

# HPVIS in the PBT Universe: Data Validity and Scope



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December 12, 2006

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## STRUCTURE

1 PBT Universe

- Identify unrecognized persistent, bioaccumulative, toxic substances
- Describe scope and capabilities of system

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## STRUCTURE

1 Background: PBT Universe

2 Integration: HPVIS

- Accessing the HPVIS
- Integrating HPVIS into our PBT Universe (Chemical Information System)

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## STRUCTURE

**1** Background: PBT Universe

**2** Integration: HPVIS

**3** Comparisons: HPVIS & PBT Universe

- Using PBT Universe to assess HPVIS data
- Using HPVIS data to screen chemicals and fulfill SIDS commitments

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## PBT UNIVERSE

Data on nearly 250,000 chemicals

Persistence, bioaccumulation, toxicity, chemical property, regulatory, & exposure data

Search on regulatory status, exposure data & PBT properties

On-the-fly data type, units, & relational recognition and conversion capabilities

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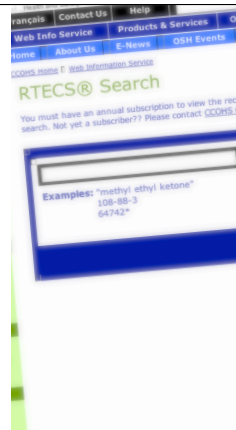
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## PBT UNIVERSE KEY DATA

### PBT

RTECS  
ECOTOX  
EFDB (Environmental Fate Database)  
HSDB (Hazardous Substances Database)  
IUCLID & HPVIS (partial)  
NSDB (Nordic Substances Database)  
OSPAR  
Environment Canada 2006  
TSCA ITC + TSCATS (planned)  
UNEP/OECD SIDS



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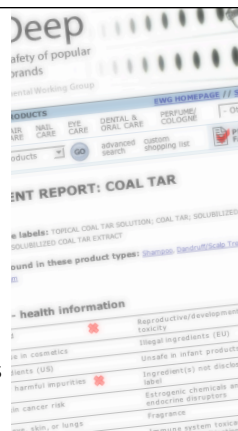
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## PBT UNIVERSE KEY DATA

### Exposure

EPA's 2003 TRI (Toxic Release Inventory), PCS (Permit Compliance System), and IUR (Inventory Update Rule)  
EWG's cosmetics, tap water, & biomonitoring data  
CDC's NHANES  
FDA's Total Diet Study  
Planned: Future/Past TRI data, USGS NAWQA

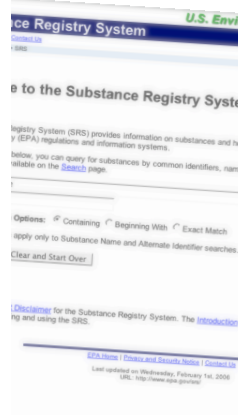


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## PBT UNIVERSE KEY DATA

### Regulatory

EPA's SRS site  
FDA's EAFUS  
International treaties:  
OSPAR (Convention for the Protection of the Marine Environment of the North-East Atlantic)  
Long-Range Transboundary Air Pollution  
Stockholm Convention on Persistent Organic Pollutants



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The goal of the HPV Challenge Program is to provide basic data on the health and environmental effects of approximately 2,200 HPV chemicals to the public... Sponsorship involves a commitment to develop data summaries of relevant existing information and to conduct testing to fill any data gaps.

### HPV Challenge Program

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The conclusions present a summary of the hazards of the chemical, written with sufficient detail and clarity as to be informative and to assist countries with classification work and other hazard based national decision making; and exposure information to put the hazard information into context.

**OECD HPV Program**

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**STATUS of HPVIS versus HPVs**

HPVIS	879 chemicals 814 HPVs 1990-2002 658 HPVs 2002
2002 IUR	2,837 HPVs
1990-2002 IUR	4,229 HPVs
OECD HPVs	4,843 HPVs

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**INTEGRATING HPVIS**

OCTOBER 2005:  
EWG examined Robust  
Summaries

- Data structures were not designed ahead of time and SIDS templates were not used
- Files were internally, but not externally structured.

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## INTEGRATING HPVIS

OCTOBER 2005:  
EWG examined Robust  
Summaries

November 2006  
HPVIS partially integrated into  
PBT Universe

- Oracle 9i export could not be imported into Oracle 10g
- XML exports via web interface malformed or incomplete data
- Requires hand-parsing via scripting language such as PHP or awk.

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## INTEGRATING HPVIS

OCTOBER 2005:  
EWG examined Robust  
Summaries

NOVEMBER 2006  
HPVIS partially integrated into  
PBT Universe

CURRENT  
PBT Universe is compared by hand  
to HPVIS

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## INTEGRATING HPVIS

- 1 HPVIS uses SIDS endpoints, but not data structures
- 2 Priority to map HPVIS to SIDS/IUCLID templates
- 3 Some fields would benefit from data picklists.
- 4 Data was well parsed compared to IUCLID data. However, many toxicity endpoints were in text fields rather than endpoint fields.

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## QUALITY of HPVIS DATA

**1** Selected five chemicals that were in both HPVIS and PBT Universe

**2** Assessed data quality in:

- Biodegradation
- Partition coefficients
- Bioaccumulation
- Ecotoxicity
- Mammalian Toxicity

- Phenol, 4(1,1,1,3,3 tetramethylbutyl) t-OP
- 1,5,9-Cyclododecatriene CDT
- Hexabromocyclododecane HBCD
- Tetrabromobisphenol A TBBPA
- 4-sec-Butyl-2,6-di-tert-butylphenol 4BTBP

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## PARTITION COEFFICIENTS

Chemical		EWG	HPVIS
t-OP	exp	<b>3-5.31 (6)</b>	<b>4.12 (1)</b>
	mod	5.28 - 5.31 (2)	5.28 (1)
CDT	exp	<b>3-6.19 (4)</b>	<b>4.97 (1)</b>
	mod	5.48 (1)	none
HBCD	exp	<b>5.81 (1)</b>	<b>5.63 (1)<sup>1</sup></b>
	mod	7.74 (1)	none
TBBPA	exp	3-5.9 (3)	4.54-5.90 (2)
	mod	6.3-7.2 (2)	none
4BTBP	exp	none	none
	mod	6.43 (1)	6.43 (1)

<sup>1</sup> Value comes from 3194-55-6's entry, but the test substance was HBCD in this case.

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## BIOCONCENTRATION

Chemical		EWG	HPVIS
t-OP	exp	<b>113 - 469 (2)</b>	<b>none</b>
	mod	<b>2291 - 45700 (6)</b>	<b>none</b>
CDT	exp	<b>2630-14800 (2)</b>	<b>none</b>
	mod	<b>3467 (1)</b>	<b>1339 (1)</b>
HBCD	exp	<b>18100 (1)</b>	<b>8974(1)<sup>1</sup></b>
	mod	<b>6166 (1)</b>	<b>none</b>
TBBPA	exp	20-1200 (4)	<b>148-3190 (5)</b>
	mod	5 - 42700	none
4BTBP	exp	none	none
	mod	6310-1.4E6 (4)	none

<sup>1</sup> The HPVIS also reports that earthworms have a bioaccumulation factor (BAF) of 4.5

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## BIODEGRADATION

Chemical		EWG	HPVIS
t-OP	ready	0-74%: 28d (3)	0-69.9%: 28-35d (3)
	inher	no (5)	none
CDT	ready	0-2%: 5-14d	<b>1%: 28d</b>
	inher	no (1)	none
HBCD	ready	no (1)	<b>0%:28d-100%:7d</b>
	inher	none	none
TBBPA	<b>ready</b>	<b>0:80d-&lt;20%: 28d(4)</b>	<b>0%:14d-60%:64d</b>
	<b>inher</b>	<b>no (6)</b>	<b>yes</b>
4BTBP	ready	weeks-p (mod)	weeks-p (mod+RA)
	inher	months-u (mod)	months-u (mod+RA)

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## ECOTOXICITY

All toxicity units in mg/L

Chemical		EWG	HPVIS
t-OP	acute LC50	0.069:24h shrp - 81:48h fish (25)	4.12 (1)
	chronic NOEC	0.006 l:60d fish - 0.030:21d daphnia (2)	11 - 0.006 l:60d fish
CDT	acute LC50	0.116: - 140: (7)	0.47: - 140: (4+3)
	chronic NOEC	none	none
HBCD	<b>acute LC50</b>	<b>0.0093:72h algae - 146: daphnia (3)</b>	<b>0.0093:72h algae - &gt;1.5:96h algae (5)<sup>1</sup></b>
	<b>chronic NOEC</b>	<b>none</b>	<b>128:56d worm - 250:28d amph. (3)<sup>1</sup></b>

<sup>1</sup> 1 test classified as acute lasted 88 days. 5 acute & 3 chronic tests demonstrated NOEC below solubility limits (0.0067mg/L). 1 21-day plant study found NOEC <5000 mg/kg soil.

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## ECOTOXICITY

All toxicity units in mg/L

Chemical		EWG	HPVIS
TBBPA	<b>acute LC50</b>	<b>0.0016:96h zebra danio- 8.2: killifish (15)</b>	<b>0.4:96h trout - 8.2:48h killifish (5)</b>
	chronic NOEC	0.16:35d minnow - 228:	0.16:35d daphnia - 0.07:70d mussel (3)
4BTBP	acute LC50	0.072:96h fish - 0.22:48h dap (mod)	0.072:96h fish - 0.22:48h dap (model)
	chronic NOEC	0.003:90d fish - 0.008:21d dap (mod)	0.003:90d fish - 0.008:21d dap (model)

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### MAMMALIAN TOXICITY

endpoints in mg/kg unless otherwise noted

Chemical		EWG	HPVIS
t-OP	<b>act</b>	<b>25-4600 (12)</b>	<b>&gt;2000-2200 (4)</b>
	<b>md</b>	<b>32-7680 (24)</b>	<b>2000 (1)</b>
	rep	250-1920 (2)	200 ppm (1 iv)
	<b>dev</b>	<b>0.014-0.14 (1)</b>	<b>75-750 (2 RA)</b>
	mut	negative (3 iv)	negative (4 iv)
	tum	5280 - 12wk (1)	none
CDT	<b>act</b>	<b>500 - 4660 (4)</b>	<b>none</b>
	md	10700 (1)	none
	rep	none	<b>100-300 (1)</b>
	dev	none	<b>25 ppm (1)</b>
	mut	negative (2 iv)	none
	tum	none	none

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### MAMMALIAN TOXICITY

Chemical		EWG	HPVIS
HBCD	act	> 10000 (1)	>10000 (3)
	md	none	<b>2560-4820 (4)</b>
	rep	none	<b>&gt;1000 (1)</b>
	dev	>2500 (1)	<b>&gt;1000-&gt;2500 (2)</b>
	mut	none	<b>&gt;2000 (1 iv)</b>
	tum	none	<b>&gt;4000 (1)</b>
	neu	none	<b>&gt;1000 (1)</b>
TBBPA	act	3160-5000 (5)	2000-5000 (4)
	md	2500-1e5 (4)	<b>780 - &gt;2500 (6)</b>
	<b>rep</b>	<b>250 (1)</b>	<b>&gt; 1000 (2)</b>
	dev	10000 (1)	none
mut	negative (1)	none	

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### MAMMALIAN TOXICITY

Chemical		EWG	HPVIS
4BTBP	act	none	<b>4800 (1)</b>
	md	none	1.08-100 (4 RA)
	rep	none	15-750 (2 RA)
	dev	none	75-750 (2 RA)
	mut	none	negative (5)
	tum	none	none

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**1** Basic data on the health and environmental effects

- HPVIS chemicals are missing studies, sometimes critically, reducing scope of results
- HPVIS adds recent and previously unpublished studies
- HPV Challenge Program has caused some new testing of HPVs

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**USING HPVIS for STATED GOALS**

**1** Basic data on the health and environmental effects

- Bioaccumulation data was not required for all chemicals, but would be required under the program guidelines where ecotoxicity was a concern
- Use/Exposure data is generally missing
- At least one study is duplicated, highlighting need for common referencing format
- Degradation products need more systematic treatment to identify PBTs

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**USING HPVIS for STATED GOALS**

**1** Basic data on the health and environmental effects

**2** Assist countries with classification work and other hazard based national decision making

- Difficult to access raw data
- Difficult to integrate data into other systems
- Countries or end-users need to develop robust unit conversions system to compare data

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**THANKS!**

**1** Collaborators

- Richard Wiles
- Jane Houlihan
- Timothy Kropp

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**THANKS!**

**1** Collaborators

**2** Funders

- NEWMOA for HPVIS support
- Luce Foundation for PBT Universe

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