

# Characterizing Chemicals in Commerce

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Development of the High Production Volume  
Information System (HPVIS)

Atlanta, Georgia

September 27, 2007

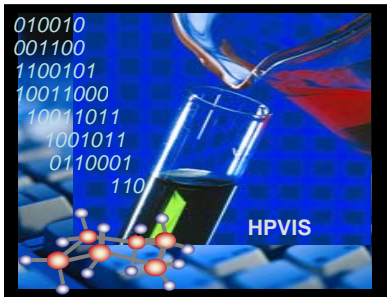


Office of Pollution Prevention and Toxics

# HPV Challenge Program Goals

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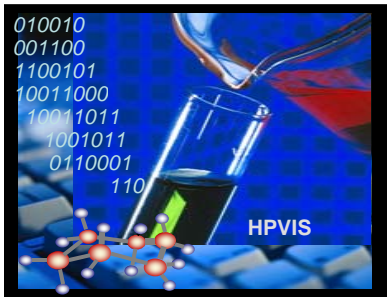
- Provide public availability of all High Production Volume (HPV) Challenge Program data
- Provide a data repository for HPV Challenge Program submissions, including test plans, robust summaries, and public comments on the HPVIS web site: [www.epa.gov/hpvis](http://www.epa.gov/hpvis)



# HPVIS Goals

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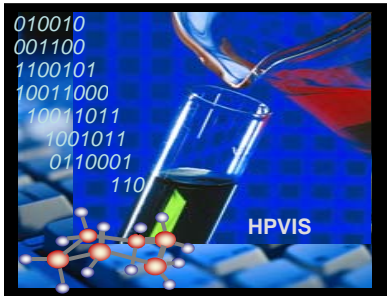
- HPVIS is a database that provides easy access to health and environmental effects information obtained through the HPV Challenge Program
- Provide robust search, query, reporting, retrieval and export capabilities balancing the various stakeholder/user-expressed wants and needs
- Provide compatibility with IUCLID



# HPVIS Development Philosophy

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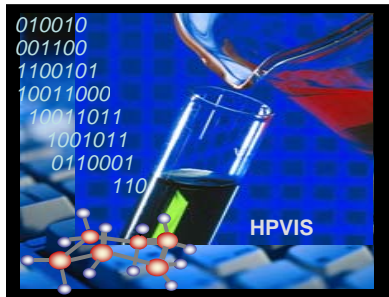
Use a rigorous, systematized approach to software development emphasizing stakeholder identification, participation, and buy-in at all stages of the development process



# Major HPVIS Design Elements

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- Web-based relational database
- Submission-based
- Robust submitter access and security features
- Submission by single company or consortium of companies for individual chemicals and/or chemical categories
- Flexible data entry and retrieval of chemicals within categories



# System Implementation

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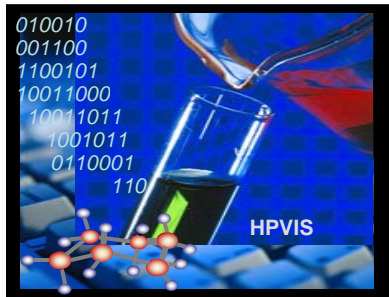
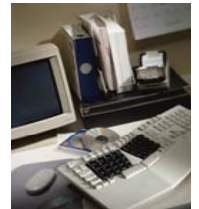
- Database

- ◆ Legacy data population in progress

- 242 Single Chemical Submissions
- 117 Category Chemical Submissions
- 912 unique Sponsored Chemicals

- ◆ Support for Sponsor direct entry of data (new and revised submissions)

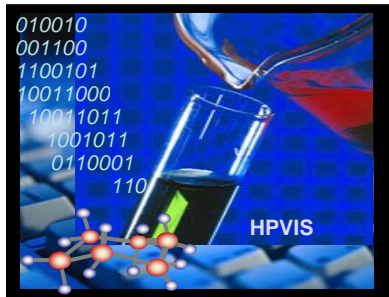
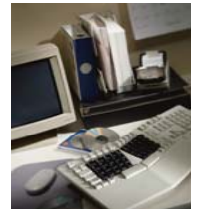
- Data entry capabilities for over 50 defined SIDS and non-SIDS endpoints



# System Implementation (continued)

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- Data Review and Characterization
  - ◆ Sponsor Validation (of EPA-entered legacy data) process
  - ◆ EPA data adequacy review process
  - ◆ Data screening algorithm to prioritize chemicals for review. Results are available to public via Hazard Characterization Screen

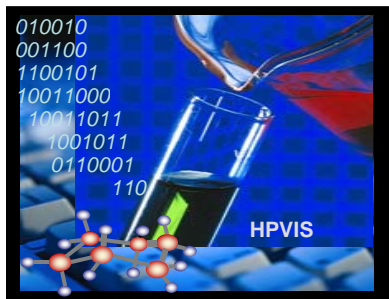


# System Implementation (continued)

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- Data Retrieval Queries

- ◆ View Robust Summaries by Chemical, partial chem. name or CAS
- ◆ View Submission (select by Chemical and/or Chemical Category, Submission Name, Submitter, and/or Sponsor)
- ◆ *Ad hoc* query (by discipline, endpoint, or across database)





# System Implementation (continued)

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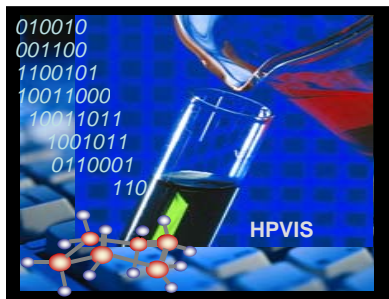
- Data Retrieval (continued)



- ◆ Matrix of Category Chemicals and Endpoints

- ◆ Endpoint Result Report

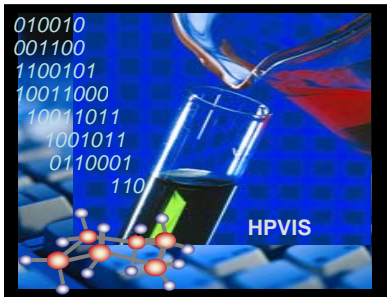
- Select endpoint and result type (e.g., Acute Toxicity and NOAEL (No Observed Adverse Effect Level )



# Hazard Characterization

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- Screening-level HCs provide public access to more than raw technical data on HPVs.
- HCs (chemicals and chemical categories) include:
  - ◆ Summary of data submitted by Challenge sponsors
  - ◆ EPA's evaluation of quality and completeness and data gaps.
  - ◆ EPA's determination of potential hazards (toxicity) of a chemical or category
- First 101 HCs – released September 2007



# Category Matrix Report Example

EPA - HPVIS - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Forward Stop Home Search Favorites Media Print Mail News RSS

Address [http://iaspub.epa.gov/opthpv/far\\_readacross.search\\_page](http://iaspub.epa.gov/opthpv/far_readacross.search_page) Go Links

**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

## Category Matrix Search

The Category Matrix Report presents results for HPV Challenge Program data that was reported in categories of chemicals. The report is 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.

**Category Selection**

Select a Category Name from the list below.

**Category Name :**

Aliphatic Esters Category

**Endpoint Discipline Selection**

Select an Endpoint Discipline from the list below.

**Endpoint Discipline :**

Physical-Chemical

**Axes selection**

Select category matrix display X and Y axes

Axes	X	Y
<input checked="" type="radio"/>	CAS Number	Endpoint
<input type="radio"/>	Endpoint	CAS Number

One CAS Number at a time

Search <<< Previous Reset

Done Internet

# Category Matrix Report Example (continued)

EPA - HPVIS - Microsoft Internet Explorer

Address: [http://iaspub.epa.gov/oppphpv/far\\_readacross.controlTable](http://iaspub.epa.gov/oppphpv/far_readacross.controlTable)

## Category Matrix Report

**Category Name :** Aliphatic Esters Category ([view chemicals](#))      **Endpoint Discipline :** Physical-Chemical

Endpoint Name	103-24-2 Nonanedioic acid, bis(2-ethylhexyl) ester	105-52-2 2-Butenedioic acid (2Z)-, bis(1,3-dimethylbutyl) ester	105-62-4 9-Octadecenoic acid (9Z)-, 1-methyl-1,2-ethanediyl ester	106-79-6 Decanedioic acid, dimethyl ester	108-63-4 Hexanedioic acid, bis(1-methylheptyl) ester	111-60-4 Octadecanoic acid, 2-hydroxyethyl ester	11138-60-6 Decanoic acid, ester with 2-ethyl-2-(hydroxymethyl)-1,3-propanediol octanoate	115-83-3 Octadecanoic acid, 2,2-bis[[[(1-oxooctadecyl)oxy]methyl]-1,3-propanediyl ester	122-62-3 Decanedioic acid, bis(2-ethylhexyl) ester
<b>Melting Point (12)</b>	Unknown Melts = -78 °C <a href="#">Summary</a>			Unknown Melts = 38 °C <a href="#">Summary</a>		Unknown Melts = 60.5 °C <a href="#">Summary</a>			Unknown Melts = -48 <a href="#">Summary</a>
<b>Boiling Point (15)</b>	Unknown Boils = 237 °C @ 5 mm Hg <a href="#">Summary</a>			Unknown Boils = 175 °C @ 20 mm Hg <a href="#">Summary</a>	Unknown Boils = 175 °C @ 2 mm Hg <a href="#">Summary</a>	Unknown Boils 189 - 191 °C @ 3 mm Hg <a href="#">Summary</a>	Measured Boils > 300 °C @ 102 kPa <a href="#">Summary</a>		Unknown Boils = 256 @ 5 mm Hg <a href="#">Summary</a>
<b>Vapor Pressure (6)</b>	Unknown = 5 mm Hg @ 237 °C <a href="#">Summary</a>						Measured < 13 Pa @ 25 °C <a href="#">Summary</a>		
<b>Partition Coefficient (5)</b>							Measured > 2.7 @ 22 °C <a href="#">Summary</a>		Unknown = 3.74 @ 2. <a href="#">Summary</a>

[View All Results](#)

[View All Results](#)

Internet 4:09 PM

# Category Matrix Report Example (continued)

**Category Matrix**

[Category Name](#)

[Endpoint Name](#)

[Melting Point \(12\)](#)

[Boiling Point \(15\)](#)

[Vapor Pressure \(6\)](#)

[Partition Coefficient \(5\)](#)

Melting Point	
<b>Test Substance - Melting Point</b>	
<b>Category Chemical:</b>	(103-24-2) Nonanedioic acid, bis(2-ethylhexyl) ester
<b>Test Substance:</b>	(103-24-2) Nonanedioic acid, bis(2-ethylhexyl) ester
<b>Test Substance Purity/Composition and Other Test Substance Comments:</b>	Purity not indicated
<b>Category Chemical Result Type:</b>	Unknown
<b>Test Substance Result Type:</b>	Unknown
<b>Results - Melting Point</b>	
<b>Melting Indicator:</b>	Melts
<b>Melting Point Value/Range (Temperature):</b>	-78 °C
<b>Results Remarks:</b>	
<b>Study/Method - Melting Point</b>	
<b>Key Study Sponsor Indicator:</b>	
<b>Year Study Performed:</b>	
<b>Method/Guideline Followed:</b>	Other
<b>Method/Guideline and Test Condition Remarks:</b>	Methods of determination were not given. Physical chemical properties were summarized for two azelate ester derivatives in Patty's Toxicology reference book (David et al. 2001).
<b>GLP:</b>	No Data
<b>Study Reference:</b>	David RM, et al. (2001). Esters of aromatic mono-, di-, and tricarboxylic acids, aromatic diacids and di-, tri-, or

# Ad hoc Query Example

**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

## HPVIS Ad Hoc Query

This query allows you to select key data elements from HPVIS to generate a query 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 selected view.

The [HPVIS Ad Hoc Query User's Guide](#) will provide you with detailed information. 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 queried.

- Submission Information
- Discipline Results
- Physical Chemical**
- Fate
- EcoToxicity
- Mammalian Health Effects
- Use and Exposure

<<< Previous

- Melting Point
- Boiling Point
- Vapor Pressure
- Partition Coefficient
- Water Solubility
- Density/Specific Gravity
- Viscosity
- Surface Tension
- Dissociation Constant
- Non-Saturated pH
- Solubility in Different Media
- Granulometry
- Flash Point
- Flammability
- AutoFlammability
- Explosivity
- Chemical Reactivity
- Oxidation Properties
- Oxidation Reduction Potential
- Physical Chemical Other

- View Data
- View Guideline

http://iaspub.epa.gov/opthpv/hpv\_ez.list?database\_type=HPVIS&table\_name=V\_PCHEM\_SIDS\_1\_EZ&query\_name=Melting Point Data

Start | Inbox - Micr... | Today's Ne... | Today's Ne... | Baseline | Microsoft P... | EPA - HPV... | 4:26 PM

# Ad hoc Query Example (continued)

**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 \(HPVIS\)](#) > HPVIS Ad hoc Query

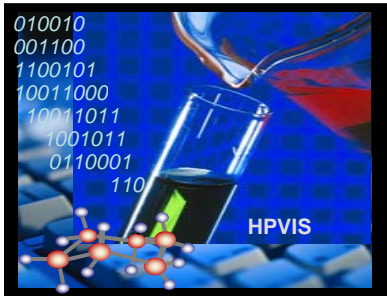
**Selection of Columns**

**STEP 2:** Select **one or more** column(s) for your output by clicking on the square box next to the column name. When you are finished selecting columns, click on the **"STEP 3: Enter Search Criteria"** button at the bottom of this page.

Select All View in Alphabetical Order

**QUERY NAME: Melting Point Data, TABLE NAME: V\_PCHEM\_SIDS\_1\_EZ**

<input checked="" type="checkbox"/>	<a href="#">Category Chemical CAS Number</a>	A standardized number assigned by the Chemical Abstracts Service (CAS) to identify a chemical (e.g., 10595-60-5).
<input type="checkbox"/>	<a href="#">Category Chemical Name</a>	The ninth collective index name of the category chemical.
<input type="checkbox"/>	<a href="#">Consortium Name</a>	The names of the companies that belong to the consortium or partnership if applicable.
<input type="checkbox"/>	<a href="#">Sponsor Name</a>	The name of the individual company or consortium (i.e., two or more companies) making a commitment in the HPV Challenge Program to provide data for a chemical or category of chemicals (e.g., Eastman Chemical Company).
<input checked="" type="checkbox"/>	<a href="#">Sponsored Chemical CAS Number</a>	A standardized number assigned by the Chemical Abstracts Service (CAS) to identify a chemical or category (e.g., 10595-60-5).
<input type="checkbox"/>	<a href="#">Sponsored Chemical Name</a>	The ninth collective index name of the sponsored chemical or category.
<input type="checkbox"/>	<a href="#">Submission Name</a>	The sponsor provided name associated with the submission.
<input type="checkbox"/>	<a href="#">Submitter's Name</a>	The name of the individual company or consortium formally providing test plan related information.



# Ad hoc Query Example (continued)

EPA - HPVIS - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Address [http://iaspub.epa.gov/opthpv/hpv\\_ez.retrieval\\_list](http://iaspub.epa.gov/opthpv/hpv_ez.retrieval_list)

**STEP 3: Enter Search Criteria and Organize the Output**

Query Name: Melting Point Data [Output Options for Selected Columns](#)

Column Name	Operator Definition	Search Value	Column Display Order	Sort Column	Sort Order	Where Only
<a href="#">Category Chemical CAS Number</a>	Equal to		<input type="checkbox"/>	<input type="checkbox"/>	Ascending	<input type="checkbox"/>
<a href="#">Sponsored Chemical CAS Number</a>	Equal to		<input type="checkbox"/>	<input type="checkbox"/>	Ascending	<input type="checkbox"/>
<a href="#">Sponsored Chemical Result Type</a>	Equal to		<input type="checkbox"/>	<input type="checkbox"/>	Ascending	<input type="checkbox"/>
<a href="#">Test Substance Result Type</a>	Equal to		<input type="checkbox"/>	<input type="checkbox"/>	Ascending	<input type="checkbox"/>
<a href="#">Melting Indicator</a>	Equal to		<input type="checkbox"/>	<input type="checkbox"/>	Ascending	<input type="checkbox"/>
<a href="#">Value Description</a>	Equal to		<input type="checkbox"/>	<input type="checkbox"/>	Ascending	<input type="checkbox"/>
<a href="#">Test Value</a>	Equal to		<input type="checkbox"/>	<input type="checkbox"/>	Ascending	<input type="checkbox"/>
<a href="#">Test Value Units</a>	Equal to		<input type="checkbox"/>	<input type="checkbox"/>	Ascending	<input type="checkbox"/>
<a href="#">Key Study Sponsor Indicator</a>	Equal to		<input type="checkbox"/>	<input type="checkbox"/>	Ascending	<input type="checkbox"/>

Done

Start | Internet | 4:18 PM



# Ad hoc Query Example (continued)

EPA - HPVIS - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Address [http://iaspub.epa.gov/opthpv/hpv\\_ez.get\\_table](http://iaspub.epa.gov/opthpv/hpv_ez.get_table)

**Query Name: Melting Point Data**

Page No. 1

Get Results in Excel Format

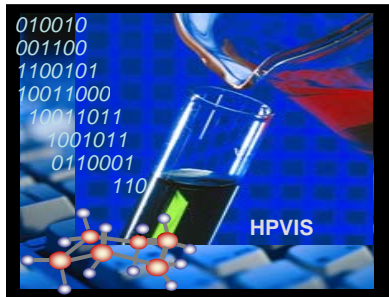
<a href="#">Category Chemical CAS Number</a>	<a href="#">Sponsored Chemical CAS Number</a>	<a href="#">Sponsored Chemical Result Type</a>	<a href="#">Test Substance Result Type</a>	<a href="#">Melting Indicator</a>	<a href="#">Value Description</a>	<a href="#">Test Value</a>	<a href="#">Test Value Units</a>	<a href="#">Key Study Sponsor Indicator</a>
	100-02-7				=	114	°C	
	100-50-5			Melts	=	2	°C	
	100-50-5				=	-100	°C	
	100-50-5				=	-96.1	°C	
	100-53-8	Measured	Measured	Melts	=	-30	°C	
	100-53-8	Measured	Measured	Melts	=	-14.9	°C	Key
	100-53-8	Measured	Measured	Melts	=	-14.8	°C	
	100-69-6					-15.16	°C	
	10081-67-1	Measured	Measured	Melts	=	95	°C	
	101-20-2	Estimated by Calculation	Estimated		=	182	°C	
	101-20-2				=	250	°C	
	101-20-2				=	255.3	°C	
	101-80-4	Measured	Measured				°C	
	101-84-8				=	28	°C	
	102-06-7	Unknown			=	142	°C	
	102-06-7	Unknown			=	147	°C	
	102-06-7	Unknown			=	151.6	°C	
	102-06-7	Unknown					°C	

Start | Internet | 4:20 PM

# Potential System Enhancements

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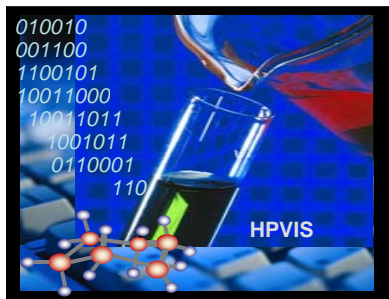
- ◆ Enhanced chemical name searches, e.g., synonyms.
- ◆ Unit-of-measure standardization
- ◆ Enhancement of Ad Hoc Query
- ◆ Support for data sharing with other EPA and external databases
- ◆ Acceptance and Identification of data from programs other than the HPV Challenge Program (e.g., eHPV).



# eChemPortal

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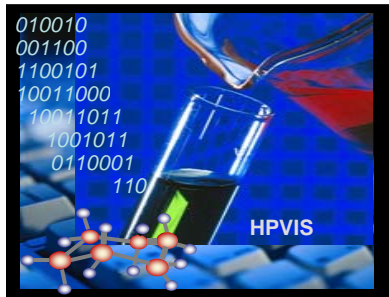
- An Internet gateway to information on the properties, hazards and risks of chemicals.
- An integrated system that allows users to simultaneously search multiple databases prepared by government chemical review programs around the world.
- Publicly launched June 2007



# eChemPortal (cont)

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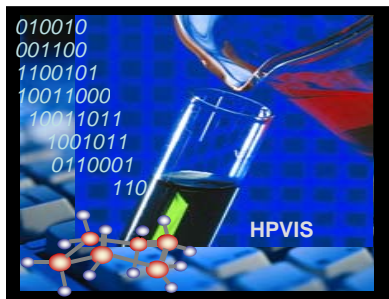
- The eChemPortal offers free public access to information on properties of chemicals:
- Physical chemical properties
- Environmental Fate and Behaviour
- Ecotoxicity
- Toxicity



# eChemPortal Participating Databases

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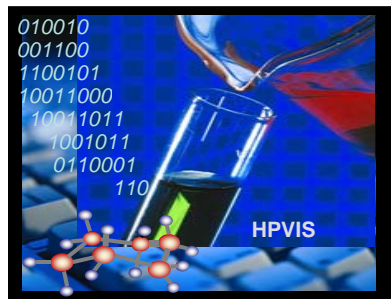
- [CHRIP](#)
  - [ESIS](#)
  - [HPVIS](#)
  - [INCHEM](#)
  - [SIDS IUCLID](#)
  - [SIDS UNEP](#)
  - [OECD HPV](#)
- 
- Users can search multiple sources of information simultaneously using a chemical NAME or CAS and obtain direct links to retrieved data within each site



# eChemPortal (continued)

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- Hosted at the Organisation for Economic Co-operation and Development (OECD)
- Will be implemented in stages.
- First phase integrated several databases that could only be accessed individually on the internet.
- Second phase: will extend these sources and incorporate advanced search and query options to retrieve and compile specific hazard or other property and effects data.



# For More Information

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High Production Volume  
Information System (HPVIS)

