

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

*Kathie Dionisio<sup>1</sup>, Richard Judson<sup>2</sup>*

*<sup>1</sup>U.S. EPA, National Exposure Research Laboratory*

*<sup>2</sup>U.S. EPA, National Center for Computational Toxicology  
Office of Research and Development*



January 23, 2014

# High throughput exposure prioritization

**Goal:** A high-throughput exposure approach to use with the ToxCast chemical hazard identification.

**Proof of Concept:** Using off-the-shelf models capable of quantitatively predicting exposure determinants in a high throughput (1000s of chemicals) manner.

To date have found only fate and transport models to have sufficient throughput.

These models predict the contribution from manufacture and industrial use to overall exposure rapidly and efficiently.

Applying and developing new high throughput models of consumer use and indoor exposure.

*Environmental Fate and Transport*



*Consumer Use and Indoor Exposure*

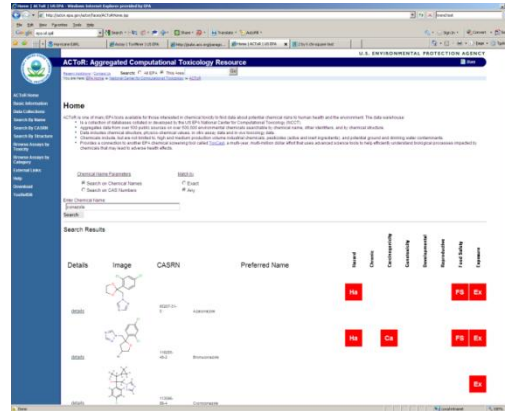
# The Origin of ACToR: The Chemical Landscape Project

- 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

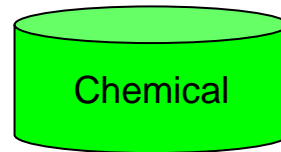
# ACToR

## Aggregated Computational Toxicology Resource

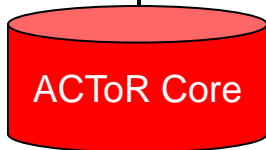
<http://actor.epa.gov/>



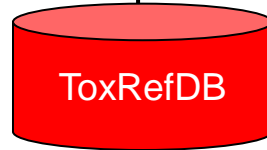
**ACToR API**



Chemical ID,  
Structure



Tabular Data,  
Links to Web  
Resources



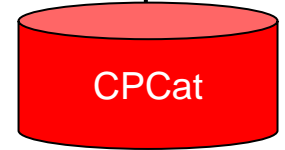
In Vivo Data  
(NCCT, OPP)



ToxCast Data  
(NCCT, ORD,  
Collaborators)



Exposure  
Biomonitoring Data  
(NERL, NCCT)



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

Internet  
Searches

# 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 (live, but work-in-progress):
  - <http://actor.epa.gov/cpcat>

# 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

# Data Sources – 43,636 total chemicals

Source	Type	Source Categories	CPCat Terms	Chemicals
CDR 2012 Industrial Function	Functional Categories	35	24	5,023
Dow	Functional Categories	20	18	104
Keml	Functional Categories	62	19	877
Toxome	Functional Categories	17	15	443
CDR 2012 Industrial Sector	Industrial Sector Categories	48	27	5,226
SPIN Industrial Sector	Industrial Sector Categories	1,934	50	4,604
SPIN NACE	Industrial Sector Categories	138	20	7,745
Retail Product Categories	Product Categories	450	74	2,778
DrugBank	Therapeutic Categories	586	460	1,755
ACToR Assays and Lists	Use Categories	137	102	35,732
ACToR UseDB	Use Categories	15	15	31,622
CDR 2012 Consumer	Use Categories	35	30	3,321
DfE	Use Categories	12	9	444
IUR 2006	Use Categories	21	20	1,152
NICNAS	Use Categories	19	17	177
SPIN detpcat	Use Categories	1,210	153	6,491
SPIN UC62	Use Categories	63	40	9,059

# 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



# CPCat term assignment

- Each data source has its own category hierarchy
- These are harmonized in CPCat by mapping categories from data sources to a common set of “terms” (keywords)
- Each original source category may be associated with several CPCat terms
- CPCat assigns ~260 unique terms, excluding drug related terms (~720 total)
- Full data dictionary of CPCat terms to be included with final database release

# CPCat term notation

- Comma (“,”) indicates a group of CPCat terms
  - baby, toy
- Underscore (“\_”) indicates a single CPCat term
  - arts\_crafts
- Suffix “\*\_ActorUseDB” indicates the CPCat term comes from one of 15 broad ACToR UseDB use categories
  - food\_additive\_ActorUseDB

# CPCat example search: Bisphenol A

actor.epa.gov/cpcat/faces/home.xhtml;jsessionid=ED1117C1267B95CC984856D7C417FDEB

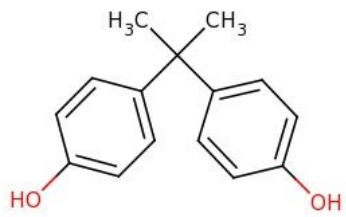
**CPCat: Chemical and Product Categories** [Contact Us](#)

You are here: [EPA Home](#) » [Computational Toxicology Research](#) » [Chemical Use](#)



[Home](#)
[Basic Info](#)
[Data Collection](#)
[Use](#)
[Download](#)
[Help](#)

**Chemical: BISPHENOL A**

**CASRN: 80-05-7**



[Export Use Data](#)
[Export Product Data](#)

**Use Information:**

CPCat Description	Source Description	ACToR Assay/List	Category	Category Type
consumer_product_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	Consumer Products	Danish Consumer Products Survey No. 102: 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	Categories from ACToR Assays and Lists	Use Categories

# CPCat example search: Bisphenol A

actor.epa.gov/cpcat/faces/home.xhtml;jsessionid=ED1117C1267B95CC984856D7C417FDEB

Product Information:		
Product ↕	Manufacturer ↕	Manufacturer
EPOLITE 2152 HARDENER	HEXCEL CORP	<a href="#">External Link</a> <a href="#">EXIT Disclaimer</a>
HYSOL KS4008 PART B KB4008, KS4008	DEXTER CORP	<a href="#">External Link</a> <a href="#">EXIT Disclaimer</a>
SCOTCH-WELD EC-3578 B/A PART A STRUCTURAL (SUPDAT)	3M GENERAL OFFICE	<a href="#">External Link</a> <a href="#">EXIT Disclaimer</a>
CHEMLOK 805 ELASTOMER ADHESIVE, 98050W	LORD CORP	<a href="#">External Link</a> <a href="#">EXIT Disclaimer</a>
3197 STEEL WORKS	HILL MFG CO INC	<a href="#">External Link</a> <a href="#">EXIT Disclaimer</a>
HSE 2411 AMINE HARDENER FOR HIGH STRENGTH EPOXY RESIN	HILTI INC	<a href="#">External Link</a> <a href="#">EXIT Disclaimer</a>
RM 698 RAPID PRIMER - HARDENER	HILTI INC	<a href="#">External Link</a> <a href="#">EXIT Disclaimer</a>
RM 698 RAPID REPAIR MORTAR - HARDENER	HILTI INC	<a href="#">External Link</a> <a href="#">EXIT Disclaimer</a>
HYSOL 50-206 R, XX0354	DEXTER CORP	<a href="#">External Link</a> <a href="#">EXIT Disclaimer</a>
EPOLITE 1350 HANDENER	HEXCEL CORP, RESINS GROUP	<a href="#">External Link</a> <a href="#">EXIT Disclaimer</a>
453 ADHESIVE GENERAL PURPOSE MIXER CUPS, 21427	LOCTITE CORP	<a href="#">External Link</a> <a href="#">EXIT Disclaimer</a>
CAT-L-INK 50-407R MEDIUM, BLUE (XX0362)	DEXTER ELECTRONIC MATERIALS	<a href="#">External Link</a> <a href="#">EXIT Disclaimer</a>
SRS SURFACE RENEWAL SYSTEM ONE, 82733	LOCTITE CORP	<a href="#">External Link</a> <a href="#">EXIT Disclaimer</a>
50-771R NC BLACK (XX1190)	DEXTER CORPORATION ELECTRONIC MATERIALS	<a href="#">External Link</a> <a href="#">EXIT Disclaimer</a>
M-O-NC	DEXTER CORPORATION/HYSOL DIVISION	<a href="#">External Link</a> <a href="#">EXIT Disclaimer</a>
RP 1135 HARDENER	CIBA-GEIGY CORP FORMULATED SYSTEMS GROUP	<a href="#">External Link</a> <a href="#">EXIT Disclaimer</a>
HYSOL 50-200 AR (XX0351)	DEXTER ELECTRONIC MATERIALS DIV	<a href="#">External Link</a> <a href="#">EXIT Disclaimer</a>
RP 1118 HARDENER	CIBA-GEIGY CORP/REN PLASTICS	<a href="#">External Link</a> <a href="#">EXIT Disclaimer</a>
DER 317	DOW CHEM.U.S.A.	<a href="#">External Link</a> <a href="#">EXIT Disclaimer</a>
D.E.R.337	DOW CHEMICAL,U.S.A.	<a href="#">External Link</a> <a href="#">EXIT Disclaimer</a>
D.E.R.341	DOW CHEMICAL U.S.A.	<a href="#">External Link</a> <a href="#">EXIT Disclaimer</a>
50-710 STENCIL INK (XX0368)	DEXTER CORP THE DEXTER ELECTRONIC MATERIAL DIV.	<a href="#">External Link</a> <a href="#">EXIT Disclaimer</a>
M-O-N-C BLACK, ME1009	HYSOL DIV DEXTER CORP	<a href="#">External Link</a> <a href="#">EXIT Disclaimer</a>
EL-CHEM NO 200 PRIMER PART.B	ELECTRO CHEMICAL ENGINEERING & MFG.CO.	<a href="#">External Link</a> <a href="#">EXIT Disclaimer</a>

# CPCat example search: Atrazine

actor.epa.gov/cpcat/faces/home.xhtml

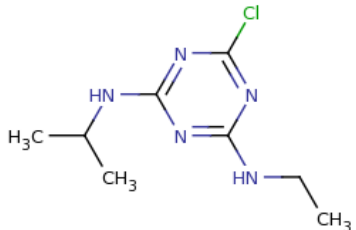
**CPCat: Chemical and Product Categories** [Contact Us](#)

You are here: [EPA Home](#) » [Computational Toxicology Research](#) » [Chemical Use](#)



[Home](#)
[Basic Info](#)
[Data Collection](#)
[Use](#)
[Download](#)
[Help](#)

**Chemical: atrazine**

**CASRN: 1912-24-9**



[Export Use Data](#)
[Export Product Data](#)

**Use Information:**

CPCat Description	Source Description	ACToR Assay/List	Category	Category Type
pesticide_ActorUseDB, herbicide	Herbicide		ACToR UseDB	Use Categories
personal_care_ActorUseDB	Personal Care Product		ACToR UseDB	Use Categories
pesticide_ActorUseDB	Pesticide		ACToR UseDB	Use Categories

# CPCat example search: Atrazine

actor.epa.gov/cpcat/faces/home.xhtml

		ground water in Southern Georgia in 2002	Assays and Lists	
pesticide, herbicide	Herbicides	USGS Herb Rain Summary:USGS: Summary of herbicides in rainwater, 1990-1991:USGS: Summary of herbicides and degradates detected in rainfall across Midwestern and Northeastern regions, 1990-91 (19 months)	Categories from ACToR Assays and Lists	Use Categories
pesticide, herbicide	Herbicides	USGS Herbicides Properties:(USGS) Properties of herbicides:Properties of herbicides of interest to USGS as part of its groundwater monitoring program	Categories from ACToR Assays and Lists	Use Categories
health_product, feminine_care	Personal Care Products: Sanitary Napkins	Danish Consumer Products Survey No. 12:Chemical Substances from Tampons:Results from the GC/MS screening of tampons	Categories from ACToR Assays and Lists	Use Categories
pesticide, drinking_water	Pesticides	Cal CDPR Pest Wells 2010:Cal CDPR Sampling For Pesticide Residues In California Well Water for 2010:Cal CDPR (California Department of Pesticide Regulation) Sampling For Pesticide Residues In California Well Water for 2010	Categories from ACToR Assays and Lists	Use Categories
pesticide, drinking_water	Pesticides	Cal CDPR Pest Wells Summary:Cal CDPR Sampling Historical Summary of Pesticide Residues In California Well Water:Cal CDPR (California Department of Pesticide Regulation) Summary of Historical and Current Pesticide Detections in Wells	Categories from ACToR Assays and Lists	Use Categories
pesticide	Pesticides	Cal CDPR PestSales 2000:California Pesticide Sales for 2000:California Department of Pesticide Regulation: Amount of active ingredient(s) in Pesticide Products sold in California for the year 2000	Categories from ACToR Assays and Lists	Use Categories
pesticide	Pesticides	Cal CDPR PestSales 2001:California Pesticide Sales for 2001:California Department of Pesticide Regulation: Amount of active ingredient(s) in Pesticide products sold in California for the year 2001	Categories from ACToR Assays and Lists	Use Categories
pesticide	Pesticides	Cal CDPR PestSales 2002:California Pesticide Sales for 2002:California Department of Pesticide Regulation: Amount of active ingredient(s) in Pesticide products sold in California for the year 2002	Categories from ACToR Assays and Lists	Use Categories
pesticide	Pesticides	Cal CDPR PestSales 2003:California Pesticide Sales for 2003:California Department of Pesticide Regulation: Amount of active ingredient(s) in Pesticide Products sold in	Categories from ACToR	Use Categories

# CPCat terms associated with ethyl paraben

agricultural  
arts\_crafts  
automobile, care\_product  
automobile, maintenance  
baby, bath  
baby, furniture  
baby, skin  
battery  
child  
child, toy  
cleaning\_washing  
cleaning\_washing, consumer  
cleaning\_washing, industrial  
cleaning\_washing, manufacturing  
construction\_activity  
consumer\_product, fragrance  
consumer\_product\_ActorUseDB  
cosmetics  
cosmetics, eye  
cosmetics, fragrance

cosmetics, hair  
cosmetics, hair, cleaning\_washing  
cosmetics, hair, colorant  
cosmetics, lips  
cosmetics, nails  
cosmetics, preservatives  
cosmetics, raw\_material  
cosmetics, skin  
cosmetics, skin, cleaning\_washing  
cosmetics, skin, colorant  
cosmetics, uv\_blocker  
drug  
drug, inactive\_ingredient  
drug, veterinary  
electronic\_component  
food, flavor  
food\_additive  
food\_additive\_ActorUseDB  
food\_contact, disinfectant  
fragrance, manufacturing

industrial, manufacturing  
industrial\_manufacturing\_ActorUseDB  
metal, manufacturing  
paint  
paraben  
personal\_care, cleaning\_washing  
personal\_care, sexual\_wellness  
personal\_care, sunscreen  
personal\_care\_ActorUseDB  
pesticide  
pesticide, biocide  
pesticide, inert\_ingredient  
pesticide, preservative  
pesticide\_ActorUseDB, inert  
photographic  
preservative  
solvent  
surface\_treatment

# CPCat terms associated with ethyl paraben

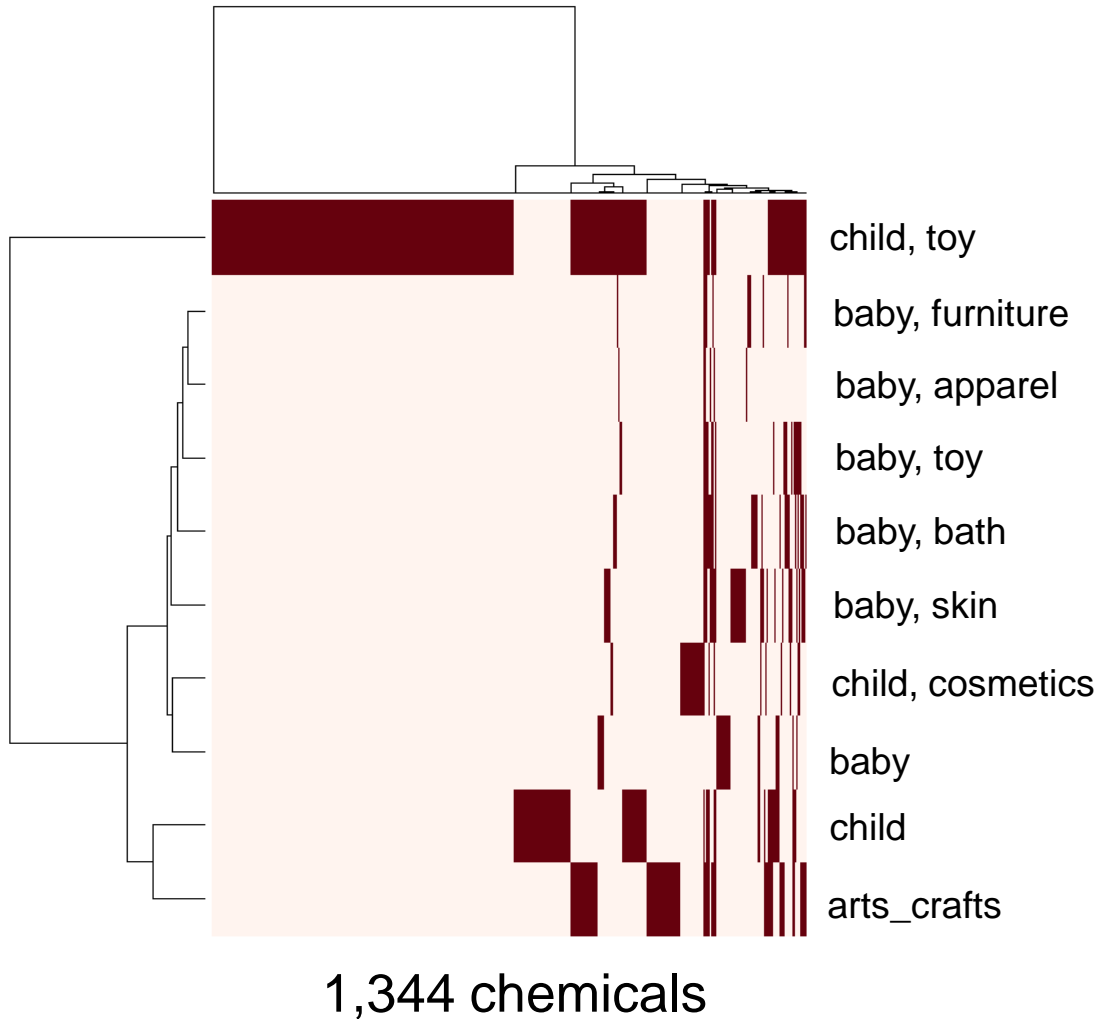
agricultural  
arts\_crafts  
automobile, care\_product  
automobile, maintenance  
baby, bath  
baby, furniture  
baby, skin  
**battery**  
child  
child, toy  
cleaning\_washing  
cleaning\_washing, consumer  
cleaning\_washing, industrial  
cleaning\_washing, manufacturing  
construction\_activity  
consumer\_product, fragrance  
consumer\_product\_ActorUseDB  
cosmetics  
cosmetics, eye  
cosmetics, fragrance

cosmetics, hair  
cosmetics, hair, cleaning\_washing  
cosmetics, hair, colorant  
cosmetics, lips  
cosmetics, nails  
cosmetics, preservatives  
cosmetics, raw\_material  
cosmetics, skin  
cosmetics, skin, cleaning\_washing  
cosmetics, skin, colorant  
cosmetics, uv\_blocker  
drug  
drug, inactive\_ingredient  
drug, veterinary  
**electronic\_component**  
food, flavor  
food\_additive  
food\_additive\_ActorUseDB  
food\_contact, disinfectant  
fragrance, manufacturing

industrial, manufacturing  
industrial\_manufacturing\_ActorUseDB  
metal, manufacturing  
paint  
paraben  
personal\_care, cleaning\_washing  
personal\_care, sexual\_wellness  
personal\_care, sunscreen  
personal\_care\_ActorUseDB  
pesticide  
pesticide, biocide  
pesticide, inert\_ingredient  
pesticide, preservative  
pesticide\_ActorUseDB, inert  
photographic  
preservative  
solvent  
surface\_treatment



# Use CPCat to enumerate chemicals for exposure scenarios



Example:

children's exposure

- Chemical is associated with the CPCat term(s)
- Chemical is not associated with the CPCat term(s)

Relevant  
CPCat terms

# Potential Use in EDSP: Exposure Routes for SDWA Chemicals

5,251 SDWA chemicals in EDSP



4,189 in CPCat



3,373 associated with at least one  
consumer-use related CPCat term

# Potential Use in EDSP: Exposure Routes for SDWA Chemicals

- 92 consumer-use related CPCat terms total associated with the SDWA compounds

adhesive, consumer	flame_retardant
apparel	food (multiple categories)
apparel_care	food_additive
arts_crafts	food_contact (multiple categories)
automobile (multiple categories)	health_product (multiple categories)
baby (multiple categories)	home (multiple categories)
battery	ink_toner
building_material	office_product
child(multiple categories)	paint
cigarette	paper
cleaning_washing (multiple categories)	personal_care (multiple categories)
consumer_product (multiple categories)	pesticide (drinking_water, food_contaminant, food_use)
cosmetics (multiple categories)	pet (multiple categories)
dental	vitamin
disinfection_byproduct	vitamin_minerals
drycleaning	water_treatment
electronic_component	writing

# EDSP / SDWA chemicals with most consumer-related terms

CASRN	Name	CPCat term hits
57-55-6	1,2-Propanediol	63
64-17-5	ethanol	62
56-81-5	glycerol	60
7647-14-5	sodium chloride	58
67-63-0	Isopropyl alcohol	53
99-76-3	methyl 4-hydroxybenzoate	52
102-71-6	2,2,2-nitrilotriethanol	50
77-92-9	citric acid	49
1310-73-2	sodium hydroxide	49
50-00-0	formaldehyde	48
94-13-3	propyl 4-hydroxybenzoate	48
13463-67-7	titanium dioxide	48
128-37-0	2,6-di-tert-butyl-p-cresol	45
2682-20-4	2-methyl-3(2H)-isothiazolone	45
7631-86-9	silicon dioxide	44
122-99-6	2-phenoxyethanol	42
14807-96-6	Talc (Mg <sub>3</sub> H <sub>2</sub> (SiO <sub>3</sub> ) <sub>4</sub> )	41
26172-55-4	5-chloro-2-methyl-3(2H)-isothiazolone	41

CASRN	Name	CPCat term hits
100-51-6	benzyl alcohol	40
67-64-1	acetone	39
471-34-1	calcium carbonate	39
1314-13-2	zinc oxide	39
57-11-4	stearic acid	38
64-02-8	EDTA, tetrasodium	37
75-28-5	isobutane	37
106-97-8	butane	37
141-78-6	ethyl acetate	37
3844-45-9	Acid blue 9	37
111-76-2	2-butoxyethanol	36
144-55-8	sodium bicarbonate	36
64-19-7	acetic acid	35
111-90-0	2-(2-ethoxyethoxy)ethanol	35
532-32-1	sodium benzoate	35
36653-82-4	cetyl alcohol	35

# Conclusions

- 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 assignment
- Exposure dose and toxicological information not included in CPCat

- Potential uses for CPCat

- High throughput exposure modeling
- Priority setting tasks (e.g., exposure based prioritization)



# EPA Office of Research and Development

## ExpoCast Team

Kathie Dionisio\*

**Peter Eghehy**

Kristin Isaacs

Richard Judson

Thomas Knudsen

Chantel Nicolas\*

Robert Pearce\*

James Rabinowitz

Woody Setzer

Cory Strobe\*

Dan Vallero

Amber Wang\*

## \*Trainees

## Chemical Safety for Sustainability (CSS) Collaborators

Michael Breen

Stephen Edwards

Rocky Goldsmith

Chris Grulke\*

Elaine Hubal

CSS Deputy National Program Director

Tina Bahadori

CSS National Program Director

Haluk Ozkaynak

Jon Sobus

Mark Strynar

Cecilia Tan

## External Collaborators

Jon Arnot (ARC)

Deborah Bennett (University of California, Irvine)

Alicia Frame (Dow Chemical)

Olivier Jolliet (University of Michigan)

Jade Mitchell (Michigan State)

Barbara Wetmore (Hamner)

Special thanks to Alicia Frame (former NCCT trainee) for the work she contributed to this project.

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