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

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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
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.
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
http://actor.epa.gov/
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

<table>
<thead>
<tr>
<th>Source</th>
<th>Type</th>
<th>Source Categories</th>
<th>CPCat Terms</th>
<th>Chemicals</th>
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<tbody>
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<td>DrugBank</td>
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<td>ACToR Assays and Lists</td>
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<td>IUR 2006</td>
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<td>20</td>
<td>1,152</td>
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<td>NICNAS</td>
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<td>SPIN detpcat</td>
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<td>Use Categories</td>
<td>63</td>
<td>40</td>
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</table>
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

CASRN: 80-05-7

Use Information:

<table>
<thead>
<tr>
<th>CPCat Description</th>
<th>Source Description</th>
<th>ACToR Assay List</th>
<th>Category</th>
<th>Category Type</th>
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<tbody>
<tr>
<td>consumer_product_ActorUseDB</td>
<td>Consumer Use</td>
<td>ACToR UseDB</td>
<td>Use Categories</td>
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<td>personal_care_ActorUseDB</td>
<td>Personal Care Product</td>
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<td>child</td>
<td>Consumer Products</td>
<td>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</td>
<td>Categories from ACToR Assays and Lists</td>
<td>Use Categories</td>
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CPCat example search: Bisphenol A

<table>
<thead>
<tr>
<th>Product</th>
<th>Manufacturer</th>
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<tbody>
<tr>
<td>EPOLITE 2162 HARDENER</td>
<td>HBCCEL CORP</td>
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<tr>
<td>HYSOL KS4008 PART B KB4008, KS4008</td>
<td>DEXTER CORP</td>
<td>External Link</td>
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<td>SCOTCH-WELD EC-3578 B/A PART A STRUCTURAL (SUPDAT)</td>
<td>3M GENERAL OFFICE</td>
<td>External Link</td>
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<tr>
<td>CHEMLOK 605 ELASTOMER ADHESIVE, 96050W</td>
<td>LORD CORP</td>
<td>External Link</td>
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<td>3197 STEEL WORKS</td>
<td>HILL MFG CO INC</td>
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<td>H1SE 2411 AMINE HARDENER FOR HIGH STRENGTH EPOXY RESIN</td>
<td>HILTI INC</td>
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<td>RM 698 RAPID PRIMER - HARDENER</td>
<td>HILTI INC</td>
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<td>RM 698 RAPID REPAIR MORTAR - HARDENER</td>
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<td>LOCTITE CORP</td>
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<td>CAT-LINK 50-407R MEDIUM, BLUE (VX0362)</td>
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<td>50-771R NC BLACK (VX1190)</td>
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<td>D.E.R.341</td>
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<td>60-710 STENCIL LINK (VX0388)</td>
<td>DEXTER CORP THE DEXTER ELECTRONIC MATERIAL DIV</td>
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<td>M-ONIC N BLACK, ME1009</td>
<td>HYSOL DIV/DEXTER CORP</td>
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<td>EL-CHEM NO 200 PRIMER PART B</td>
<td>ELECTRO CHEMICAL ENGINEERING &amp; MFG CO</td>
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CPCat example search: Atrazine

CASRN: 1912-24-9
### CPCat example search: Atrazine

<table>
<thead>
<tr>
<th>Health Product, Feminine Care</th>
<th>Personal Care Products: Sanitary Napkins</th>
<th>Danish Consumer Products Survey: No. 12: Chemical Substances from Tampons Results from the GC/MS screening of tampons</th>
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<tr>
<td>Pesticide, Drinking Water</td>
<td>Pesticides</td>
<td>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</td>
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<td>Pesticides</td>
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<tr>
<td>Pesticide</td>
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</table>
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
consumer_product_ActorUseDB
consumer_product, raw_material
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

1,344 chemicals
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
apparel
apparel_care
arts_crafts
automobile (multiple categories)
baby (multiple categories)
battery
building_material
child (multiple categories)
cigarette
cleaning_washing (multiple categories)
consumer_product (multiple categories)
cosmetics (multiple categories)
dental
disinfection_byproduct
drycleaning
electronic_component

flame_retardant
food (multiple categories)
food_additive
food_contact (multiple categories)
health_product (multiple categories)
home (multiple categories)
ink_toner
office_product
paint
paper
personal_care (multiple categories)
pesticide (drinking_water, food_contaminant, food_use)
pet (multiple categories)
vitamin
vitamin_minerals
water_treatment
writing
### EDSP / SDWA chemicals with most consumer-related terms

<table>
<thead>
<tr>
<th>CASRN</th>
<th>Name</th>
<th>CPCat term hits</th>
</tr>
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<tbody>
<tr>
<td>57-55-6</td>
<td>1,2-Propanediol</td>
<td>63</td>
</tr>
<tr>
<td>64-17-5</td>
<td>ethanol</td>
<td>62</td>
</tr>
<tr>
<td>56-81-5</td>
<td>glycerol</td>
<td>60</td>
</tr>
<tr>
<td>7647-14-5</td>
<td>sodium chloride</td>
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</tr>
<tr>
<td>67-63-0</td>
<td>Isopropyl alcohol</td>
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<tr>
<td>99-76-3</td>
<td>methyl 4-hydroxybenzoate</td>
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<tr>
<td>102-71-6</td>
<td>2,2,2-nitroltriethanol</td>
<td>50</td>
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<td>77-92-9</td>
<td>citric acid</td>
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<tr>
<td>1310-73-2</td>
<td>sodium hydroxide</td>
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<tr>
<td>50-00-0</td>
<td>formaldehyde</td>
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<tr>
<td>94-13-3</td>
<td>propyl 4-hydroxybenzoate</td>
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<td>13463-67-7</td>
<td>titanium dioxide</td>
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<tr>
<td>128-37-0</td>
<td>2,6-di-tert-butyl-p-cresol</td>
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<td>2682-20-4</td>
<td>2-methyl-3(2H)-isothiazolone</td>
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<tr>
<td>7631-86-9</td>
<td>silicon dioxide</td>
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<tr>
<td>122-99-6</td>
<td>2-phenoxyethanol</td>
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<td>14807-96-6</td>
<td>Talc (Mg3H2(SiO3)4)</td>
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<tr>
<td>26172-55-4</td>
<td>5-chloro-2-methyl-3(2H)-isothiazolone</td>
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<table>
<thead>
<tr>
<th>CASRN</th>
<th>Name</th>
<th>CPCat term hits</th>
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<td>100-51-6</td>
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<td>acetone</td>
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<td>471-34-1</td>
<td>calcium carbonate</td>
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<td>1314-13-2</td>
<td>zinc oxide</td>
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<td>57-11-4</td>
<td>stearic acid</td>
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<td>64-02-8</td>
<td>EDTA, tetrasodium</td>
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<td>75-28-5</td>
<td>isobutane</td>
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<td>106-97-8</td>
<td>butane</td>
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<td>141-78-6</td>
<td>ethyl acetate</td>
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<td>Acid blue 9</td>
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<td>532-32-1</td>
<td>sodium benzoate</td>
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<tr>
<td>36653-82-4</td>
<td>cetyl alcohol</td>
<td>35</td>
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</tbody>
</table>
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

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Barbara Wetmore (Hamner)

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