo Striplash Adhesive (2016 formulation)	Personal care - makeup and related - eye makeup	Formulation	Bulk Assignment

Products | Documents | Function

Functions Associated with "Formaldehyde"

Show All Functions

Show 10 entries Search: Download Functions

Data Type	Document	Reported Function	Harmonized Function
Composition	wellmade performance flooring	binder	Binder
Composition	zep tri foam	Preservative	Preservative
Composition	zep tri foam	Preservative	Preservative
Composition	heavy duty glass cleaner concentrate	Preservative	Preservative
Composition	aap clear coat protectant yellow pina colada	Preservative	Preservative
Composition	clean ems disinfectant twls	Preservative	Preservative
Composition	zep blue foaming clear coat protectant	Preservative	Preservative
Composition	zep pink foaming clear coat protectant	Preservative	Preservative

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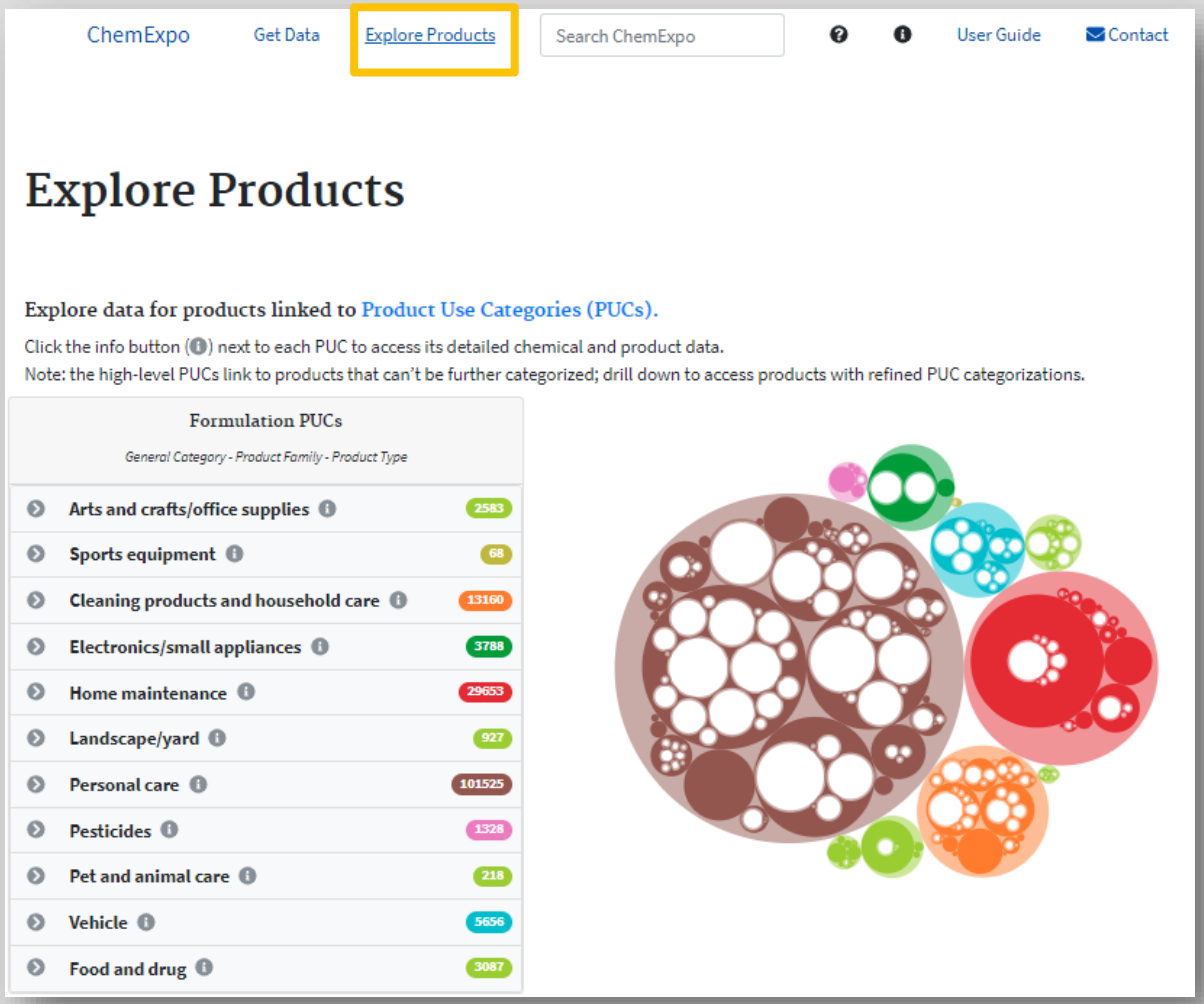
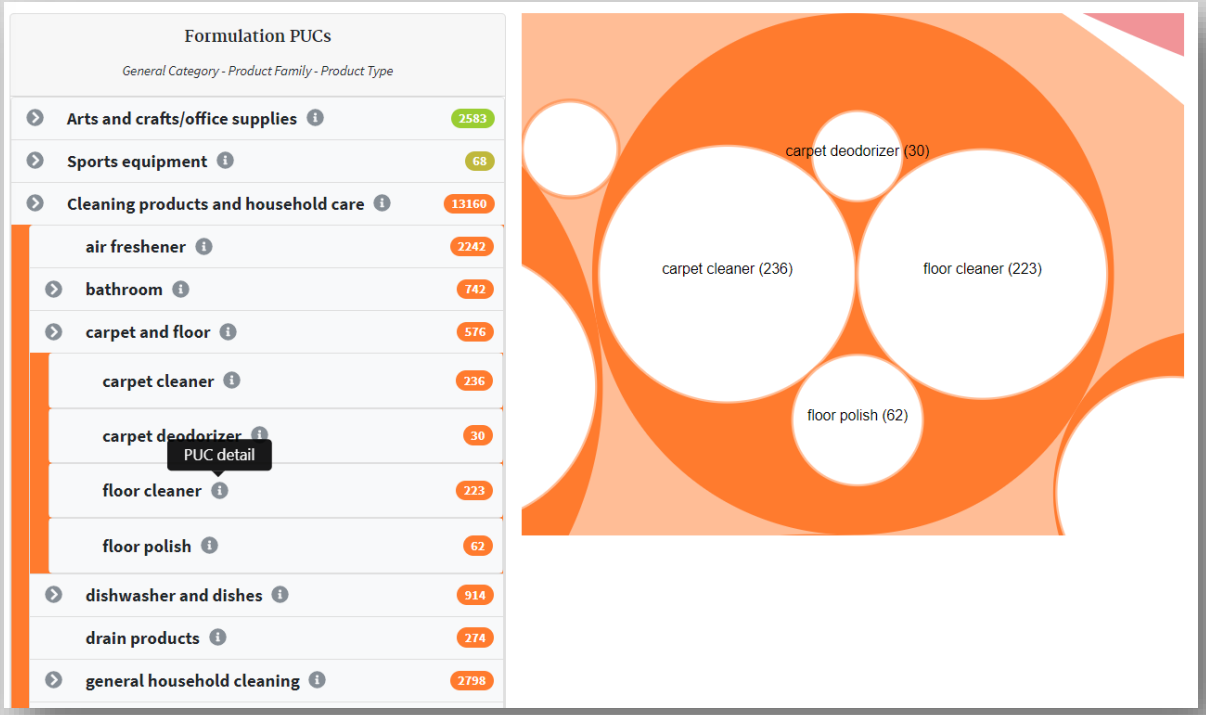
EXPLORE PRODUCTS





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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 sp

Additional Statistics

Products	223
Cumulative Products	223
Documents	222
Curated Chemicals	231

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

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

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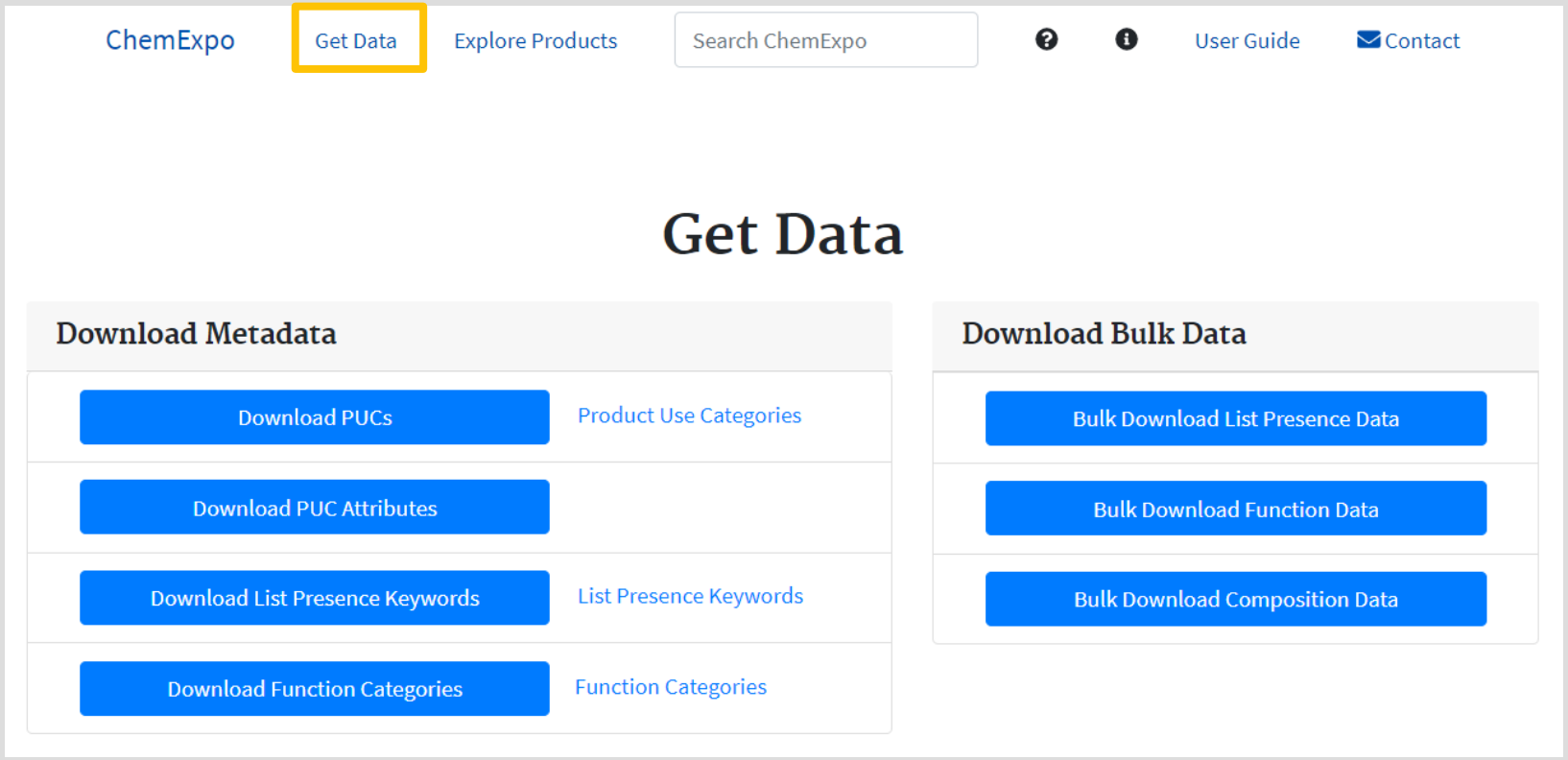
DOWNLOAD DATA



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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...

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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	

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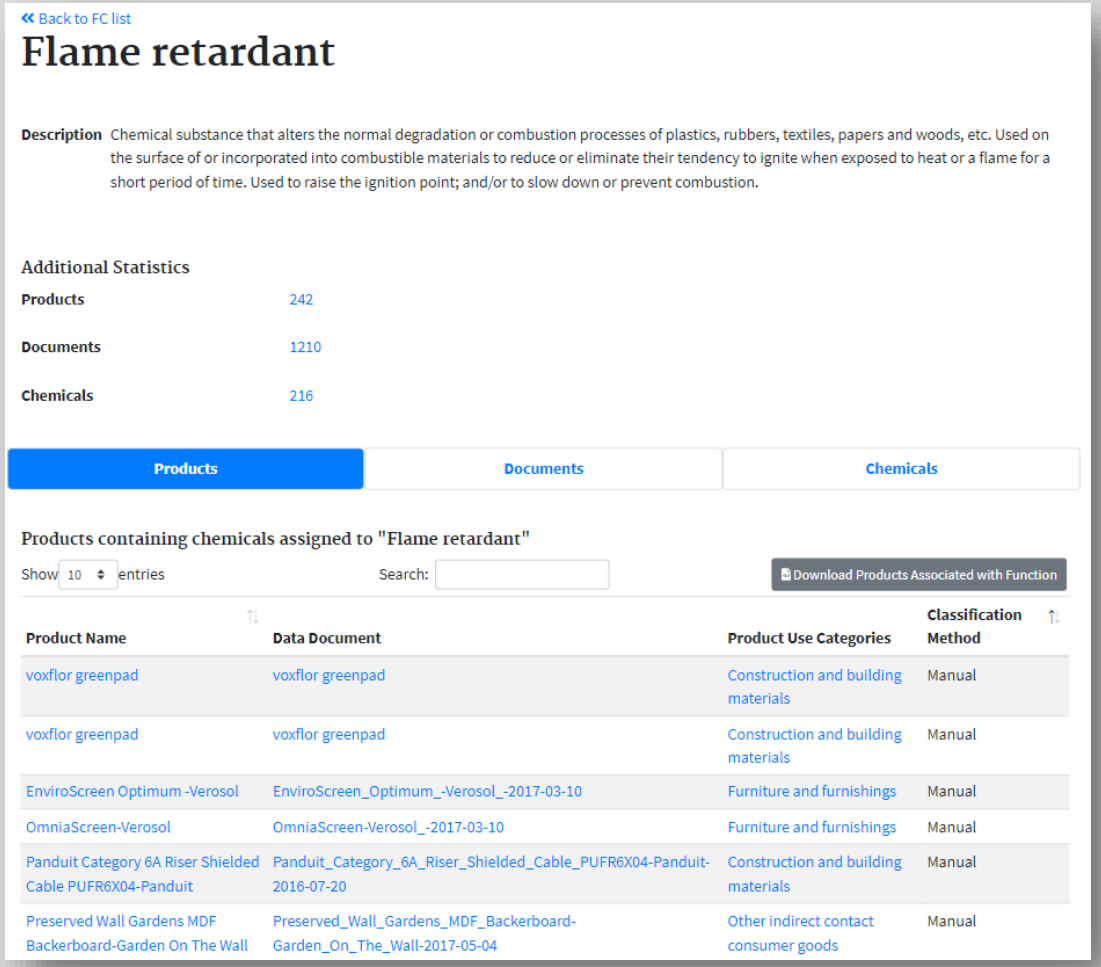
FUNCTION DETAIL PAGE: FLAME RETARDANT



« 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

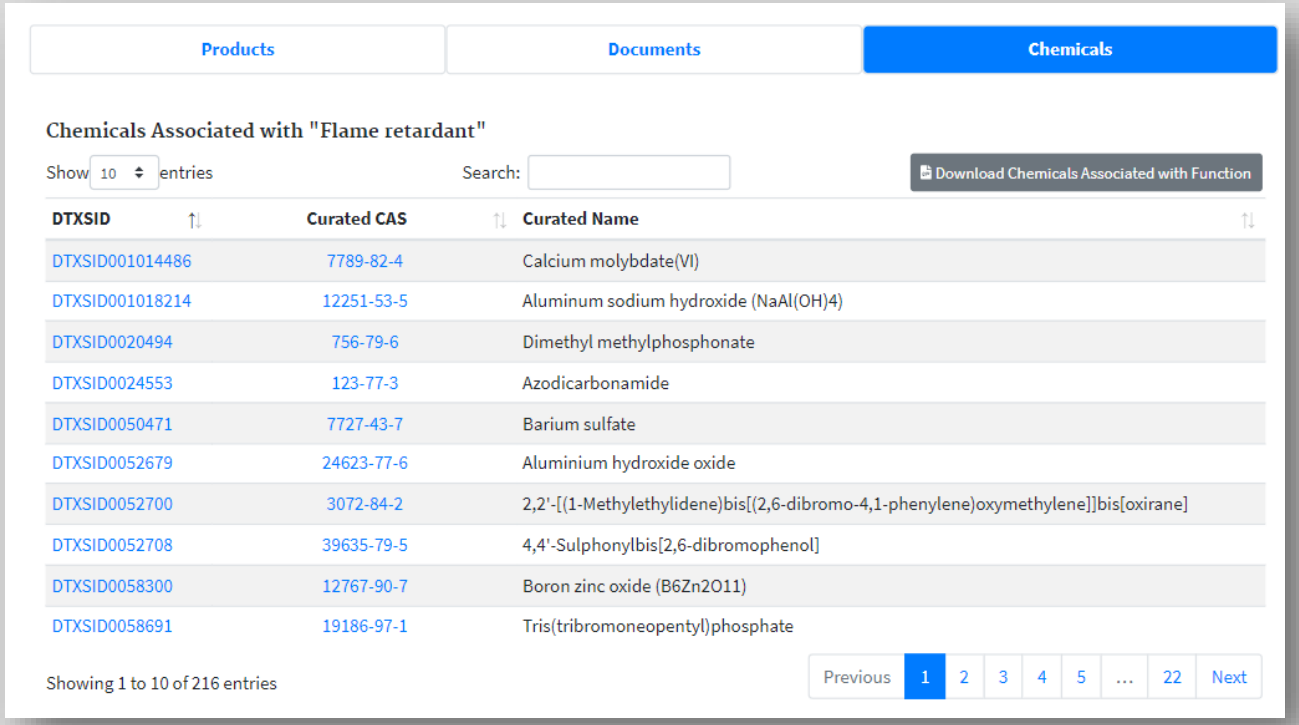
Products	242
Documents	1210
Chemicals	216

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 PUFR6X04-Panduit	Panduit_Category_6A_Riser_Shielded_Cable_PUFR6X04-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

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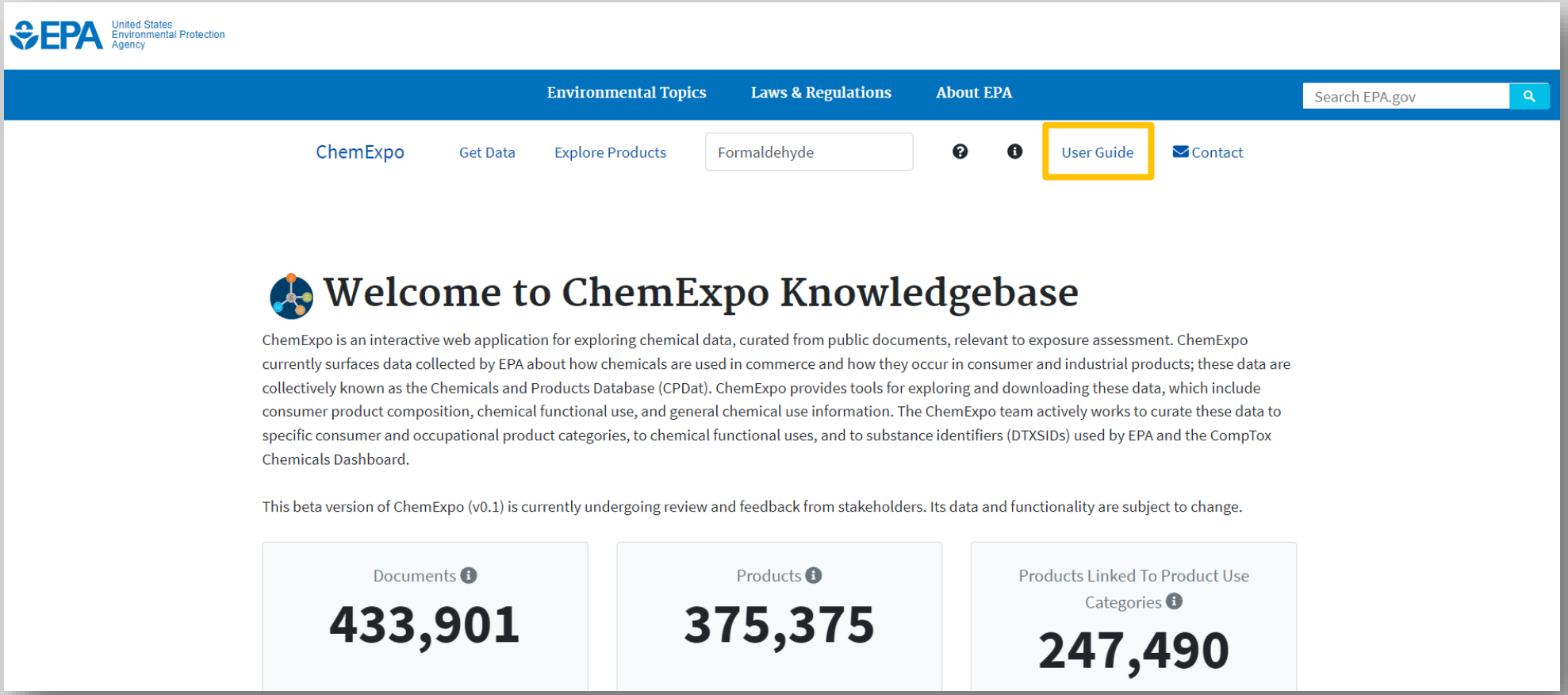

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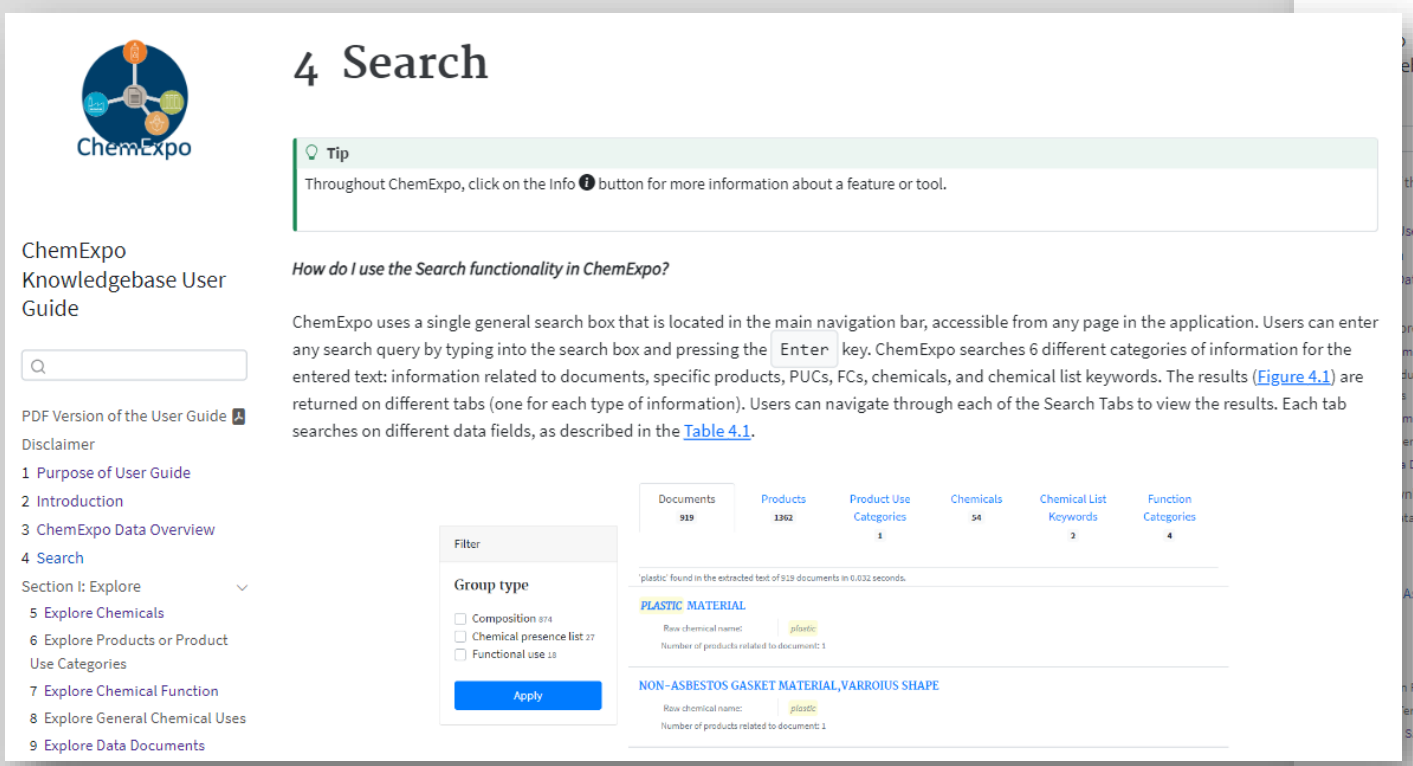
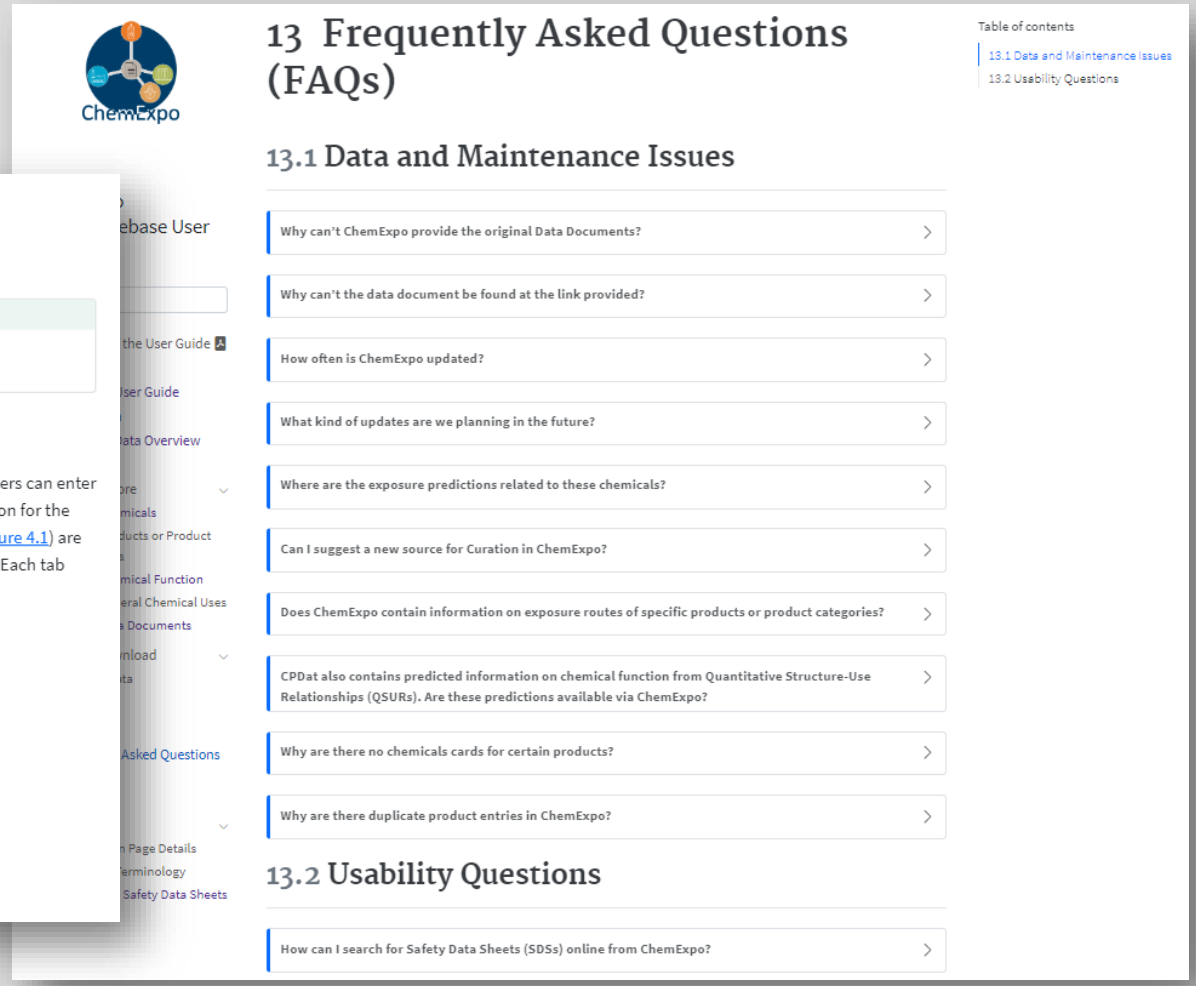
CHEMEXPO USER GUIDE





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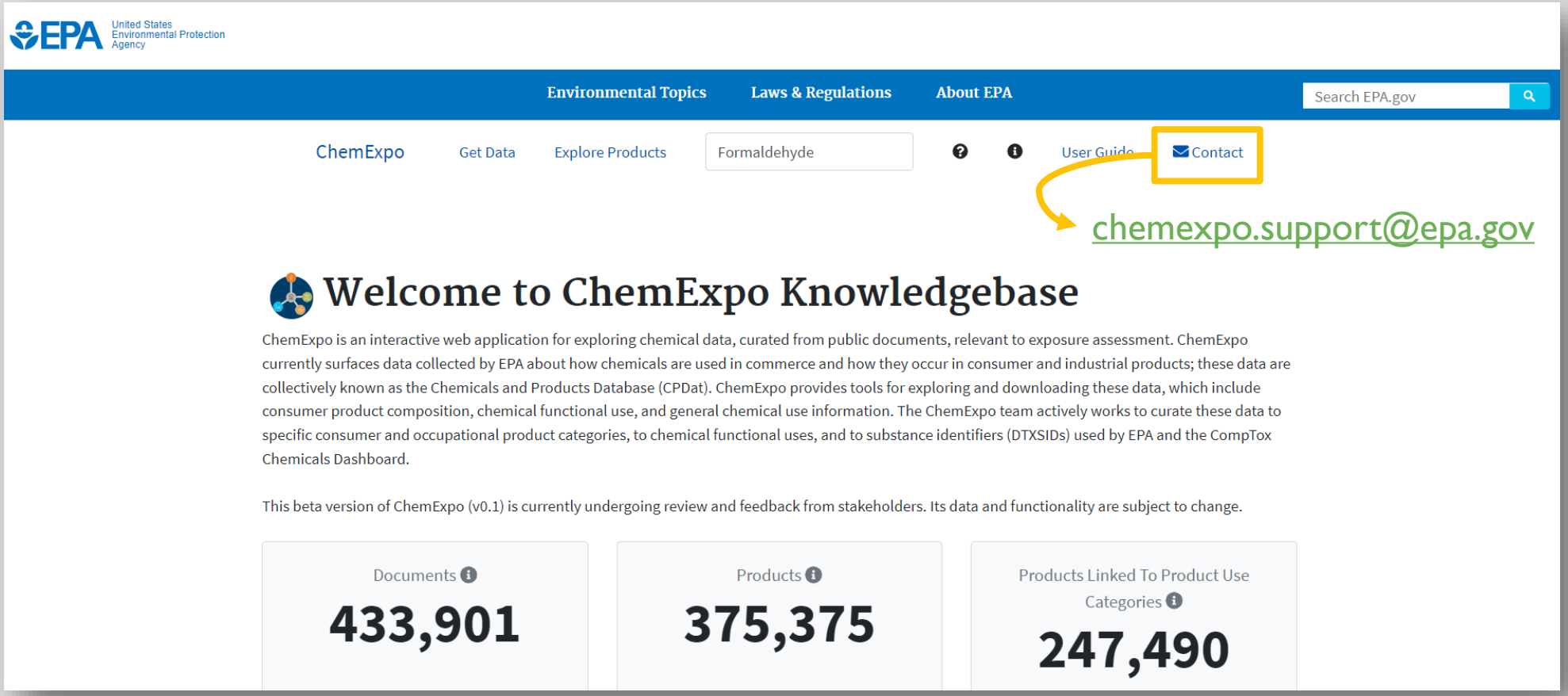
CHEMEXPO HELP



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WRAPPING UP

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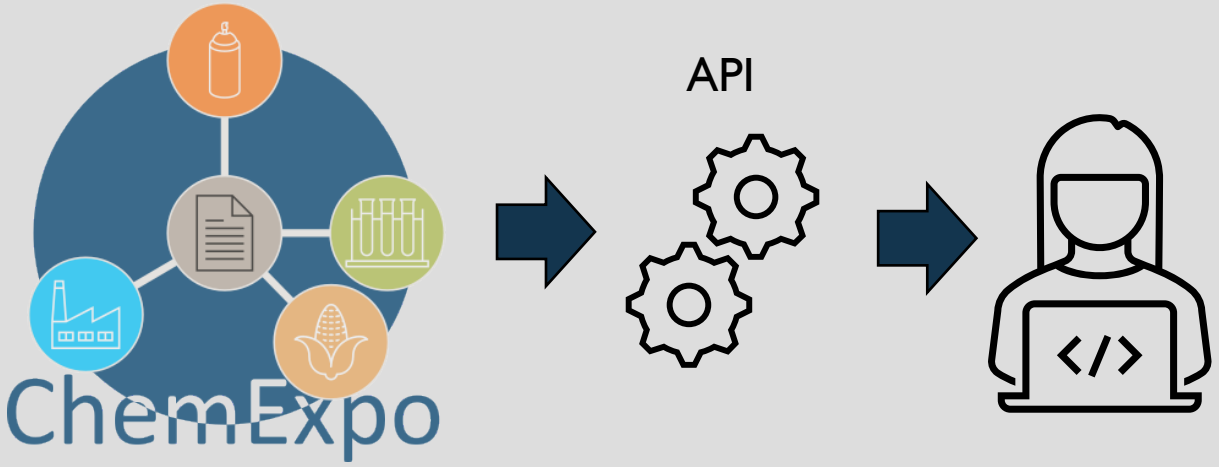
FUTURE WORK

- Formal peer-review of ChemExpo
- CPDat v4.0 and accompanying peer review manuscript
- Development and release of ChemExpo Application Programming Interfaces (APIs)



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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!

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THANK YOU!!

U.S. EPA

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GDIT

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