Exploring consumer exposure pathways and patterns of use for chemicals in the environment through the Chemical/Product Categories Database (CPCat)

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Resources

- CPCPdb
  - Goldsmith et al., Development of a consumer product ingredient database for chemical exposure screening and prioritization. *Food & Chemical Toxicology.* 2014.
- CPCat
  - Dionisio et al., Exploring consumer exposure pathways and patterns of use for chemicals in the environment. *Toxicology Reports*. 2015.
  - http://actor.epa.gov/cpcat
  - NCCT Communities of Practice talk, 1/23/2014, available online at: http://www.epa.gov/ncct/communities_of_practice.html

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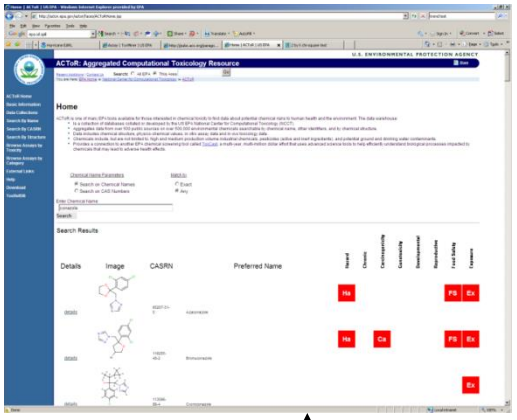
The Origin of ACToR: The Chemical Landscape Project

- ACToR (Aggregated Computational Toxicology Resource)
- What is the unique set of chemicals EPA is most concerned with?
  - Targets for the overall ToxCast Program
- How much is known about these chemicals?
- Where are the data gaps?
- Collaboration across EPA
  - Office of Research and Development (ORD)
  - Office of Pesticide Programs (OPP)
  - Office of Pollution Prevention and Toxics (OPPT)
  - Office of Water (OW)
  - Great Lakes National Program Office (GLNPO)
  - Endocrine Disruptor Screening Program (EDSP)
- Running this study required building a database

ACToR: An Optimal Home for CPCat

Aggregated Computational Toxicology Resource

http://actor.epa.gov/



ACToR API

Chemical

Chemical ID, Structure

Internet Searches

ACToR Core

Tabular Data, Links to Web Resources

ToxRefDB

In Vivo Data (NCCT, OPP)

ToxCastDB

ToxCast Data (NCCT, ORD, Collaborators)

ExpoCastDB

Exposure Biomonitoring Data (NERL, NCCT)

CPCat

Chemical and Product category and use data (NCCT, NERL)

CPCat: Chemical and Product Category Database

- There is a need to catalog how chemicals are used
- One major input to exposure modeling
- Information exists but was widely dispersed
- Use ACToR to help bring this data together
- Create CPCat database
  - Chemical use categories
  - Product use categories
  - Mapping from chemicals to products
- ACToR UseDB one part of CPCat
- Access CPCat through ACToR:
  - http://actor.epa.gov/cpcat

General classes of chemical use categories

- Use associated categories
  - e.g., a chemical used in lipstick
- Functional-use categories
  - e.g., a solvent
- Product-use categories
  - e.g., chemicals used in bathtub toys
- Therapeutic-use categories
  - e.g., antibiotics
- Industrial sector-use categories
  - e.g., mining

CPCat data sources (>40,000 unique chemicals included)

Original data source	Class of categories	Original categories	CPCat cassettes	Chemicals
ACToR Data Sets and Lists	General-use	131	173	35,838
ACToR UseDB	General-use	15	15	31,622
CDR 2012:				
Consumer	General-use	34	36	3,321
Industrial Function	Functional-use	34	27	5,023
Industrial Sector	Industrial sector-use	42	43	5,226
DfE	Functional-use	11	9	444
Dow	Functional-use	19	18	104
DrugBank	Therapeutic-use	582	460	1,754
2006 IUR	General-use	19	24	1,152
KemI	Functional-use	61	31	876
NICNAS	General-use	17	17	177
Retail Product Categories	Product-use	359	191	2,778
SPIN:				
detpcat	General-use	781	284	6,491
Industrial Sector	Industrial sector-use	580	221	4,603
NACE	Industrial sector-use	57	52	7,745
UC62	General-use	61	59	9,059
Toxome	Functional-use	16	16	442

ACToR UseDB

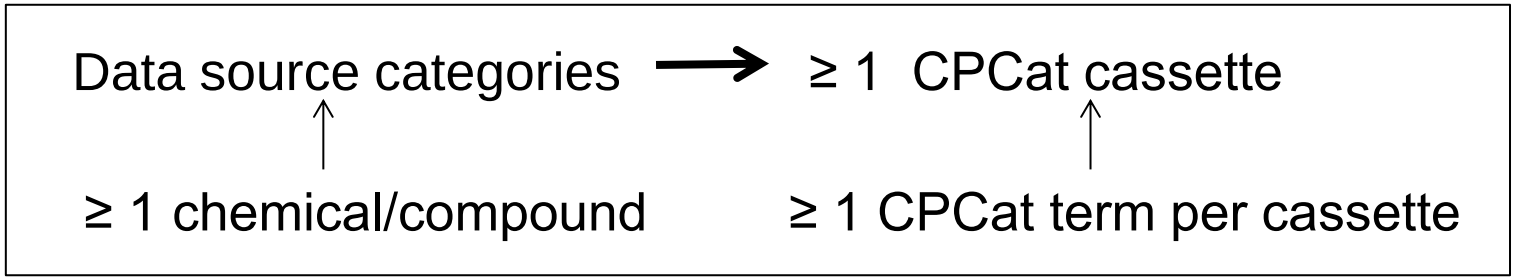
- Mined the ACToR database and assigned chemicals to a small number of high-level chemical use categories

  - Antimicrobials
  - Chemical/industrial process
  - Chemical warfare
  - Colorants/dyes
  - Consumer use
  - Fertilizer
  - Flame retardant
  - Food use/food additive
  - Fragrances
  - Herbicide
  - Inert ingredients in pesticides
  - Personal care products
  - Pesticides
  - Petrochemicals
  - Pharmaceuticals

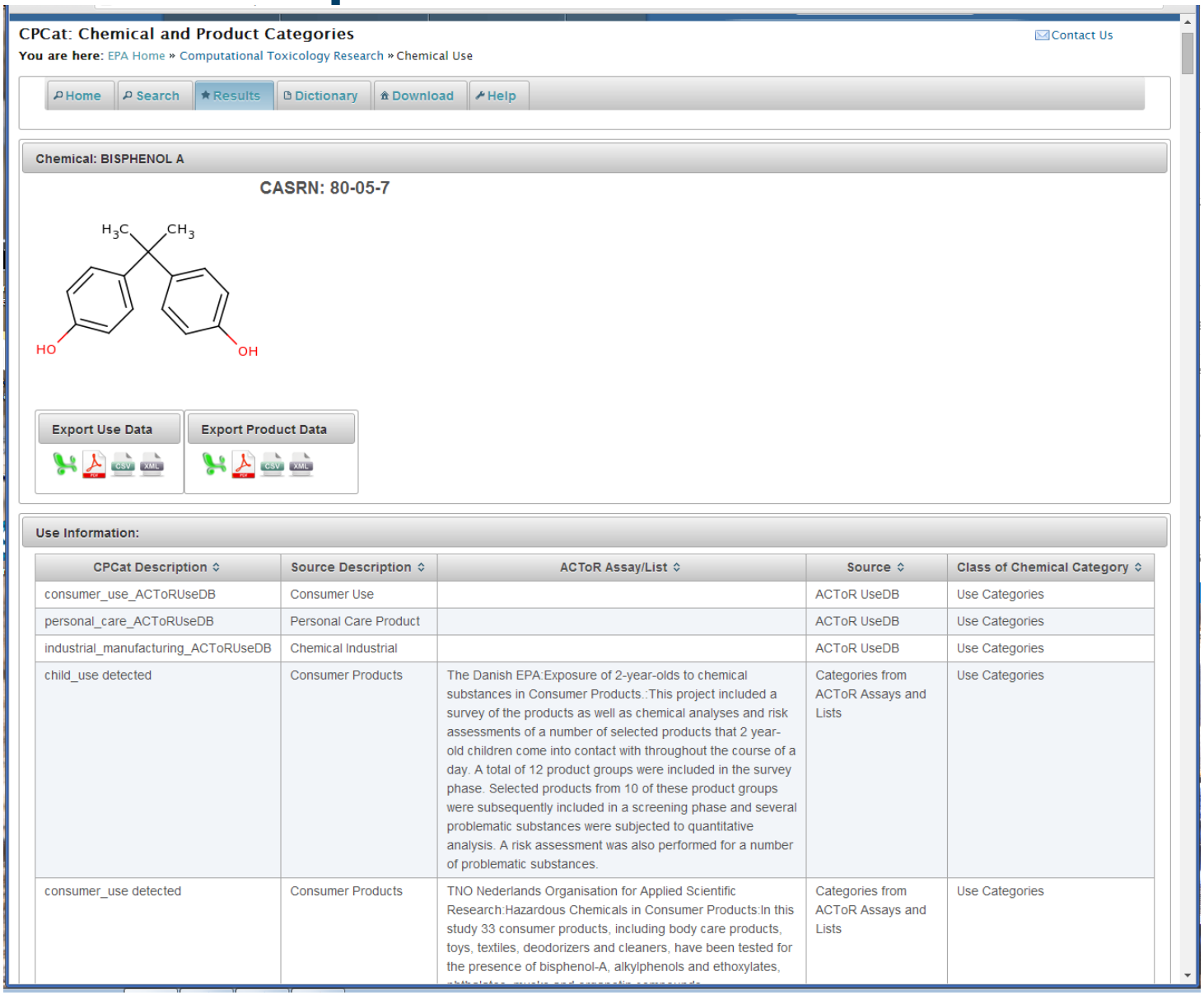
For an example of application of the above use categories, see: Wambaugh et al., “High Throughput Heuristics for Prioritizing Human Exposure to Environmental Chemicals.” *Environ Sci Technol* 2014.

CPCat term/cassette assignment

- Each data source has its own category hierarchy
- These are harmonized in CPCat by manually mapping categories from data sources to a common set of “terms” (keywords/categories)
- Categories from data sources were manually mapped to one or more CPCat “cassettes”
- Each CPCat cassette is made up of one or more CPCat terms describing the product or usage
- CPCat assigns 377 unique terms and 824 unique cassettes, excluding drug related terms/cassettes (833 terms and 1,297 cassettes total)



CPCat Example Search Screenshot: Bisphenol A



CPCat: Chemical and Product Categories

Contact Us

You are here: EPA Home » Computational Toxicology Research » Chemical Use

Home | Search | Results | Dictionary | Download | Help

Chemical: BISPHENOL A

CASRN: 80-05-7

Export Use Data | Export Product Data

Use Information:

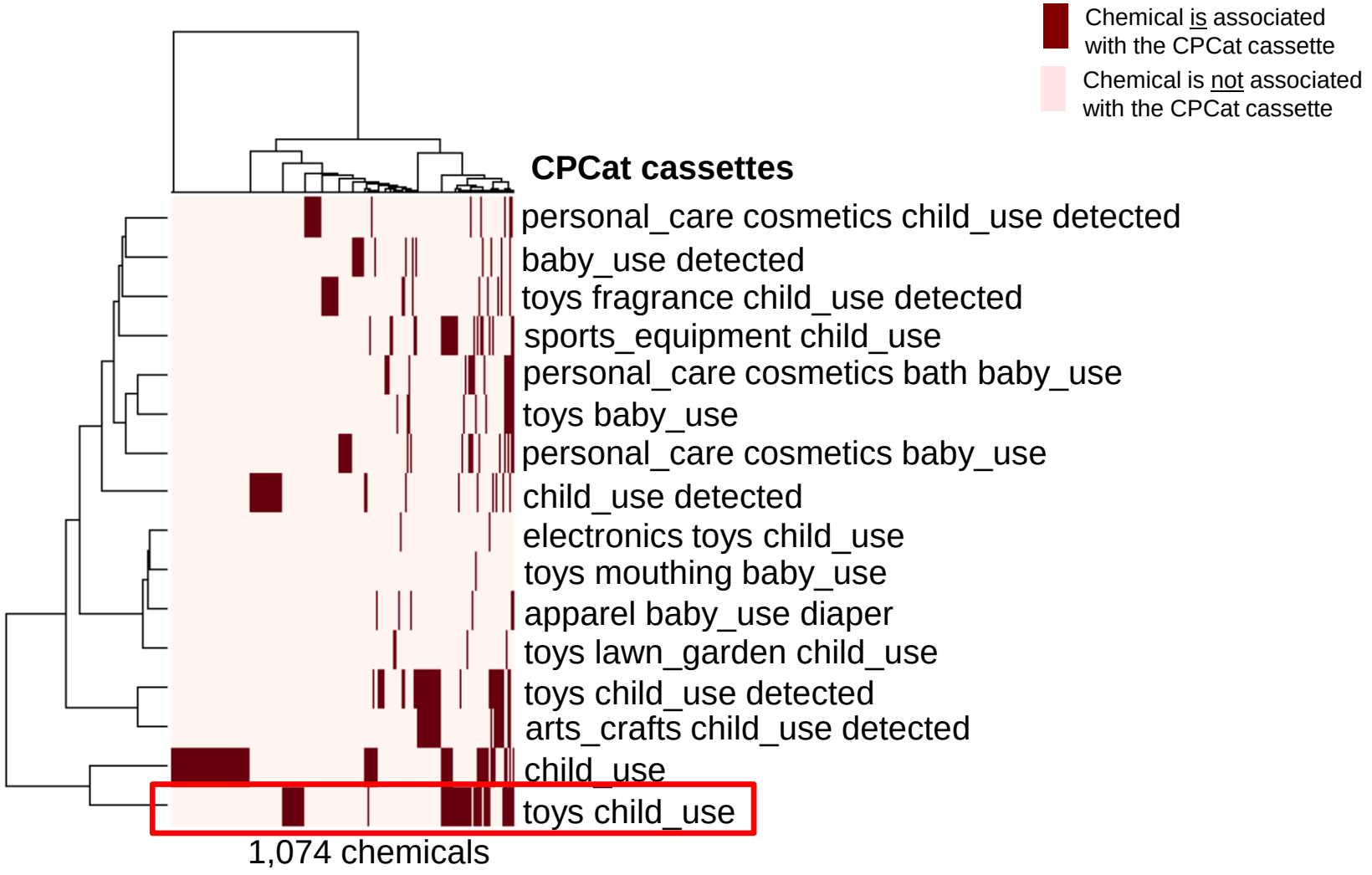
CPCat Description	Source Description	ACToR Assay/List	Source	Class of Chemical Category
consumer_use_ACToRUseDB	Consumer Use		ACToR UseDB	Use Categories
personal_care_ACToRUseDB	Personal Care Product		ACToR UseDB	Use Categories
industrial_manufacturing_ACToRUseDB	Chemical Industrial		ACToR UseDB	Use Categories
child_use detected	Consumer Products	The Danish EPA:Exposure of 2-year-olds to chemical substances in Consumer Products.:This project included a survey of the products as well as chemical analyses and risk assessments of a number of selected products that 2 year-old children come into contact with throughout the course of a day. A total of 12 product groups were included in the survey phase. Selected products from 10 of these product groups were subsequently included in a screening phase and several problematic substances were subjected to quantitative analysis. A risk assessment was also performed for a number of problematic substances.	Categories from ACToR Assays and Lists	Use Categories
consumer_use detected	Consumer Products	TNO Nederlands Organisation for Applied Scientific Research:Hazardous Chemicals in Consumer Products:In this study 33 consumer products, including body care products, toys, textiles, deodorizers and cleaners, have been tested for the presence of bisphenol-A, alkylphenols and ethoxylates,	Categories from ACToR Assays and Lists	Use Categories

CPCat terms associated with ethyl paraben

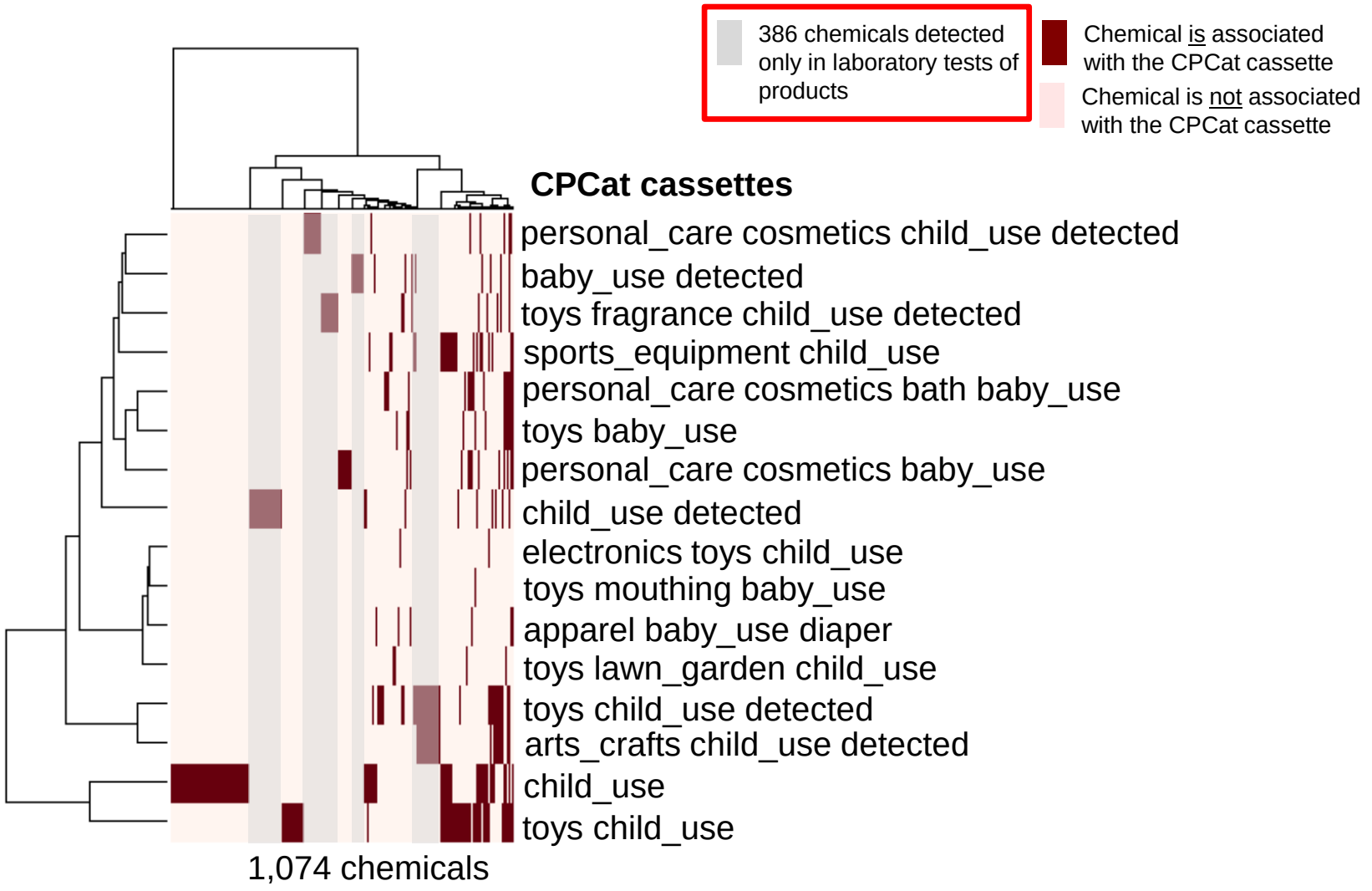
agricultural*
arts_crafts*
automotive_care
child_use
cleaning_washing*
construction
consumer_use_ACToRUseDB
detergent
drug*
electronics batteries*
facility salon detected
fluid_property_modulator
food_additive*
food_additive_ACToRUseDB
food_contact
fragrance consumer_use
hunting
industrial cleaning_washing
industrial_manufacturing_ACToRUseDB
inert_ACToRUseDB
manufacturing chemical
manufacturing cleaning_washing polish
manufacturing detergent
manufacturing drug
manufacturing export
manufacturing metals
manufacturing personal_care*
manufacturing soap
paint
paraben
personal_care
personal_care bath
personal_care cosmetics*
personal_care sanitizer hand
personal_care sexual_wellness gel detected
personal_care shower gel
personal_care soap*
personal_care sunscreen*
personal_care wash*
personal_care_ACToRUseDB
pesticide*
photographic
preservatives
raw_material personal_care cosmetics
sports_equipment
surface_treatment
tools personal_care hair
toys*

A * indicates multiple cassettes containing additional CPCat terms

Use CPCat to enumerate chemicals for child exposure scenario



Use CPCat to enumerate chemicals for child exposure scenario



Potential Use in EDSP: Exposure Routes for SDWA Chemicals

- Select consumer exposure related CPCat cassettes

adhesive consumer_use*
air_fresheners consumer_use*
air_treatment consumer_use
apparel*
apparel_care*
appliance consumer_use*
arts_crafts*
automotive_care consumer_use
automotive_component consumer_use*
baby_use detected*
batteries consumer_use
beverage*
building_material consumer_use*
child_use*
cleaning_washing*
colorant consumer_use detected
consumer_use
consumer_use_ACToRUseDB
décor*
drinking_water*
drinking_water_contaminant*
electronics*
explosives consumer_use
extermination consumer_use
fertilizer consumer_use
flame_retardant
food*
food_additive*
food_contact*
food_residue*
fragrance consumer_use
fuel automotive
fuel consumer_use
fungicide consumer_use
furniture*
heating*
hunting
impregnation consumer_use detected
lawn_garden consumer_use
leather consumer_use
lubricant consumer_use*
personal_care*
personal_care ACToRUseDB
pesticide consumer_use
pet
polish apparel_care footwear
solvent consumer_use
sports_equipment*
stoves consumer_use
surface_treatment consumer_use
tea_coffee
textile consumer_use*
toilets baby_use
tools consumer_use*
tools lawn_garden
tools personal_care*
toys*
water_treatment consumer_use
writing*

A * indicates multiple cassettes containing additional CPCat terms

Potential Use in EDSP: Exposure Routes for SDWA Chemicals

5,251 SDWA chemicals in EDSP

↓

~4,000 in CPCat

↓

3,514 associated with at least one consumer-use related CPCat cassette

- Use CPCat for prioritization of chemicals for screening based on potential exposure routes (more "hits" → more potential exposure routes)

EDSP / SDWA chemicals with most consumer-related cassette hits

CAS	*Name*	*CPCat consumer cassette hits*
57-55-6	1,2-propanediol	121
64-17-5	ethanol	114
56-81-5	glycerol	110
67-63-0	isopropyl alcohol	90
77-92-9	citric acid	85
99-76-3	methyl 4-hydroxybenzoate	85
1310-73-2	sodium hydroxide	84
13463-67-7	titanium dioxide	82
7647-14-5	sodium chloride	80
102-71-6	2,2,2-nitrilotriethanol	78
106-97-8	butane	74
75-28-5	isobutane	73
94-13-3	propyl 4-hydroxybenzoate	72

versus ~2,500 chemicals with <5 consumer-related cassette hits

Conclusions

- CPCat is the first publically available, large scale database to harmonize disparate sources of chemical use categorization
- Potential uses for CPCat
  - Grouping chemicals by potential types of exposure sources, or by diversity of potential sources
  - High throughput exposure modeling
  - Priority setting tasks (e.g., high throughput chemical exposure prioritization)
- Limitations
  - Source data used “as is” (e.g., methodology for compiling SPIN database, a major source, is unclear)
  - Exposure potential and exposure routes must be inferred from CPCat term/cassette assignment
  - Exposure dose and toxicological information not included in CPCat

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CPCat Data Sources

- IUR/CDR (Inventory Update Reporting Modifications Rule/Chemical Data Reporting Rule)
  - Information on commercial chemical substances and mixtures on TSCA Chemical Substance Inventory
- SPIN
  - Joint effort from government environmental agencies of Norway, Sweden, Denmark, and Finland
  - Data from product registries
- ACToR Data Sets and Lists
  - ACToR Data Set: Data set linking chemicals to physico-chemical values
  - ACToR List: chemicals meeting a given criteria
- ACToR UseDB
  - Chemicals assigned to small number of high-level chemical-use categories