Suspect Screening of Chemicals in Consumer Products

Katherine Phillips, Kristin Isaacs, John Wambaugh

The views expressed in this presentation are those of the authors and do not necessarily represent the views or policies of the U.S. Environmental Protection Agency. Reference to commercial products or services does not constitute endorsement.
• The timely characterization of the human and ecological risk posed by thousands of existing and emerging commercial chemicals is a critical challenge.

• **High throughput risk prioritization** relies on three components:
  1. high throughput hazard characterization
  2. high throughput exposure forecasts
  3. high throughput toxicokinetics (i.e., dosimetry)

• While advances have been made in HT toxicity screening, exposure methods applicable to 1000s of chemicals are needed.

**Graph:**
- High Risk
- Medium Risk
- Low Risk

**Axes:**
- Toxicity
- Exposure

**Units:**
mg of substance / kg of bodyweight / day

*Slide from Kristin Isaacs*
Available Information

Many manufacturers of consumer product formulations release a (Material) Safety Data Sheet, or (M)SDS, for products. This is less common for articles, however some manufacturers release Health Product Declarations (HPDs) which are similar.

Exact concentrations are not known.

Trade secret chemicals are not disclosed.

Fragrances and colorants may not be disclosed with the product.
Suspect Screening of House Dust

- 56 dust samples were analyzed using liquid chromatography
- Formulas of potentially identified chemicals were matched against database of chemicals
- Exposure, bioactivity, instrument abundance, and detection frequency were used to rank chemicals for confirmation
Analytical Analyses

**Targeted Analysis**
- Uses analytical techniques to look for a predetermined list of 10s to 100s chemicals
- These chemicals make up much less than 1% of the exposome

**Suspect Screening Analysis**
- Uses analytical techniques and spectral databases to compare spectra from a sample to 100s or 1000s of chemicals in the database
- These chemicals make up approximately 5 – 10% of the exposome

**Non-targeted Analysis**
- Identity of potential chemicals in samples are proposed without the aid of list or database
- These chemicals make up approximately 90 – 95% of the exposome

Slide adapted from Jon Sobus
SSA Workflow

- 100 different products were purchased across retail stores
- Products were spread across 20 product categories (5 different products from each category)
- Product Categories covered:
  - Articles: long term products in the home (e.g., carpet, upholstery)
  - Formulations: short term products that are used up (e.g., shampoo, lotion)
  - Food

Experimental results provided by Alice Yau and Kristin Favela (Southwest Research Institute)
Caveats of this Study

• Presence of a chemical does not imply exposure
• Presence of a chemical does not imply bioavailability
• Homogenized samples are created from products for SSA
• Chemicals in samples are extracted with organic solvents
• Different exposure pathways exist for different products
• Toxicity of chemical exposure is not evaluated here (i.e., exposure alone is not risk)
## Chemicals Tentatively Identified

<table>
<thead>
<tr>
<th>Chemical List</th>
<th>Number of Chemicals in List</th>
<th>Number of Ident. Spect. Matches in List</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPCPdb</td>
<td>1797</td>
<td>199</td>
</tr>
<tr>
<td>EDSP</td>
<td>177</td>
<td>19</td>
</tr>
<tr>
<td>ToxCast ER Agonist</td>
<td>64</td>
<td>10</td>
</tr>
<tr>
<td>Flame Retardant</td>
<td>67</td>
<td>9</td>
</tr>
<tr>
<td>NHANES</td>
<td>452</td>
<td>36</td>
</tr>
<tr>
<td>Pharmaceuticals</td>
<td>670</td>
<td>1</td>
</tr>
<tr>
<td>Tox21</td>
<td>8948</td>
<td>522</td>
</tr>
<tr>
<td>ToxCast</td>
<td>4745</td>
<td>443</td>
</tr>
<tr>
<td>ToxRef</td>
<td>1172</td>
<td>105</td>
</tr>
</tbody>
</table>

### Articles
- Carpet
- Carpet Padding
- Cotton Clothing
- Fabric Upholstery
- Shower Curtain
- Vinyl Upholstery
- Plastic Children’s Toy
- Lipstick
- Toothpaste
- Sunscreen
- Indoor House Paint
- Shaving Cream
- Hand Soap
- Skin Lotion
- Baby Soap
- Deodorant
- Shampoo
- Glass Cleaner
- Air Freshener

### Formulations

### Foods

<table>
<thead>
<tr>
<th>Unique Chemicals</th>
<th>Cereal</th>
<th>log$_{10}$ (μg/g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>250</td>
<td></td>
<td></td>
</tr>
<tr>
<td>200</td>
<td></td>
<td></td>
</tr>
<tr>
<td>150</td>
<td></td>
<td></td>
</tr>
<tr>
<td>100</td>
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</tr>
<tr>
<td>50</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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*EPA*
Prevalence of Chemicals

- The majority of tentative hits were found in only 1 or 2 products
- Many confirmed hits were found in larger number of products
Prevalence of Chemicals

- 1603 spectra from samples were mapped to spectra in NIST 08
- 119 were confirmed with 200+ internal standards
- 119 + 738 + 1006 ≠ 1603; some chemicals are in more than one identification category
**ER Agonists**

- Propylparaben is commonly used in personal care products typically used as a preservative.
- Bisphenol A was confirmed in vinyl upholstery, shampoo, and a shower curtain with tentative identifications in one toothpaste and one plastic children’s toy.
- 4-tert-butylphenol is typically used in adhesive/sealant and coating applications.
Flame Retardants

- ToxCast chemical annotations and public information were used to generate a list of chemicals used as flame retardants.
- Chemicals with flame retardant applications were indicated most in carpet padding, vinyl materials, and cotton clothing.
- Tributyl phosphate has multiple uses and was likely in cereals serving some other functional role or is an unintentionally added chemical.
Identify functional use of chemicals in commerce

Obtain structural features of chemicals

Build models that predict functional use from chemical structure

FUse DB has ~14000 chemicals with reported uses
ID Bolstering with Functional Use

- Only looked at tentatively identified (1541) chemicals
- 550 IDs had at least one reported use in FUSE
- An additional 317 IDs had validated predicted functional uses from QSURs
- Can prioritize chemicals for confirmation by first looking at those with reported uses, and then those with predicted uses
Comparison with Ingredient Lists

- Only 931 ingredients were reported in total for all 100 products (either on packaging or manufacturer’s website)
- Only 65 products (formulations and food) should have reported ingredients
- Only 821 could be mapped back to chemical identifiers
- 95 of 821 ingredients were actually identified in the SSA

<table>
<thead>
<tr>
<th>Product Category</th>
<th>Number of Chemicals Identified</th>
</tr>
</thead>
<tbody>
<tr>
<td>air freshener</td>
<td>4</td>
</tr>
<tr>
<td>baby soap</td>
<td>9</td>
</tr>
<tr>
<td>deodorant</td>
<td>6</td>
</tr>
<tr>
<td>glass cleaner</td>
<td>4</td>
</tr>
<tr>
<td>hand soap</td>
<td>10</td>
</tr>
<tr>
<td>lipstick</td>
<td>14</td>
</tr>
<tr>
<td>shampoo</td>
<td>10</td>
</tr>
<tr>
<td>shaving cream</td>
<td>9</td>
</tr>
<tr>
<td>skin lotion</td>
<td>10</td>
</tr>
<tr>
<td>sunscreen</td>
<td>7</td>
</tr>
<tr>
<td>toothpaste</td>
<td>6</td>
</tr>
</tbody>
</table>
Comparison with CPDat

- 37 CASRN-product pairs were found from MSDS data in CPDat among the 1603 identified spectral matches
- Mean values of MSDS reported weight fractions were compared to estimated concentration from SSA
- SSA values tend to be an underestimate of reported values
Comparison with Product Testing Data

- MSDS is only provided for formulations
- Information on article concentration were found through State of Washington’s reporting data
- Reporting data results from targeted analysis of products
- SSA values were still underestimated

Reported data obtained from State of Washington Department of Ecology’s Product Testing Data (https://fortress.wa.gov/ecy/ptdbpublicreporting/)
Comparison with Active Ingredients

- Actual weight fractions are required to be reported for active ingredients in a personal care product.
- Only sunscreens had active ingredients in the SSA.
- Much better comparison here than with the ranges of MSDS concentration or reported concentrations of articles.
Summary

• Limited information for the tens of thousands of chemicals in commerce
• 100 different products across 20 product categories were analyzed via SSA
• 1603 of the 4270 spectral matches were tentatively identified (119 confirmed)
• 652 chemicals were tentatively identified in formulations that were not previously known to be in formulations
• 867 chemicals could be prioritized for confirmation using functional use
• Estimated concentrations from SSA was typically lower than either manufacturer or state reported values of ingredients
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