

Using existing chemical datasets to assess the HPVIS: Finding PBTs in HPVs

STRUCTURE

1 Background: EWG Datasets

- Identify emerging persistent, bioaccumulative, toxic contaminants
- Describe scope and capabilities of system

STRUCTURE

1 Background: EWG Datasets

2 Integration: HPVIS

- Accessing the HPVIS
- Integrating HPVIS into the EWG Datasets

STRUCTURE

1 Background: EWG Datasets

2 Integration: HPVIS

3 Comparisons: HPVIS & EWG Datasets

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

EWG DATASETS

Persistence, bioaccumulation, toxicity, chemical property, regulatory, & exposure data on nearly 250,000 chemicals

- RTECS
- ECOTOX
- EFDB
- HSDB
- IUCLID
- HPVIS (partial)
- NSDB
- OSPAR
- Environment Canada
- TSCA ITC + TSCATS

EWG DATASETS

Persistence, bioaccumulation, toxicity, chemical property, regulatory, & exposure data on nearly 250,000 chemicals

Able to search and group on the above data (in implementation)

EWG DATASETS

Persistence, bioaccumulation, toxicity, chemical property, regulatory, & exposure data on nearly 250,000 chemicals

Able to search and group on the above data (in implementation)

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

“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 webpages](#)

“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 Guidelines -
from website**

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.
- Data used to validate TRI

INTEGRATING HPVIS

OCTOBER 2005:

EWG examined Robust Summaries

NOVEMBER 2006

HPVIS partially integrated into EWG Datasets

- 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

INTEGRATING HPVIS

OCTOBER 2005:

EWG examined Robust
Summaries

NOVEMBER 2006

HPVIS partially integrated into EWG
Datasets

CURRENT

EWG Datasets compared manually
by hand to HPVIS

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 is well parsed compared to IULCID data, however, many toxicity endpoints remain text rather than endpoint fields.

COMPARISONS: HPVIS & EWG DATASETS

1 Selected five chemicals that were in both HPVIS and EWG Datasets

2 Assessed data quality in:

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

| | |
|---------------------------------------|----------------------------------|
| • Phenol, 4(1,1,3,3 tetramethylbutyl) | t-OP 04/02 06/06 |
| • 1,5,9-Cyclododecatriene | CDT 12/01 12/03 |
| • Hexabromo-cyclododecane | HBCD 12/02 07/05 |
| • Tetrabrom-bisphenol A | TBBPA 12/02 11/04 03/06 |
| • 4-sec-Butyl-2,6-di-tert-butylphenol | 4BTBP 04/02 06/06 |

PARTITION COEFFICIENTS

| Chemical | | EWG | HPVIS |
|----------|-----|-----------------|-----------------------|
| t-OP | exp | 3-5.31 (6) | 4.12 (1) |
| | mod | 5.28 - 5.31 (2) | 5.28 (1) |
| CDT | exp | 3-6.19 (4) | 4.97 (1) |
| | mod | 5.48 (1) | none |
| HBCD | exp | 5.81 (1) | 5.63 (1) ¹ |
| | 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) |

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

BIOCONCENTRATION

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

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

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 (2) | 1%: 28d (1) |
| | inher | no (1) | none |
| HBCD | ready | no (1) | 0%:28d-100%:7d (6) |
| TBBPA | ready | 0:80d-<20%: 28d(4) | 0%:14d-60%:64d |
| | inher | no (6) | yes |
| 4BTBP | ready | weeks-p (mod) | weeks-p (mod+RA) |
| | inher | months-u (mod) | months-u (mod+RA) |

ECOTOXICITY

All toxicity units in mg/L

| Chemical | | EWG | HPVIS |
|----------|--------------|--|---|
| t-OP | acute LC50 | 0.069:24h shrimp -81:48h fish (25) | .019:96h shrimp - 4.2:72h algae (4) |
| | chronic NOEC | 0.0061:60d trout -0.030:21d daphnia (2) | 0.0061:60d trout - <1:35d trout (3) |
| CDT | acute LC50 | 0.116:24h goldfish- 140:96h algae (7) | 0.47:96h mysids- 140:96h algae (4) |
| HBCD | acute LC50 | 0.0093:72h algae -146: daphnia (3) | 0.0093:72h algae - >1.5:96h algae (5)¹ |
| | chronic NOEC | none | 128:56d worm - 250:28d amph. (3)¹ |

¹ 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.

ECOTOXICITY

All toxicity units in mg/L

| Chemical | | EWG | HPVIS |
|----------|-----------------|---|---|
| TBBPA | acute LC50 | 0.0016:96h zebra danio- 8.2: killifish (15) | 0.4:96h trout - 8.2:48h killifish (5) |
| | 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) |

MAMMALIAN TOXICITY

endpoints in mg/kg unless otherwise noted

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

MAMMALIAN TOXICITY

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

MAMMALIAN TOXICITY

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

MISSED IN THE HPVVIS

North-East Atlan-
d HBCD on its list
priority action to
fine environment.
official position ex-
a POP candidate,
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nt Programme. At
is included in nei-
7 chemicals under
convention on Pris-
ent (PIC) nor the
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LC/MS in all ap-
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the Toxicological
(Belgium). Georg
Janak is a senior
cientist in the de-
se Norwegian In-

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2005 ES&T HBCD cover story

- 11 studies before/ initial 2002 R.S. submission
- 5 on Env. Monitoring
- 1 on bioaccumulation
- 1 on ecotoxicity
- 2 on mam. toxicity
- 22 studies before revised 2005 submission
- 6 on env. monitoring
- 9 on bioaccumulation
- 2 on ecotoxicity
- 5 on mam. toxicity

MISSED IN THE HPVIS



U.S. Environmental Protection Agency
High Production Volume Information System (HPVIS)

Recent Additions | Contact Us Search: **GO**

EPA Home > Prevention, Pesticides & Toxic Substances > Pollution Prevention & Toxics > High Production Volume (HPV) Challenge Program > High Production Volume Information System (HPVIS) > Detailed Chemical Results

Detailed Chemical Results

Chemical Name: Cyclohexane, 1,2,5,6,9,10-hexabromo-
CAS Number: 3194-55-6

Click on the endpoint link to see the data on a tab page.

Physical-Chemical SIDS

- [Melting Point\(1\)](#)
- [Vapor Pressure\(1\)](#)
- [Partition Coefficient\(1\)](#)
- [Water Solubility\(2\)](#)

Physical-Chemical Other

- [Solubility in Different Media\(1\)](#)
- [Granulometry\(1\)](#)

Fate SIDS

- [Transport Between Environmental Compartments Fugacity/Dist\(1\)](#)
- [Biodegradation\(6\)](#)

Fate Other

- [Stability in Soil\(2\)](#)
- [Bioaccumulation\(2\)](#)
- [Monitoring Data\(1\)](#)
- [Other\(1\)](#)

EcoToxicity SIDS

- [Acute Toxicity to Aquatic Vertebrates\(2\)](#)
- [Acute Toxicity to Aquatic Invertebrates\(1\)](#)
- [Acute Toxicity to Aquatic Plants\(3\)](#)

EcoToxicity Other

- [Chronic Aquatic Vertebrate Toxicity\(1\)](#)
- [Chronic Aquatic Invertebrate Toxicity\(1\)](#)
- [Toxicity to Terrestrial Plants\(1\)](#)
- [Toxicity to Soil Dwelling Organisms\(2\)](#)
- [Other\(3\)](#)

Mammalian Health Effects SIDS

- [Acute Toxicity\(3\)](#)
- [Repeated-Dose Toxicity\(4\)](#)
- [Genetic Toxicity in vivo\(1\)](#)
- [Genetic Toxicity in vitro\(3\)](#)
- [Reproductive Toxicity\(1\)](#)
- [Developmental Toxicity/Teratogenicity\(2\)](#)

Mammalian Health Effects Other

HPV Challenge Program Home
How to Participate
Who's Participating
Information on HPV Chemicals
HPV Challenge Program Robust Summaries, Test Plans & Comments
Vol. Children's Chemical Eval. Pgm.
Related Websites

2005 HPVIS

- 11 studies before/ initial 2002 R.S. submission
 - 1 on mam. toxicity
- 22 studies before revised 2005 submission
 - 1 on env. monitoring/bioaccumulation, however most env. monitoring studies are in RS from 2003 EU risk assessment. Data was truncated in HPVIS

CONCLUSIONS

1 Basic data on the health and environmental effects

- HPVIS chemicals are missing studies from standard databases reducing scope of results
- HPVIS integrates some recent and previously unpublished studies not in other databases
- HPV Challenge Program is at least partially responsible for some new testing of HPVs

CONCLUSIONS

1 Basic data on the health and environmental effects

- Bioaccumulation data was included always included for these chemicals, but would be required under the program guidelines
- Use/Exposure data is generally missing from HPVIS though not necessarily the Robust Summaries
- For at least two HPVIS endpoints, studies are duplicated
- Units are sometimes incorrectly reported within studies

CONCLUSIONS

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

RECOMMENDATIONS

1 Database structure and information delivery

- Tests involving proxy chemicals should also be included under those chemicals
- Degradation products need more systematic treatment to identify PBTs
- Better options to access raw data need to be implemented
- Common referencing system should be implemented

RECOMMENDATIONS

1 Database structure and information delivery

2 HPVIS Data

- Entries should reflect understanding and full existing scope of data at time of submission.
- Each HPVIS chemical needs a data scope review as there are not systemic holes
- Bioaccumulation data needs to be included whenever there is a potential PBT concern

RECOMMENDATIONS

1 Database structure and information delivery

2 HPVIS data

3 Future work

- Mechanism to add existing studies as well as ongoing/future studies must be created for database to become/remain relevant
- Web-based encrypted electronic submissions with AJAX pre-filling technology and data validation

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1 Collaborators

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