

Chemical Selection Update

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Presentation to Scientific Guidance Panel

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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

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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

March 2011 – Example Screening Table

Chem	Type of use	Vol [Trend]	Persistence (P) Bioaccumulation (B)		Tox	Environ Sample	Biota Sample	Biomon Study
			P US EPA	B LogK _{ow}				
XYZ	consumer product	1-10 M [↑]	++	5.0	✓	house dust	bird eggs	urine; blood

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

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

*U.S. EPA TSCA data

Persistence, bioaccumulation, other physical chemical properties

Chemical	Persistence	Bioaccumulation		Vapor pressure mmHg	Water solubility mg/L
	P/vP	B/vB	Log k_{ow}		
Dibutyltins	vP*				
DBT dichloride			1.6	8×10^{-2} **	92 (20°C)
DBT dilaurate			3.1	3×10^{-10}	3
Tributyltins	vP*	vB*			
TBT benzoate			4.7	1.5×10^{-6}	0.26
TBT chloride	vP	vB	4.8	9.7×10^{-3}	17 (20°C)
TBT oxide	vP	vB	4.0	7.5×10^{-6} (20°C)	19

*Summary conclusion in report for EU

**Blue text indicates estimated values

Toxicity descriptors, endpoints

Chemical	Extent of toxicity information	Toxicity endpoints
Dibutyltins	Multiple positive studies	Developmental neurotoxicity; immunotoxicity; neurotoxicity
Tributyltins	Multiple positive studies	Endocrine disruption; immunotoxicity; developmental toxicity; obesogenic

Environmental & biota samples, biomonitoring studies

Chemical	Environmental samples	Biota	Human
Dibutyltins	House dust; drinking water/PVC pipes; some foods	Fish/shellfish CA sea otter	Blood; liver; breast milk
Tributyltins	House dust; some foods	Fish/shellfish CA sea otter	Blood

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?