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**Use of the US EPA's High
Production Volume Information
System to Identify Persistent,
Bioaccumulative, Toxic
Chemicals Used in Personal
Care Products**

Presentation purpose:

To demonstrate the use of HPVIS as a tool to screen high volume chemicals for qualities that may pose a threat to human health and the environment.

Potential uses for HPVVIS

- **Screen for high volume chemicals used in pharmaceuticals, PCPs, household cleaners**
- **Identify candidates for environmental monitoring**
- **Identify candidates for replacement with less toxic alternatives**



EPA HPVIS

- **Access to environmental and health effects data for chemicals produced in amounts \geq 1 million pounds**
 - Goal: 2,200 CAS submissions
 - Current number: 1,022 (as of July 2007)

- **Includes over 50 endpoints**
 - 4 endpoint categories
 - Physical/chemical properties
 - Environmental fate and pathways
 - Ecotoxicity
 - Mammalian health effects



EPA HPVIS

- **Purpose: public has a “right to know” about high volume chemicals in their environment**
- **Data sets consist of published and unpublished studies**
- **Voluntary submission, self-reported**

Navigating EPA HPVIS

EPA High Production Volume Information System (HPVIS)

U.S. Environmental Protection Agency

High Production Volume Information System (HPVIS)

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The High Production Volume Information System (HPVIS) provides access to select health and environmental effect information on chemicals that are manufactured in exceptionally large amounts. Information in this database are submitted through EPA's [High Production Volume \(HPV\) Challenge Program](#). HPVIS allows users to search for summary information, test plans, and new data on high production volume chemicals as they are developed. Read [basic information about high production volume chemicals](#).

As of April 2007, HPVIS contains 348 submissions, representing 873 chemical substances, either as a single chemical submission or as a member of a chemical category. [High Production Volume Information System \(HPVIS\)](#)

How does this work?

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. Companies, such as chemical manufacturers and trade associations, voluntarily sponsor a set of HPV chemicals, perform tests on the chemicals, and submit their test data to this database.

To ensure consistency, sponsors follow the Screening Information Data Set (SIDS), developed by the Organization for Economic Cooperation and Development. SIDS provides internationally agreed upon tests for screening chemicals for human and environmental hazards. These data can help environmental managers and public decision-makers make informed preliminary judgements about the hazards of chemical substances.

HPVIS submissions contain data on up to 50 endpoints organized into the following four disciplines. Click on any of the disciplines to view a list of the HPVIS endpoints included in that discipline. Click on any of the individual endpoints to view the specific data fields defined for each endpoint. Note: this information is metadata - information describing the data that is included in HPVIS. To view the actual data, use the Search box on the right side of this page.

- [Physical/chemical properties \(e.g., melting point, vapor pressure\)](#)
- [Environmental fate and pathways \(e.g., biodegradation, stability in soil\)](#)
- [Ecotoxicity \(e.g., fish toxicity, toxicity to terrestrial plants\)](#)
- [Mammalian health effects \(e.g., reproductive toxicity, developmental toxicity\)](#)

Disclaimer: Data available in HPVIS have been entered from the robust summaries and test plans as submitted by the HPV Challenge program sponsors. This self-reported information is also available on the HPV website at <http://www.epa.gov/hpv>. EPA has verified the data in HPVIS to ensure that it is consistent with the information that was submitted under the HPV Challenge program. Industry sponsors also have the opportunity to verify their submitted data.

EPA also plans to assess the quality of the data but that effort has not yet begun.

HPVIS includes both initial and final submissions. The Agency intends to mark the data accordingly as our HPVIS efforts proceed.

EPA plans to follow the [recommendation of the National Pollution Prevention and Toxics Advisory Committee](#) to review the HPV Challenge data.

Start here to look up data on a high production volume chemical.

Enter partial chemical name or CAS # to search the 873 chemical substances in the HPVIS database.

[Search](#)

Other options:

[Browse a list of chemical, categories, sponsors, and submitters](#) if you don't know a specific chemical name to look up.

[Create a special report with the query tool](#) to select specific data elements to build a special report that you can review online or download to your computer.

[Create a matrix of the individual chemical members](#) of the category as one axis and the HPVIS endpoints as the other. The intent of the report is to assist users in performing a "read-across" analysis to estimate values for chemicals in the category without a result reported for a specific endpoint.

[Create an Endpoint Result Report](#), providing a frequency of distribution of the units-of-measure reported for any specific result value within the system.

Done

Start | EPA High Production V... | Downloads | Microsoft PowerPoint - [...]

8:45 PM

<http://www.epa.gov/hpvis/index.html>

Search by CAS

The screenshot shows a Mozilla Firefox browser window displaying the EPA's High Production Volume Information System (HPVIS) website. The browser's address bar shows the URL: <http://iaspub.epa.gov/jopthpv/quicksearch.display?pChem=101315>. The website header includes the EPA logo and the text "U.S. Environmental Protection Agency". The main heading is "High Production Volume Information System (HPVIS)". Below this, there is a search bar with a "GO" button and a breadcrumb trail: "EPA Home > Prevention, Pesticides & Toxic Substances > Pollution Prevention & Toxics > High Production Volume (HPV) Challenge Program > High Production Volume Information System (HPVIS) > Detailed Chemical Results".

The main content area is titled "Detailed Chemical Results" and displays the following information:

- Chemical Name:** Urea, N-(4-chlorophenyl)-N'-(3,4-dichlorophenyl)-
- CAS Number:** 101-20-2

Below the chemical name, there is a note: "Click on the endpoint link to see the data on a tab page." The results are organized into several categories, each with a list of links and counts:

- Physical-Chemical SIDS**
 - Melting Point(3)
 - Boiling Point(1)
 - Vapor Pressure(1)
 - Partition Coefficient(3)
 - Water Solubility(1)
- Physical-Chemical Other**
 - Density/Specific Gravity(1)
- Fate SIDS**
 - Photodegradation(1)
 - Stability in Water(1)
 - Transport Between Environmental Compartments Fugacity/Dist(4)
 - Biodegradation(3)
- Fate Other**
 - Bioaccumulation(1)
 - Monitoring Data(13)
- EcoToxicity SIDS**
 - Acute Toxicity to Aquatic Vertebrates(6)
 - Acute Toxicity to Aquatic Invertebrates(15)
 - Acute Toxicity to Aquatic Plants(5)
- EcoToxicity Other**
 - Chronic Aquatic Vertebrate Toxicity(2)
 - Chronic Aquatic Invertebrate Toxicity(15)
 - Other(5)
- Mammalian Health Effects SIDS**
 - Acute Toxicity(5)
 - Repeated-Dose Toxicity(3)
 - Genetic Toxicity in vitro(3)
 - Reproductive Toxicity(1)
 - Developmental Toxicity/Teratogenicity(1)
- Mammalian Health Effects Other**
 - Skin Irritation(5)

The browser's taskbar at the bottom shows the Start button, several open applications including "EPA - HPVIS - Mozilla ..." and "Microsoft PowerPoint - [...]", and the system clock showing "8:51 PM".

Robust summary

Study 1 Study 2 Study 3

Print Robust Summary

Partition Coefficient	
CAS Number :	101-20-2
Sponsored Chemical Name :	Urea, N-(4-chlorophenyl)-N'-(3,4-dichlorophenyl)-
Test Substance - Partition Coefficient	
Test Substance:	(101-20-2) Urea, N-(4-chlorophenyl)-N'-(3,4-dichlorophenyl)-
Test Substance Purity/Composition and Other Test Substance Comments:	molecular structure of triclocarban, CAS# 101-20-2 Estimated by Calculation
Test Substance Result Type:	Estimated
Results - Partition Coefficient	
Partition Coefficient Value/Range (Log K_{ow}):	= 4.9
Results Remarks:	Log pow : = 4.9 at °C
Study/Method - Partition Coefficient	
Key Study Sponsor Indicator:	
Year Study Performed:	1999
Method/Guideline Followed:	Other

Internet

Physical-Chemical Property Comparisons Between Studies for Triclocarban (CAS # 101-20-2)

	HPVIS	Halden and Paull (2005)	Sapkota <i>et al.</i> (2007)	CEE 502* (2007)
Melting point	250°C ^a	140°C ^d	-	-
Percent in each medium				
Water	70.2	-	7	12.5
Soil	0	-	77	70.3
Sediment	29.8	-	16	17.2
Air	0	-	0	0
Log Kow at 25°C	4.9 ^e	4.9 ^e	4.9 ^e	4.6 ^h
Water Solubility mg/L	0.11 at 20°C ^b	0.65-1.55 at 25°C ^{d,f}	0.65 at 25°C ^g	
Bioconcentration factor	137 ^c	-	1200 ^f	1200 ^d

^a Hawley's Chemical Dictionary, 11th ed.

^b Bayer AG study 1995

^c Monstanto study 1980

^d Calculated using PBT Profiler

^e Calculated using K_{ow} WIN

^f Calculated using ECOSAR

^g Calculated using Solaris V4.67

^h Estimated using Schwarzenbach *et al.* 2003

*Pepping, Stone, Haughwout. Unpublished data.

Query endpoints

U.S. Environmental Protection Agency

High Production Volume Information System (HPVIS)

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HPVIS Ad Hoc Query

This query allows you to select key data elements from HPVIS to build a tabular report or a Microsoft Excel Spreadsheet for downloading.

There are 3 steps to follow to generate a query:

1. First, select one view of interest from the list below.
2. Select columns (data elements or fields) from the selected view.
3. Enter your search criteria to target specific records from the database.

The [HPVIS Ad Hoc Query User's Guide](#) will provide you with detailed information on how to use the HPVIS Ad Hoc Query. For additional help, select the [Online Tutorial](#).

To view the below table in tabular form, click [Tabular Selection Form](#)

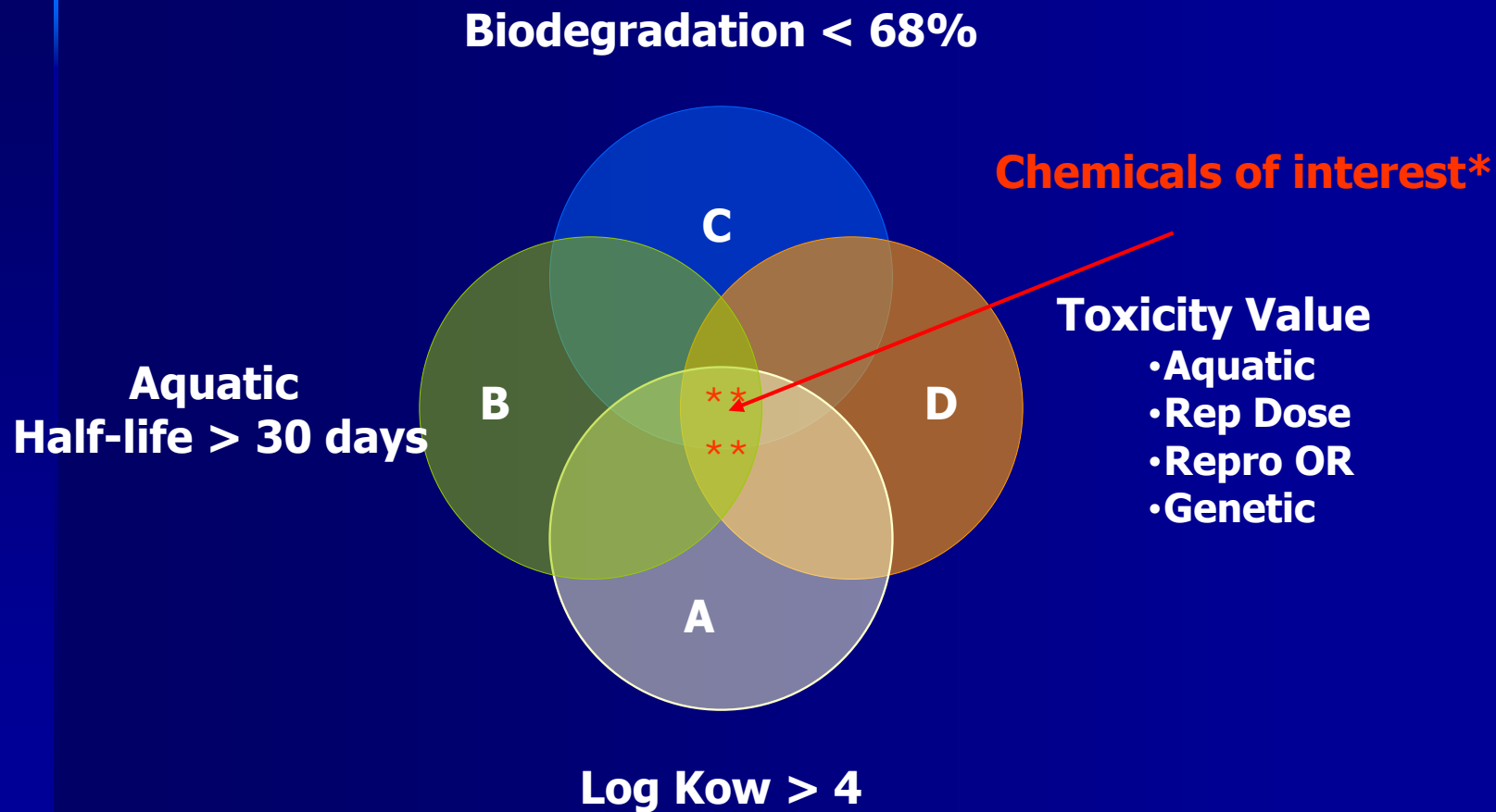
Step 1: Start by selecting one view to be the focus of your query.

▶ Submission Information	
▶ Discipline Results	
▶ Physical Chemical	
▶ Fate	▶ Photodegradation
▶ EcoToxicity	▶ Stability in Water
▶ Mammalian Health Effects	▶ Transport Between Environmental Compartments
▶ Use and Exposure	▶ FugacityDist
	▶ Biodegradation
	▶ Stability in Soil
	▶ Adsorption/Desorption to Soil
	▶ Bioaccumulation
	▶ Mode of Degradation in Actual Use
	▶ BOD5, COD or BOD5/COD Ratio
	▶ Monitoring Data
	▶ Field Studies Data
	▶ Fate Other

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http://www.epa.gov/hpvis/ez.html#

Finding chemicals of interest



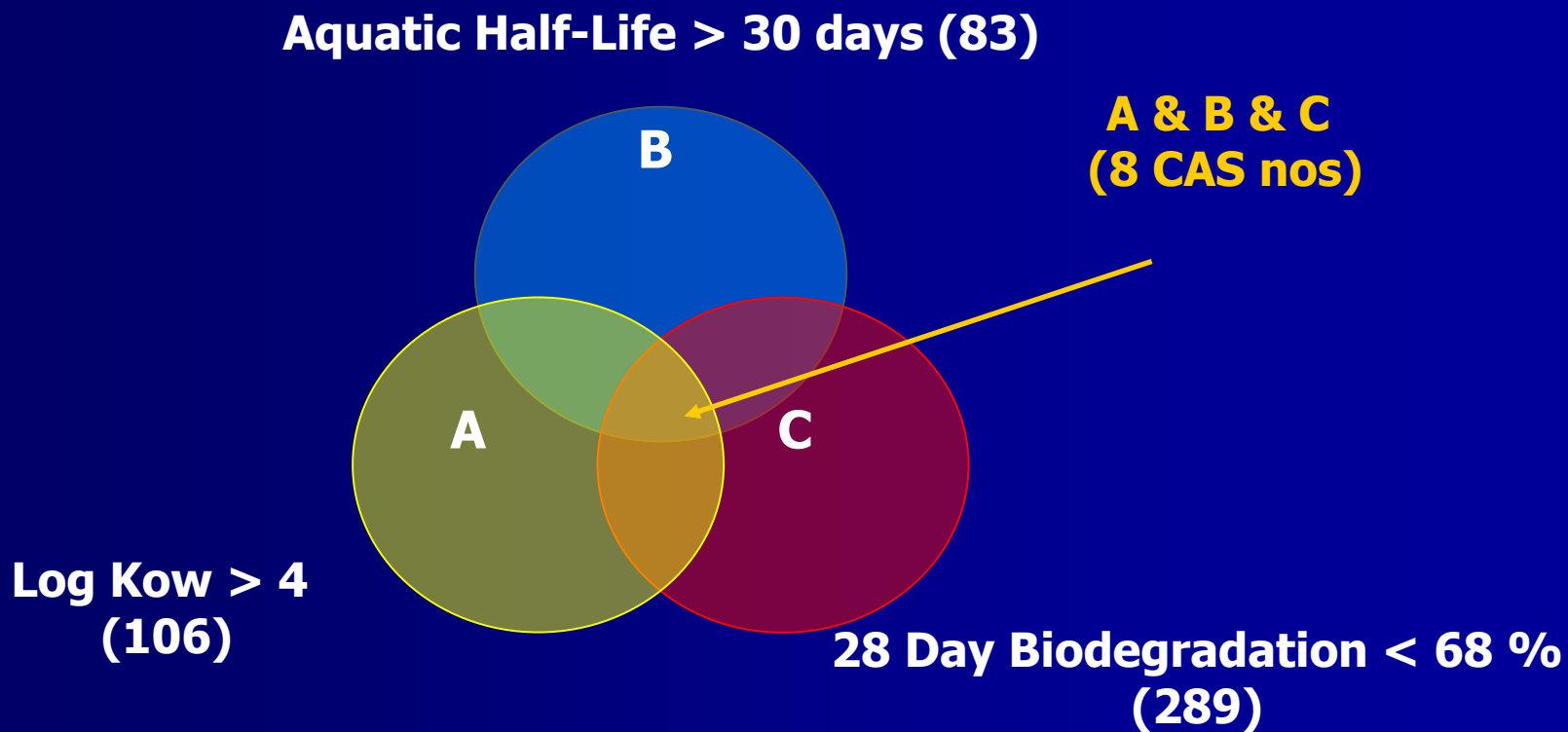
Methods Used

- 1. HPVIS was queried for each endpoint**
- 2. Data was exported to Excel files**
- 3. Files were edited using Excel and imported into MS Access**
- 4. MS Access queries were used to match chemicals that met study criteria for each endpoint**

Data in HPVIS

<u>Endpoint</u>	<u>No of CAS numbers</u>
■ At least one endpoint	879
■ Log Kow	339
■ Ready Biodegradation	375
■ Aquatic Half-Life	127
■ Aquatic Toxicity NOAEL	254
■ Repeat Dose NOAEL	233
■ Genotoxicity	335
■ Reproductive Toxicity	80

Chemicals that meet environmental fate criteria



Of 8 Chemicals That Met Fate Criteria

- 5 identified as potentially toxic, persistent and bioaccumulative

<u>CAS No.</u>	<u>Chemical Name</u>	<u>Uses</u>
101-20-2	Triclocarban	Antimicrobial in soaps
118-58-1	Benzyl salicylate	Flavor/fragrance Naturally occurring
2050-08-0	Amyl salicylate	Flavor/fragrance Naturally occurring?
32687-78-8	Antioxidant 1024	Rubber additive
68526-82-9	EP-290, C6-C10 Alkenes	Defoamer, lubricant

Database Problems

- **Multiple data values**

- Users need to decide which value to use (minimum, maximum, mean, median, most recent, etc).

- **Units vary for some endpoints**

- Half-lives provided in seconds, minutes, days, weeks, etc.
- Doses given as ppm, mg/kg, % diet, mg/L, and mg/kg/day

- **Some field names were vague and not linked to an endpoint**

- **Numeric fields created as text fields**

Data Quality

- **Test methods for HPVIS data are not standardized**
- **Some numbers are “better” than others**
 - Outdated test results
- **Test conditions, exposure times and species can vary**

Conclusions

- **HPVIS provides a large amount of data that can be accessed at no cost**
- **HPVIS provides a valuable tool that can be used to prioritize chemicals for further evaluation**
- **Although HPVIS is incomplete, we were able to evaluate data for 55 HPV chemicals**