Chemical Selection Update

Gail Krowech, Ph.D.
Office of Environmental Health Hazard Assessment

Presentation to Scientific Guidance Panel
July 14, 2011 – Sacramento, CA
Purpose of agenda item

- Update on chemical selection activities
- Update on screening tool for potential designated chemicals
  - Review Panel’s feedback on draft tool
  - Present a revised screening tool, illustrated using some organotins
- Obtain Panel’s input and recommendations
Student assistants

- Bo Hu
- Eileen Leung
Current chemical selection activities

- Screening potential designated chemicals
  - Organotins
  - Pesticides from CDPR Top 100 List
  - Emerging drinking water disinfection by-products

- Preparing document on non-halogenated aromatic organophosphate flame retardants as potential designated chemicals
<table>
<thead>
<tr>
<th>Chem</th>
<th>Type of use</th>
<th>Vol [Trend]</th>
<th>Persistence (P)</th>
<th>Bioaccumulation (B)</th>
<th>Tox</th>
<th>Environ Sample</th>
<th>Biota Sample</th>
<th>Biomon Study</th>
</tr>
</thead>
<tbody>
<tr>
<td>XYZ</td>
<td>consumer product</td>
<td>1-10 M [↑]</td>
<td>++</td>
<td>5.0</td>
<td>✓</td>
<td>house dust</td>
<td>bird eggs</td>
<td>urine; blood</td>
</tr>
</tbody>
</table>
Feedback from Panel at March meeting

- Production volume can be misleading
  - Low volume chemicals can have significant toxicity concerns
  - Production volumes can change rapidly once a chemical gets on to the market

- Checkmark to indicate toxicity is insufficient
  - Include some indication of toxicity concern and extent of information
Panel feedback (cont.)

- Broaden categories on persistence and bioaccumulation
  - Very persistent (vP) and very bioaccumulative (vB)
  - Pseudo-persistence of certain chemicals

- Add more components of the screen, e.g.,
  - Likely routes of exposure
  - Types and numbers of products
  - Additional physical chemical properties
  - Reference doses
New “Reason for Concern” category

- High import/production volume
- Indications of toxicity
- vB or vP chemical
- Potential for exposure (e.g., from consumer products, from food)
- Substitute coming on market (e.g., new plasticizer)
Expand toxicity information

- Descriptive phrase, e.g.,
  - No information found
  - Multiple positive studies
  - Suggestive *in vitro* data
  - Structurally similar to known toxicant

- Type of toxicity, e.g.,
  - Immunotoxicity
  - Developmental toxicity
Example: Screening organotins

Category includes:
- butyltins, methyltins, octyltins, phenyltins

For this example: a subset of butyltins
- dibutyl– and tributyltins
## Reason for concern, use information

<table>
<thead>
<tr>
<th>Chemical</th>
<th>Reason for concern</th>
<th>Type of use</th>
<th>Products/applications</th>
<th>Production volume (2006) lbs*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dibutyltins (DBTs)</td>
<td>Developmental neurotoxicant; exposure from consumer products</td>
<td>PVC stabilizer; catalyst for silicone and polyurethane</td>
<td>PVC flooring, handbags, water pipes, wallpaper, wine corks</td>
<td>Varies; highest, 1-10 M [varies]</td>
</tr>
<tr>
<td>Tributyltins (TBTs)</td>
<td>Endocrine disruptor; vPvB</td>
<td>Biocide</td>
<td>Anti-fouling paint, building materials, consumer products, livestock facilities</td>
<td>Varies; highest, 1-10M [varies]</td>
</tr>
</tbody>
</table>

*U.S. EPA TSCA data*
### Persistence, bioaccumulation, other physical chemical properties

<table>
<thead>
<tr>
<th>Chemical</th>
<th>Persistence</th>
<th>Bioaccumulation</th>
<th>Vapor pressure mmHg</th>
<th>Water solubility mg/L</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>P/vP</td>
<td>B/vB</td>
<td>Log $k_{ow}$</td>
<td></td>
</tr>
<tr>
<td><strong>Dibutyltins</strong></td>
<td>vP*</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DBT dichloride</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.6</td>
<td>$8 \times 10^{-2}$**</td>
<td>92 (20°C)</td>
</tr>
<tr>
<td>DBT dilaurate</td>
<td></td>
<td>3.1</td>
<td>$3 \times 10^{-10}$</td>
<td>3</td>
</tr>
<tr>
<td><strong>Tributyltins</strong></td>
<td>vP*</td>
<td>vB*</td>
<td></td>
<td></td>
</tr>
<tr>
<td>TBT benzoate</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.7</td>
<td>$1.5 \times 10^{-6}$</td>
<td>0.26</td>
</tr>
<tr>
<td>TBT chloride</td>
<td>vP</td>
<td>vB</td>
<td>4.8</td>
<td>$9.7 \times 10^{-3}$</td>
</tr>
<tr>
<td>TBT oxide</td>
<td>vP</td>
<td>vB</td>
<td>4.0</td>
<td>$7.5 \times 10^{-6}$ (20°C)</td>
</tr>
</tbody>
</table>

*Summary conclusion in report for EU

**Blue text indicates estimated values
## Toxicity descriptors, endpoints

<table>
<thead>
<tr>
<th>Chemical</th>
<th>Extent of toxicity information</th>
<th>Toxicity endpoints</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dibutyltins</td>
<td>Multiple positive studies</td>
<td>Developmental neurotoxicity; immunotoxicity; neurotoxicity</td>
</tr>
<tr>
<td>Tributyltins</td>
<td>Multiple positive studies</td>
<td>Endocrine disruption; immunotoxicity; developmental toxicity; obesogenic</td>
</tr>
</tbody>
</table>
## Chemical & biota samples, biomonitoring studies

<table>
<thead>
<tr>
<th>Chemical</th>
<th>Environmental samples</th>
<th>Biota</th>
<th>Human</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dibutyltins</td>
<td>House dust; drinking water/PVC pipes; some foods</td>
<td>Fish/shellfish</td>
<td>Blood; liver; breast milk</td>
</tr>
<tr>
<td></td>
<td></td>
<td>CA sea otter</td>
<td></td>
</tr>
<tr>
<td>Tributyltins</td>
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</table>
Some challenges with screening tool

- Limited information that may be out of date
- Certain types of information not included in current screen
- Difficult to indicate complexities and uncertainties
Questions on screening approach

- What are the highest priority categories?
- How much detail is needed in the screening table?
- How far should we go in researching certain questions?

Proposal: Use a flexible, iterative approach, depending on the specific chemicals and research questions.
Panel input on organotins

- Should the Program move forward on organotins?
- If so, should the Program develop:
  - More screening information on butyltins?
  - Screening information on additional organotins, such as octyltins?
  - Potential designated document(s)?
    - Narrow class, such as di– or tributyltins?
    - Broader class, such as butyltins?