ExpoCastDB: A Publicly Accessible Database for Observational Exposure Data

Presented to: CompTox Communities of Practice

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Overview

• ExpoCast project
  • ExpoCast DB motivation and goals

• ACToR – Aggregated Computational Toxicology Resource
  • Exposure taxonomy

• ExpoCastDB initial release
  • Studies Included and QC of data
  • Demo
  • Applications
  • Future phases
Expocast™: Exposure science for prioritization and toxicity testing

- Recognizes critical need for exposure info to inform
  - Chemical design and evaluation
  - Health risk management
- Goal
  - Advance characterization of exposure required to translate findings in comptox to support exposure and risk assessment
  - Together with ToxCast™ help EPA determine priority chemicals
- Approach
  - Mine and apply scientific advances and tools
  - Develop novel approaches for evaluating chemicals based on biologically-relevant human exposure

Cohen Hubal et al., J Toxicol Environ Health, Part B, 2010

Priority Exposure Research for Computational Toxicology
- Accessible and linkable exposure databases
- Exposure-based screening tools for accelerated chemical prioritization
Motivation for ExpoCastDB

- Increase access to human exposure data
  - Support exposure modeling
  - Advance public health through improved management of chemical risks
    - Sexton et al., Arch Environ Health, 1992;
    - Wagener et al., Annu Rev Public Health, 1995

- Linkages between exposure and toxicity data must be implemented
  - Sheldon and Cohen Hubal, EHP, 2009

- Achieve vision of better integration of exposure considerations into the risk assessment process

- Consolidation facilitates bioinformatic interrogation
  - Estimated proportion of human disease attributable to environmental pollutants is roughly the same as that attributable to genetic factors
    - Rappaport, JESEE, 2011
ExpoCastDB goals

- Consolidate observational human exposure data, improve access and provide links to health related data
  - House measurements from human exposure studies
  - Encourage standardized reporting of observational exposure information
- Provide separate interface with inner workings of ACToR
  - Facilitate linkages with toxicity data, environmental fate data, chemical manufacture information
- Provide basic user functions
  - Visualization (e.g., scatterplots, probability plots, goodness-of-fit)
  - Obtain summary statistics and estimate distributional parameters
  - Download customized datasets

http://actor.epa.gov/
ACToR
Aggregated Computational Toxicology Resource

http://actor.epa.gov/
ACToR goals and data sources

- Compile all publicly available information on environmental chemicals
- Make data available for downloading, data mining
  - Available through data.gov
  - Entire DB can be downloaded and installed locally
- Make it easy to see data gaps
  - Provides resource for EPA testing programs
- Make it widely used
  - over 2000 regular users

### Category Count

<table>
<thead>
<tr>
<th>Category</th>
<th>Count</th>
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</thead>
<tbody>
<tr>
<td>Data Sets</td>
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<tr>
<td>Chemicals</td>
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<td>3,213</td>
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<td>Data Points</td>
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- EPA (OPP, OPPT, NCEA, NERL)
- FDA, NIH, CDC, OSHA, USDA
- States and other countries
- Universities
- NGOs
- Companies
ACToR exposure taxonomy

Egeghy, Judson, Gangwal, Cohen Hubal et al., 2011 (in review) “The Exposure Data Landscape for Manufactured Chemicals”
ExpoCastDB initial release

- Data from NERL studies
  1) American Health Homes Survey
  2) HUD Child Care Center Survey (“CCC”)
  3) CTEPP – NC
  4) CTEPP – OH

- Full raw data sets available to download

- Browse data capability
  - By study name, chemical list, media list

- Descriptive statistics capabilities:
  - Detection Freq., N, max, MDL (if result concentration is < MDL, then result = 2/3 * MDL), Units
  - Mean, Std. dev., geometric mean, geometric std. dev. (GSD), 25th and 75th percentile

House chemical exposure concentration measurements from different media

Gangwal et al., 2011 (in prep.)
ExpoCastDB: Initial studies from NERL

- American Health Home Survey (AHHS):
  - 500 homes underwent pesticide sampling across US.
  - Isopropanol wetted wipe media used to sample floor surfaces.
  - 24 residential-use insecticides represented by 5 chemical classes:
    - Organochlorines, Organophosphates, Neonicotinoid, Synergist, Pyrethrins/Pyrethroids

- HUD Child Care Center Survey (“CCC”)
  - 168 child care centers in 30 primary US sampling units.
  - Wipe samples from indoor surfaces (floors, tabletops, desks) and soil samples collected.
  - Samples for pesticides (organophosphates and pyrethroids), lead, and allergens collected at multiple locations in each center.
• Children's Total Exposure to Persistent Pesticides and Other Persistent Organic Pollutants (CTEPP) – NC, OH
  • Observation measurement study designed to determine what commonly used chemicals are found in home and/or day care environments in six NC and six OH counties.
  • Samples of food, drinking water, air, urine, dust, soil, transferable residues on floors, and surface wipes collected.
  • Measured total exposure of 257 preschool children (ages 2 to 5 years) and their primary adult caregivers to more than 50 different pesticides and other chemicals.
Quality control of ExpoCastDB data

- Study exposure data provided by NERL
- Source data loaded into ExpoCastDB
- Data processed to obtain descriptive statistics (Java code)
- Descriptive stats produced from original data (SAS)
- Results compared to make sure they match
ExpoCastDB demo

ExpoCastDB:
http://actorpreprod.epa.gov/actor/faces/ExpoCastDB/Home.jsp (beta)

http://134.67.216.45:9192/actor/faces/ExpoCastDB/Home.jsp (beta)
ExpoCastDB: Applications

- Investigate occurrence and co-occurrence of chemicals
  - How frequently was a particular pesticide (e.g., esfenvalerate) detected in nationwide AHHS study?

- Comparisons across studies
  - How does avg. permethrin loading differ between homes in AHHS and daycares in CCC?

- Download individual sample-level structured data
  - Derive input distributions for probabilistic exposure models (such as SHEDS)
  - Use with readily available algorithms (U.S. EPA, 1992) and exposure factors (U.S. EPA, 1997) to produce quick deterministic estimates of uptake resulting from exposure to specific chemicals
### ExpoCastDB: Applications

#### Chemical: CHLORPYRIFOS

<table>
<thead>
<tr>
<th>CASRN</th>
<th>2921-88-2</th>
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<tr>
<td>ACToR</td>
<td></td>
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<td>Find in ACToR DB</td>
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#### American Healthy Homes Survey (AHHS)

<table>
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<tr>
<th>Media/Sample Type</th>
<th>N</th>
<th>Detection Freq. (%)</th>
<th>Median MDL Units</th>
<th>Max</th>
<th>Mean</th>
<th>SD</th>
<th>Geom. Mean</th>
<th>Geom. SD</th>
<th>25th %</th>
<th>75th %</th>
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</thead>
<tbody>
<tr>
<td>Exposure; Media; Surfaces - Total Residue</td>
<td>479</td>
<td>78.0</td>
<td>8.61E-4 ng/cm²</td>
<td>136.0</td>
<td>0.493</td>
<td>6.28</td>
<td>0.0138</td>
<td>10.7</td>
<td>0.00266</td>
<td>0.0627</td>
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</table>

#### Child Care Center Survey (CCC)

<table>
<thead>
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<th>Media/Sample Type</th>
<th>N</th>
<th>Detection Freq. (%)</th>
<th>Median MDL Units</th>
<th>Max</th>
<th>Mean</th>
<th>SD</th>
<th>Geom. Mean</th>
<th>Geom. SD</th>
<th>25th %</th>
<th>75th %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exposure; Media; Soil</td>
<td>117</td>
<td>13.0</td>
<td>5.0 ng/g</td>
<td>1150.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>Exposure; Media; Surfaces - Total Residue</td>
<td>248</td>
<td>38.0</td>
<td>0.084 ng/cm²</td>
<td>27.6</td>
<td>0.34</td>
<td>1.89</td>
<td>0.0968</td>
<td>2.82</td>
<td>0.056</td>
<td>0.132</td>
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#### CTEPP NC

<table>
<thead>
<tr>
<th>Media/Sample Type</th>
<th>N</th>
<th>Detection Freq. (%)</th>
<th>Median MDL Units</th>
<th>Max</th>
<th>Mean</th>
<th>SD</th>
<th>Geom. Mean</th>
<th>Geom. SD</th>
<th>25th %</th>
<th>75th %</th>
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<tbody>
<tr>
<td>Exposure; Biomonitoring; Dermal</td>
<td>223</td>
<td>80.0</td>
<td>0.00317 ng/cm²</td>
<td>0.744</td>
<td>0.04</td>
<td>0.0799</td>
<td>0.0152</td>
<td>4.07</td>
<td>0.00495</td>
<td>0.0365</td>
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<tr>
<td>Exposure; Media; Air</td>
<td>288</td>
<td>92.0</td>
<td>0.09 ng/m³</td>
<td>391.0</td>
<td>9.48</td>
<td>29.4</td>
<td>1.45</td>
<td>7.65</td>
<td>0.28</td>
<td>6.7</td>
</tr>
<tr>
<td>Exposure; Media; Air; Residential</td>
<td>288</td>
<td>92.0</td>
<td>0.09 ng/m³</td>
<td>391.0</td>
<td>9.48</td>
<td>29.4</td>
<td>1.45</td>
<td>7.65</td>
<td>0.28</td>
<td>6.7</td>
</tr>
<tr>
<td>Exposure; Media; Air; Residential; Indoor</td>
<td>148</td>
<td>100.0</td>
<td>0.09 ng/m³</td>
<td>391.0</td>
<td>17.5</td>
<td>39.3</td>
<td>6.45</td>
<td>3.96</td>
<td>2.25</td>
<td>17.4</td>
</tr>
<tr>
<td>Exposure; Media; Air; Residential; Outdoor</td>
<td>140</td>
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<td>0.09 ng/m³</td>
<td>45.9</td>
<td>0.998</td>
<td>4.02</td>
<td>0.299</td>
<td>3.64</td>
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<tr>
<td>Exposure; Media; Food</td>
<td>153</td>
<td>63.0</td>
<td>0.08 ng/g</td>
<td>19.7</td>
<td>0.513</td>
<td>1.68</td>
<td>0.188</td>
<td>3.4</td>
<td>0.0533</td>
<td>0.39</td>
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<tr>
<td>Exposure; Media; Food</td>
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<tr>
<td>Exposure; Media; House Dust</td>
<td>141</td>
<td>100.0</td>
<td>2.0 ng/g</td>
<td>15100.0</td>
<td>389.0</td>
<td>1330.0</td>
<td>137.0</td>
<td>3.66</td>
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<td>293.0</td>
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<tr>
<td>Exposure; Media; House Dust</td>
<td>141</td>
<td>100.0</td>
<td>3.47 ng/m²</td>
<td>51600.0</td>
<td>1540.0</td>
<td>5990.0</td>
<td>174.0</td>
<td>7.6</td>
<td>38.2</td>
<td>766.0</td>
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<td>Exposure; Media; Soil</td>
<td>142</td>
<td>10.0</td>
<td>0.49 ng/g</td>
<td>1170.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>Exposure; Media; Surfaces - Dislodgable Residue</td>
<td>18</td>
<td>94.0</td>
<td>4.39 ng/m²</td>
<td>719.0</td>
<td>142.0</td>
<td>230.0</td>
<td>47.4</td>
<td>4.62</td>
<td>16.2</td>
<td>140.0</td>
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<td>Exposure; Media; Surfaces - Total Residue</td>
<td>50</td>
<td>90.0</td>
<td>6.9 ng/m²</td>
<td>2080.0</td>
<td>212.0</td>
<td>414.0</td>
<td>67.3</td>
<td>4.54</td>
<td>29.1</td>
<td>135.0</td>
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</tbody>
</table>

#### CTEPP OH

<table>
<thead>
<tr>
<th>Media/Sample Type</th>
<th>N</th>
<th>Detection Freq. (%)</th>
<th>Median MDL Units</th>
<th>Max</th>
<th>Mean</th>
<th>SD</th>
<th>Geom. Mean</th>
<th>Geom. SD</th>
<th>25th %</th>
<th>75th %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exposure; Biomonitoring; Dermal</td>
<td>221</td>
<td>60.0</td>
<td>0.00303 ng/cm²</td>
<td>14.8</td>
<td>0.104</td>
<td>1.01</td>
<td>0.00785</td>
<td>0.0002824</td>
<td>4.9</td>
<td>0.000242</td>
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<tr>
<td>Exposure; Media; Air</td>
<td>273</td>
<td>88.0</td>
<td>0.09 ng/m³</td>
<td>98.0</td>
<td>3.54</td>
<td>10.6</td>
<td>0.74</td>
<td>5.49</td>
<td>0.21</td>
<td>2.08</td>
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<tr>
<td>Exposure; Media; Air; Residential</td>
<td>273</td>
<td>88.0</td>
<td>0.09 ng/m³</td>
<td>98.0</td>
<td>3.54</td>
<td>10.6</td>
<td>0.74</td>
<td>5.49</td>
<td>0.21</td>
<td>2.08</td>
</tr>
<tr>
<td>Exposure; Media; Air; Residential; Indoor</td>
<td>147</td>
<td>99.0</td>
<td>0.09 ng/m³</td>
<td>98.0</td>
<td>6.24</td>
<td>13.8</td>
<td>2.26</td>
<td>3.75</td>
<td>0.93</td>
<td>5.82</td>
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<td>Exposure; Media; Air; Residential; Outdoor</td>
<td>126</td>
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<td>0.389</td>
<td>0.749</td>
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<td>7.2</td>
<td>0.03 ng/mL</td>
<td>0.65</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Exposure; Media; House Dust</td>
<td>143</td>
<td>100.0</td>
<td>2.0 ng/g</td>
<td>49600.0</td>
<td>775.0</td>
<td>4610.0</td>
<td>81.0</td>
<td>4.83</td>
<td>25.6</td>
<td>178.0</td>
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<td>Exposure; Media; House Dust</td>
<td>143</td>
<td>100.0</td>
<td>3.38 ng/m²</td>
<td>54100.0</td>
<td>1200.0</td>
<td>5120.0</td>
<td>102.0</td>
<td>7.58</td>
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<td>400.0</td>
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<td>Exposure; Media; Soil</td>
<td>143</td>
<td>39.0</td>
<td>0.5 ng/g</td>
<td>2930.0</td>
<td>23.7</td>
<td>245.0</td>
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<td>3.47</td>
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<tr>
<td>Exposure; Media; Surfaces - Dislodgable Residue</td>
<td>13</td>
<td>85.0</td>
<td>4.39 ng/m²</td>
<td>32200.0</td>
<td>2500.0</td>
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<td>25.5</td>
<td>11.5</td>
<td>4.87</td>
<td>41.0</td>
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<tr>
<td>Exposure; Media; Surfaces - Total Residue</td>
<td>39</td>
<td>69.0</td>
<td>6.9 ng/m²</td>
<td>38600.0</td>
<td>1270.0</td>
<td>6260.0</td>
<td>27.7</td>
<td>8.63</td>
<td>4.6</td>
<td>65.9</td>
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</tbody>
</table>
CTEPP NC chemicals – sorted by heatmap

**Group 1**
- Benzo[a]pyrene
- Benzo[k]fluoranthene
- Benzo(e)pyrene
- Benzo(g,h,i)perylene
- Indeno [1,2,3-cd]pyrene
- Chrysene
- Benzo[b]fluoranthene
- Benz[a]anthracene
- TRANS–CHLORDANE
- CIS–CHLORDANE
- Diazinon
- Pentachlorophenol
- cis–Permethrin
- trans–Permethrin
- Di–n–butylphthalate
- Butyl benzyl phthalate
- 3,5,6–Trichloro–2–pyridinol
- CHLORPYRIFOS
- Bisphenol A

**Group 2**
- Dieldrin
- DDT
- 2,2,4,5,5′–Pentachlorobiphenyl
- 2,3,3′,4′,6–Pentachlorobiphenyl
- 2,2′,3,5′–Tetrachlorobiphenyl
- 2,3′,4′,5–Tetrachlorobiphenyl
- Aldrin
- Endrin
- 2,6–Dichlorobiphenyl
- 2,3′,4,4′,5–Pentachlorobiphenyl
- Hexachlorocyclohexane
- 2,2′,4,4′,5,5′–Hexachlorobiphenyl
- Dicamba
- 2,2′,3,4,4′,5,5′–Heptachlorobiphenyl
- 2,4,4′–Trichlorobiphenyl
- 4–Nonylphenol
- Pentachloronitrobenzene
- 4,4′–Dichlorobiphenyl
- 3,3′,4,4′,5–Pentachlorobiphenyl
- 3,3′,4,4′,5,5′–Hexachlorobiphenyl
- 3,3′,4,4′–Tetrachlorobiphenyl
- 2,4,5–Trichlorophenoxyacetic
- 2,3,3′,4,4′–Pentachlorobiphenyl

**Group 3**
- 2,4–D ACID
- DDE
- Cyfluthrin
- Dibenz[a,h]anthracene
- 2,2′,5,5′–Tetrachlorobiphenyl
- 2,2′,3,5′,6–Pentachlorobiphenyl
- Heptachlor

Bzp = Benzopyrenes
PAHs = Polycyclic aromatic hydrocarbons
OP = Organophosphate pesticides
OC = Organochlorine insecticide

Pyr = Pyrethroid pesticides
Phth = Phthalate plasticizer
PCB = Polychlorinated biphenyls (PCBs)
Aly = Alykylphenol

Molecular structures for each group are shown in blue, with benzopyrenes (Bzp), polycyclic aromatic hydrocarbons (PAHs), organochlorine insecticides (OCs), organophosphate pesticilides (OP), pyrethroid pesticides (Pyr), phthalate plasticizers (Phth), PCBs, and chlorophenoxy acetic acid herbicide (Herb).
Heatmap of CTEPP NC & OH chemical detection frequencies in different media

- **Liquid Food OH**
- **Liquid Food NC**
- **Solid Food OH**
- **Solid Food NC**
- **Indoor Air OH**
- **Indoor Air NC**
- **Outdoor Air OH**
- **Outdoor Air NC**
- **Dermal NC**
- **Surfaces**
- **Total Res. NC**
- **House Dust NC**
- **House Dust OH**
- **Soil NC**
- **Soil OH**
- **Dislodgeable Res. NC**
- **Dislodgeable Res. OH**
- **Dermal OH**
- **Surface Total Res. OH**

Chemicals listed:
- Benzo[k]fluoranthene
- Benzo[a]pyrene
- Benzo[b]fluoranthene
- Benzo[a]pyrene
- Indeno [1,2,3-cd]pyrene
- Chrysene
- Benzo[k]fluoranthene
- Benzo[j]anthracene
- cis-Permethrin
- trans-Permethrin
- Butyl benzyl phthalate
- TRANS-CHLORDANE
- CIS-CHLORDANE
- Diazinon
- Pentachlorophenol
- CHLORPYRIFOS
- Di-n-butyl phthalate
- 3,5,6-Trichloro-2-pyridinol
- Bisphenol A
- 2,3,7,8-Tetrachlorodibenzop-dioxin
- 2,3,7,8-Tetrachlorodibenzo-p-dioxin
- 2,2,4,5,5'-Pentachlorobiphenyl
- 2,2',3,4,4',5,5'-Heptachlorobiphenyl
- 2,2',3,4,4',5,5'-Heptachlorobiphenyl
- 2,2',3,4,5,5'-Hexachlorobiphenyl
- 2,2',3,4,5,6,6,7,8,9,9'-Decachlorobiphenyl
- Dieldrin
- 2,2',4,5,5'-Pentachlorobiphenyl
- 2,3,7,8-Tetrachlorodibenzo-p-dioxin
- 2,2',3,5,5'-Pentachlorobiphenyl
- 2,2',3,4,4',5,5'-Heptachlorobiphenyl
- 2,2',3,4,4',5,5'-Heptachlorobiphenyl
- 2,2',3,4,5,5'-Hexachlorobiphenyl
- Dicamba
- Hexachlorocyclohexane
- Aldrin
- 4-Nonylphenol
- Pentachlorophenol
- 2,4,5-Trichlorophenoxyacetic acid
- 4,4'-Dichlorodiphenyl ether
- 3,5,4,8,3',4'-Pentachlorodibenzo-p-dioxin
- 2,2',5,5'-Tetrachlorobiphenyl
- 2,2',3,5,6,6,7,9,9'-Decachlorobiphenyl
- 2,2',3,4,5,6,6,7,8,9,9'-Dodecachlorobiphenyl
- 2,6-Dichlorophenol
- 2,4-DICL
- DDE
- Cyfluthrin
- Dichlorodiphenyldichloroethylene
- 2,3,5,8-Tetrachlorodibenzofuran
- Hexachlorocyclohexane
Chemical overlap of CTEPP (NC, OH), AHHS, CCC studies

Only 5 chemicals overlap:

- **Name**
  - CHLORPYRIFOS
  - cis-Permethrin
  - Cyfluthrin
  - Diazinon
  - trans-Permethrin

- **CASRN**
  - 2921-88-2
  - 61949-76-6
  - 68359-37-5
  - 333-41-5
  - 61949-77-7
Next phase study data sets that can be added:

• National Human Exposure Assessment Survey (NHEXAS) – Arizona, “MD” (longitudinal), Region 5

• Minnesota Children’s Pesticide Exposure survey (MNCPES ~ 90 kids)

• Non-occupational pesticide exposure study (NOPES)

• Total Exposure Assessment Methodology Study (TEAM)

• Particle Total Exposure Assessment Methodology (PTEAM)

• NHANES – National Health and Nutrition Examination Survey

• Other exposure data curated from literature . . .
  • Nanomaterials exposure data (measured particle counts in air)
    Gangwal et al. 2011, Environ Health Perspect
    “Informing Selection of Nanomaterial Concentrations for ToxCast In Vitro Testing based on Occupational Exposure Potential”
ExpoCastDB prototype application: Future phases

Next phase website application capabilities:

• Combine chemical concentration measurements from multiple studies and allow filters/search criteria:
  • Chemical concentrations must be in same media.
  • Allow for user input of entering chemicals, media, or study.
  • When combining data sets, calculate detection frequency criteria (>= 25%) based on entire data set for all studies selected.

• Data visualization including log probability plots.

• Additional meta data browsing by ancillary information (location, subject, etc.).
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