

Characterizing Chemicals in Commerce



Development of the High Production Volume
Information System (HPVIS)

December 12, 2006

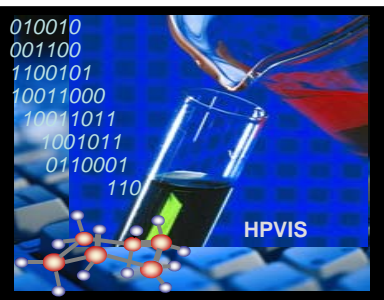


Office of Pollution Prevention and Toxics



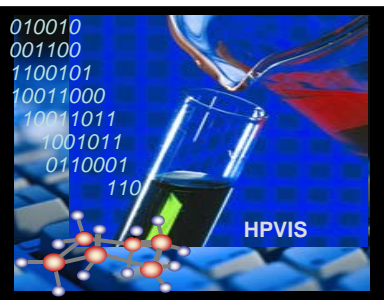
HPV Goals

- Provide public availability of all High Production Volume (HPV) Challenge Program data on the EPA web site
- Provide a data repository for HPV Challenge Program submissions, including test plans, robust summaries, and public comments



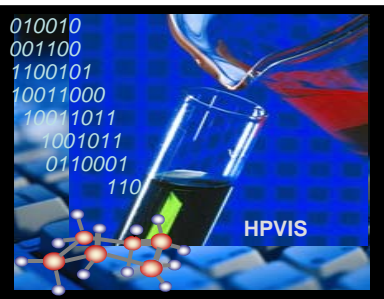
HPVIS Goals

- Provide robust search, query, reporting, retrieval and export capabilities balancing the various stakeholder/user-expressed wants and needs
- Ensure transparency in all operations
- Provide compatibility with IUCLID
- Contribute to development of international HPV information systems



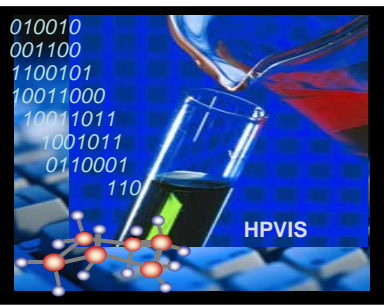
HPVIS Development Philosophy

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



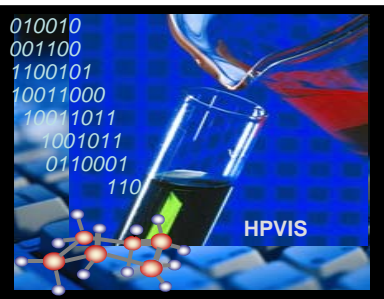
Software Development Steps

- Define a management structure
- Gather and prioritize requirements
- Design system to meet short and long-term requirements
- Design and build database
- Develop and test software
- Populate database with legacy data and field the application



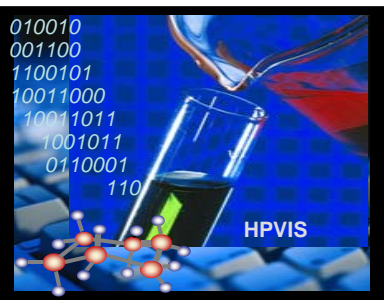
Requirements Gathering

- Over 200 initial system requirements were collected from approximately 100 participants
 - ◆ 4 workshops with OPPT staff
 - ◆ 15 interviews with OPPT managers
 - ◆ 4 sessions with outside stakeholders
 - Environmental and chemical organizations
 - EPA Regional staff and State and tribal representatives via FOSTTA



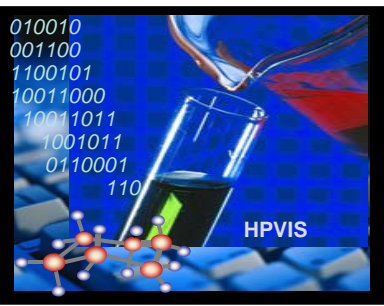
Major HPVIS Design Elements

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



International Elements

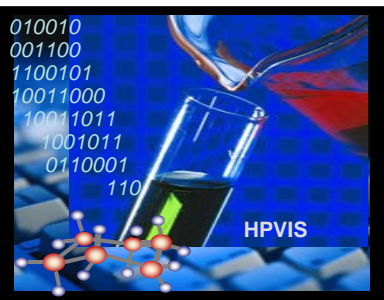
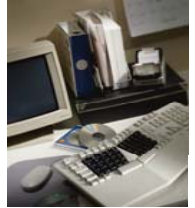
- HPV was built taking into account other international HPV program systems
 - ◆ IUCLID 4
 - ◆ IUCLID 5 and REACH IT
- Compatibility with OECD efforts to provide global access to HPV data and meet commitments made at the World Summit on Sustainable Development
- eChemPortal implementation 2007



System Implementation

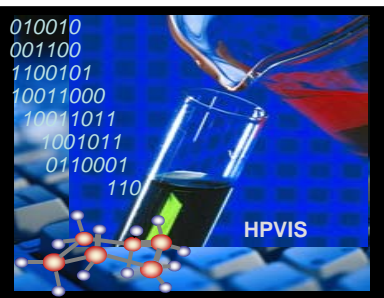
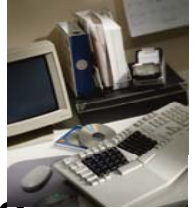
- Database

- ◆ Database structure defined
- ◆ Legacy data population in progress
 - 236 Single Chemical Submissions Complete (92%)
 - 91 Category Chemical Submissions Complete (69%)
 - 848 Sponsored Chemicals Complete (58%)
- ◆ Support for Sponsor direct entry of data (new and revised submissions)
 - Data entry functionality for over 50 defined SIDS and non-SIDS endpoints



System Implementation (continued)

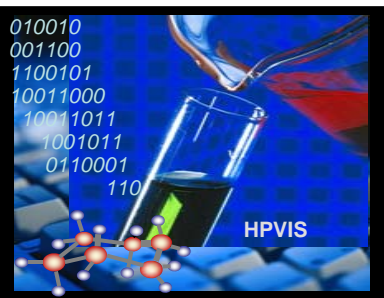
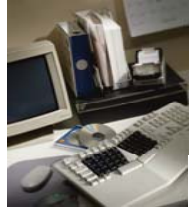
- Data Review and Characterization
 - ◆ Sponsor QC (of EPA-entered legacy data) process
 - ◆ EPA data adequacy review process
 - ◆ Data screening algorithm to identify potential chemicals of interest



System Implementation (continued)

- Data Retrieval

- ◆ View Robust Summaries by Chemical (however chemical is entered)
- ◆ View Submission (select by Chemical, Submission Name, Submitter, and/or Sponsor)
- ◆ *Ad hoc* query (by discipline, endpoint, or across database)



System Implementation (continued)

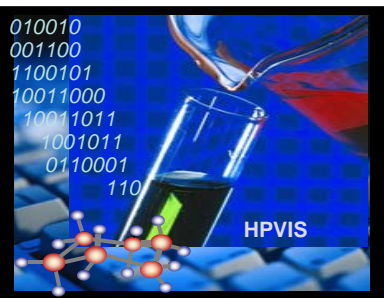
- Data Retrieval (continued)

- ◆ Matrix of Category Chemicals and Endpoints

- Single Discipline or All Disciplines
 - User-specified X and Y axis (chemicals by endpoint or endpoints by chemical)

- ◆ Frequency Distribution of Units of Measure (Endpoint Result Report)

- Select endpoint and result type (e.g., Acute Toxicity and NOAEL)



Category Matrix Report Example

EPA - HPVIS - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Address http://iaspub.epa.gov/opthpv/far_readacross.search_page

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

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Category Matrix Report Example (continued)

EPA - HPVIS - Microsoft Internet Explorer

Address: 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-ethanediy l 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
Melting Point (12)	Unknown Melts = -78 °C Summary			Unknown Melts = 38 °C Summary		Unknown Melts = 60.5 °C Summary			Unknown Melts = -48 Summary
Boiling Point (15)	Unknown Boils = 237 °C @ 5 mm Hg Summary			Unknown Boils = 175 °C @ 20 mm Hg Summary	Unknown Boils = 175 °C @ 2 mm Hg Summary	Unknown Boils 189 - 191 °C @ 3 mm Hg Summary	Measured Boils > 300 °C @ 102 kPa Summary		Unknown Boils = 256 @ 5 mm Hg Summary
Vapor Pressure (6)	Unknown = 5 mm Hg @ 237 °C Summary						Measured < 13 Pa @ 25 °C Summary		
Partition Coefficient (5)							Measured > 2.7 @ 22 °C Summary		Unknown = 3.74 @ 2. Summary

[View All Results](#)

[View All Results](#)

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Category Matrix Report Example (continued)

Category Matrix Report Example (continued)

Category Name

Endpoint Name

Melting Point (12)

Boiling Point (15)

Vapor Pressure (6)

Partition Coefficient (5)

http://iaspub.epa.gov/opptpv/Public_Search.PublicEndPointReport?robust_summary_id=24956532&Whi - Microsoft Internet Explorer

Address http://iaspub.epa.gov/opptpv/Public_Search.PublicEndPointReport?robust_summary_id=24956532&WhichButton=PrintCat&ep_name=Melt

Melting Point	
Test Substance - Melting Point	
Category Chemical:	(103-24-2) Nonanedioic acid, bis(2-ethylhexyl) ester
Test Substance:	(103-24-2) Nonanedioic acid, bis(2-ethylhexyl) ester
Test Substance Purity/Composition and Other Test Substance Comments:	Purity not indicated
Category Chemical Result Type:	Unknown
Test Substance Result Type:	Unknown
Results - Melting Point	
Melting Indicator:	Melts
Melting Point Value/Range (Temperature):	-78 °C
Results Remarks:	
Study/Method - Melting Point	
Key Study Sponsor Indicator:	
Year Study Performed:	
Method/Guideline Followed:	Other
Method/Guideline and Test Condition Remarks:	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).
GLP:	No Data
Study Reference:	David RM, et al. (2001). Esters of aromatic mono-, di-, and tricarboxylic acids, aromatic diacids and di-, tri-, or

Done

http://iaspub.epa.gov/opptpv/Public_Search.PublicEndPointReport?robust_summary_id=24956532&WhichButton=PrintCat&ep_name=Meltin

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Ad hoc Query Example

EPA - HPVIS - Microsoft Internet Explorer
File Edit View Favorites Tools Help
Back Forward Stop Home Search Favorites Media
Address <http://www.epa.gov/hpvis/ez.html> 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

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	▶

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	▶

<<< Previous

http://iaspub.epa.gov/opthpv/hpv_ez.list?database_type=HPVIS&table_name=V_PCHEM_SIDS_1_EZ&query_name=Melting Point Data Internet

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Ad hoc Query Example (continued)

EPA - HPVIS - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Address http://iaspub.epa.gov/oppphpv/hpv_ez.list

U.S. Environmental Protection Agency

High Production Volume Information System (HPVIS)

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[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"/>	Category Chemical CAS Number	A standardized number assigned by the Chemical Abstracts Service (CAS) to identify a chemical (e.g., 10595-60-5).
<input type="checkbox"/>	Category Chemical Name	The ninth collective index name of the category chemical.
<input type="checkbox"/>	Consortium Name	The names of the companies that belong to the consortium or partnership if applicable.
<input type="checkbox"/>	Sponsor Name	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"/>	Sponsored Chemical CAS Number	A standardized number assigned by the Chemical Abstracts Service (CAS) to identify a chemical or category (e.g., 10595-60-5).
<input type="checkbox"/>	Sponsored Chemical Name	The ninth collective index name of the sponsored chemical or category.
<input type="checkbox"/>	Submission Name	The sponsor provided name associated with the submission.
<input type="checkbox"/>	Submitter's Name	The name of the individual company or consortium formally providing test plan related information.

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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

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
Category Chemical CAS Number	Equal to		<input type="checkbox"/>	<input type="checkbox"/>	Ascending	<input type="checkbox"/>
Sponsored Chemical CAS Number	Equal to		<input type="checkbox"/>	<input type="checkbox"/>	Ascending	<input type="checkbox"/>
Sponsored Chemical Result Type	Equal to		<input type="checkbox"/>	<input type="checkbox"/>	Ascending	<input type="checkbox"/>
Test Substance Result Type	Equal to		<input type="checkbox"/>	<input type="checkbox"/>	Ascending	<input type="checkbox"/>
Melting Indicator	Equal to		<input type="checkbox"/>	<input type="checkbox"/>	Ascending	<input type="checkbox"/>
Value Description	Equal to		<input type="checkbox"/>	<input type="checkbox"/>	Ascending	<input type="checkbox"/>
Test Value	Equal to		<input type="checkbox"/>	<input type="checkbox"/>	Ascending	<input type="checkbox"/>
Test Value Units	Equal to		<input type="checkbox"/>	<input type="checkbox"/>	Ascending	<input type="checkbox"/>
Key Study Sponsor Indicator	Equal to		<input type="checkbox"/>	<input type="checkbox"/>	Ascending	<input type="checkbox"/>

Done

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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

Query Name: Melting Point Data

Page No. 1

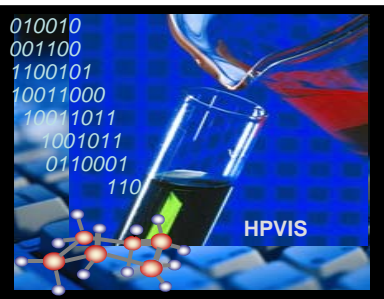
Get Results in Excel Format

Category Chemical CAS Number	Sponsored Chemical CAS Number	Sponsored Chemical Result Type	Test Substance Result Type	Melting Indicator	Value Description	Test Value	Test Value Units	Key Study Sponsor Indicator
	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	

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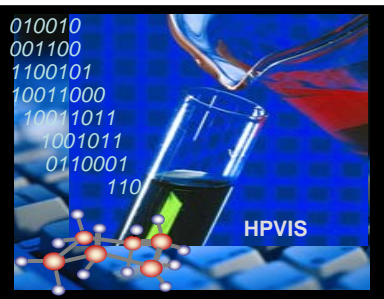
HPVIS Training/Demonstration

- 4 (identical) sessions of HPVIS training/demonstration available at this conference:
 - ◆ Today 1:30 to 3:00 – Session 1C
 - ◆ Today 3:30 to 5:00 – Session 2C
 - ◆ Tomorrow 10:45 to 12:15 – Session 3B
 - ◆ Tomorrow 1:30 to 3:00 – Session 4B



HPVIS Training (continued)

- HPVIS demonstrations will be informal and concentrate on data retrieval
- Data entry functions may also be demonstrated if participants desire



For More Information

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High Production Volume
Information System (HPVIS)

