Characterizing Chemicals in Commerce

Development of the High Production Volume Information System (HPVIS)

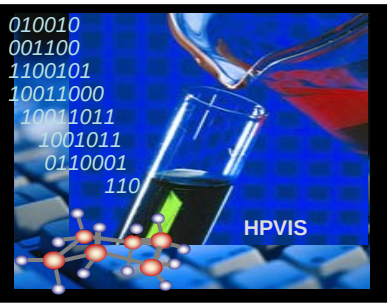
December 12, 2006

Information Management Division

Office of Pollution Prevention and Toxics

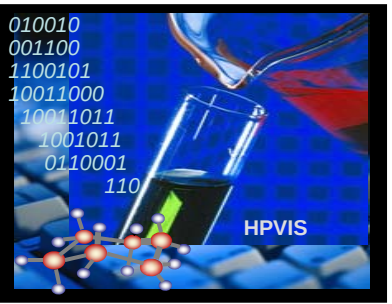
HPV Goals

- 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



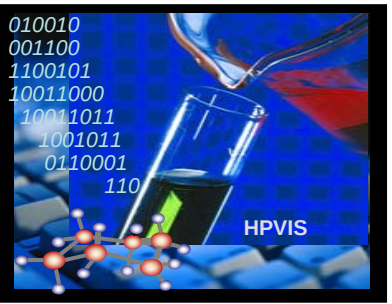
HPVIS Goals

- 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



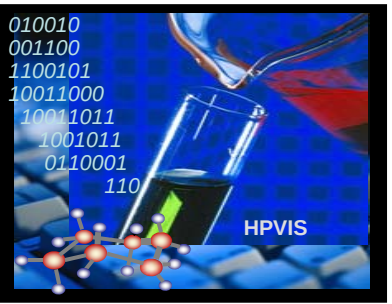
HPVIS Development Philosophy

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



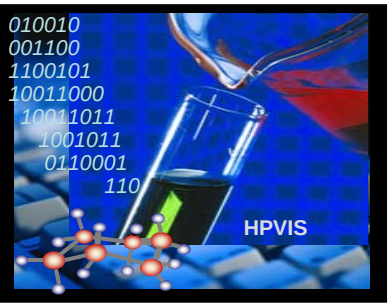
Software Development Steps

- 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



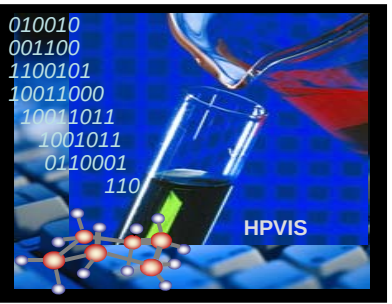
Requirements Gathering

- 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



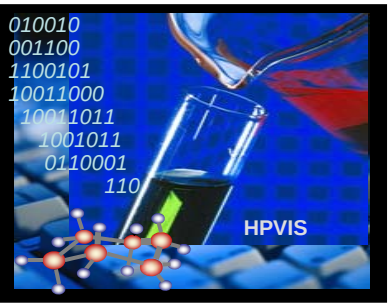
Major HPVIS Design Elements

- 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



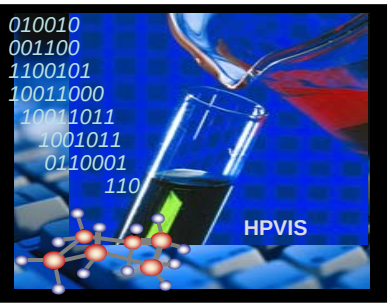
International Elements

- 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



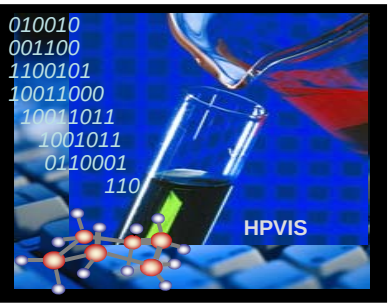
System Implementation

- 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



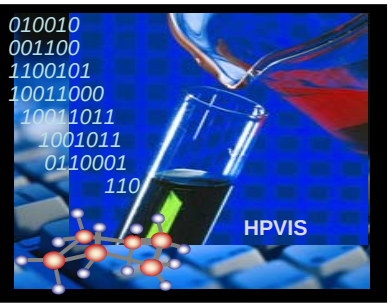
System Implementation (continued)

- 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



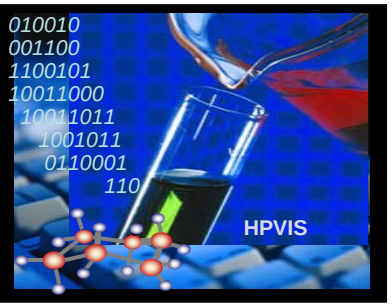
System Implementation (continued)

- 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)

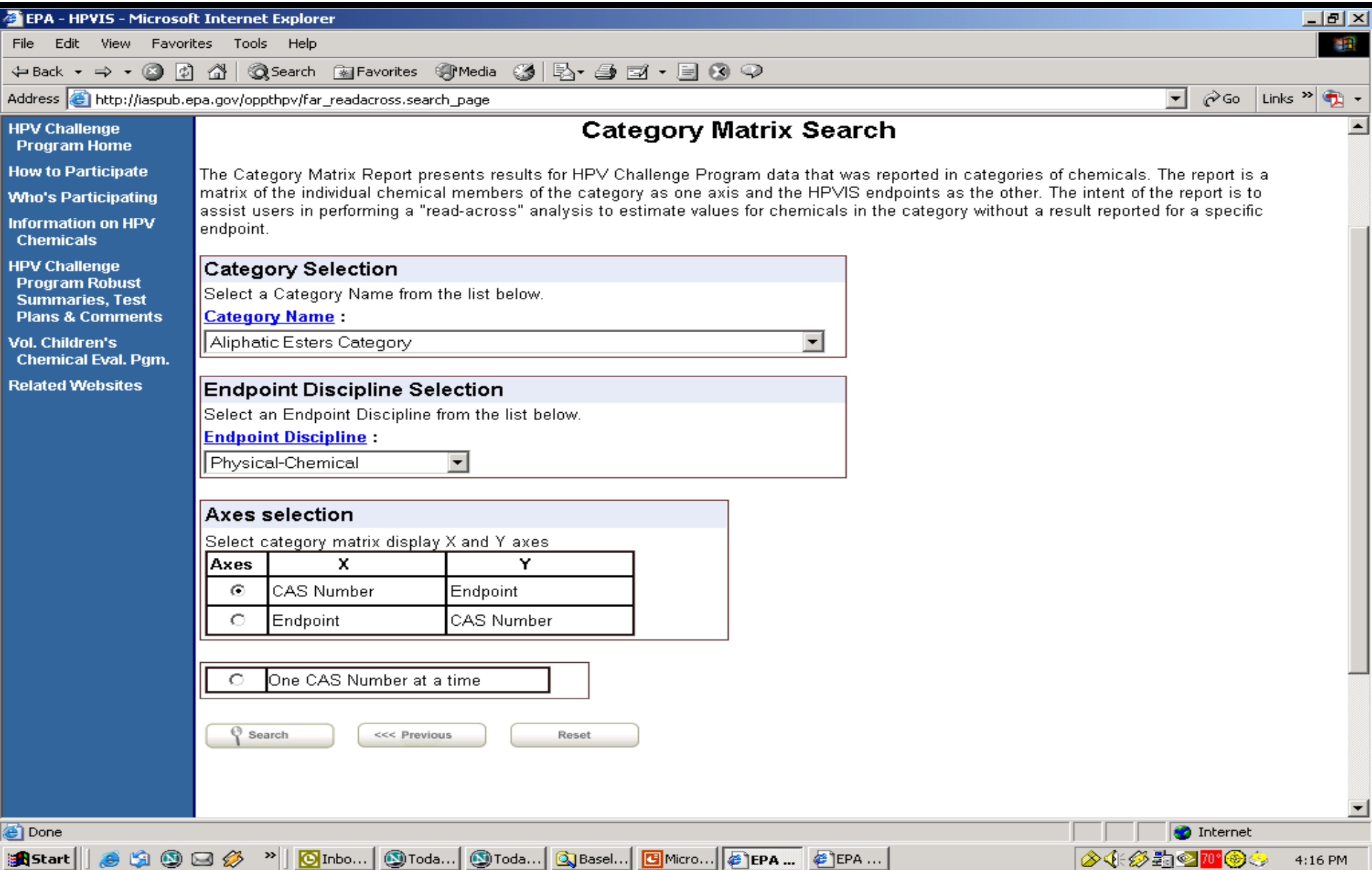


System Implementation (continued)

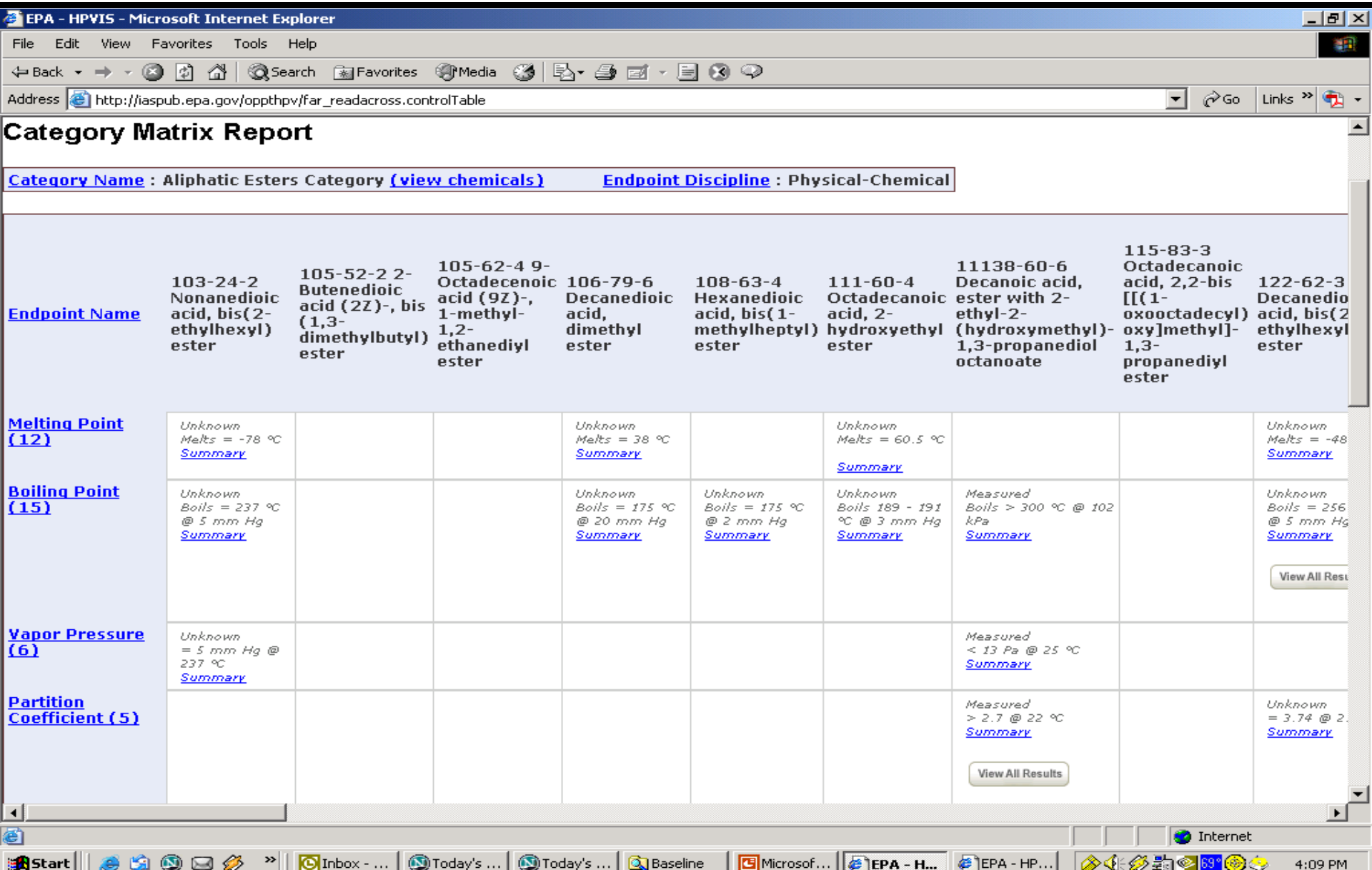
- Data Retrieval (continued)
  - Matrix of Category Chemicals and Endpoints
    - Single Discipline or All Disciplines
    - User-specified X and Y axis (chemicals by endpoint or endpoints by chemical)
  - Frequency Distribution of Units of Measure (Endpoint Result Report)
    - Select endpoint and result type (e.g., Acute Toxicity and NOAEL)



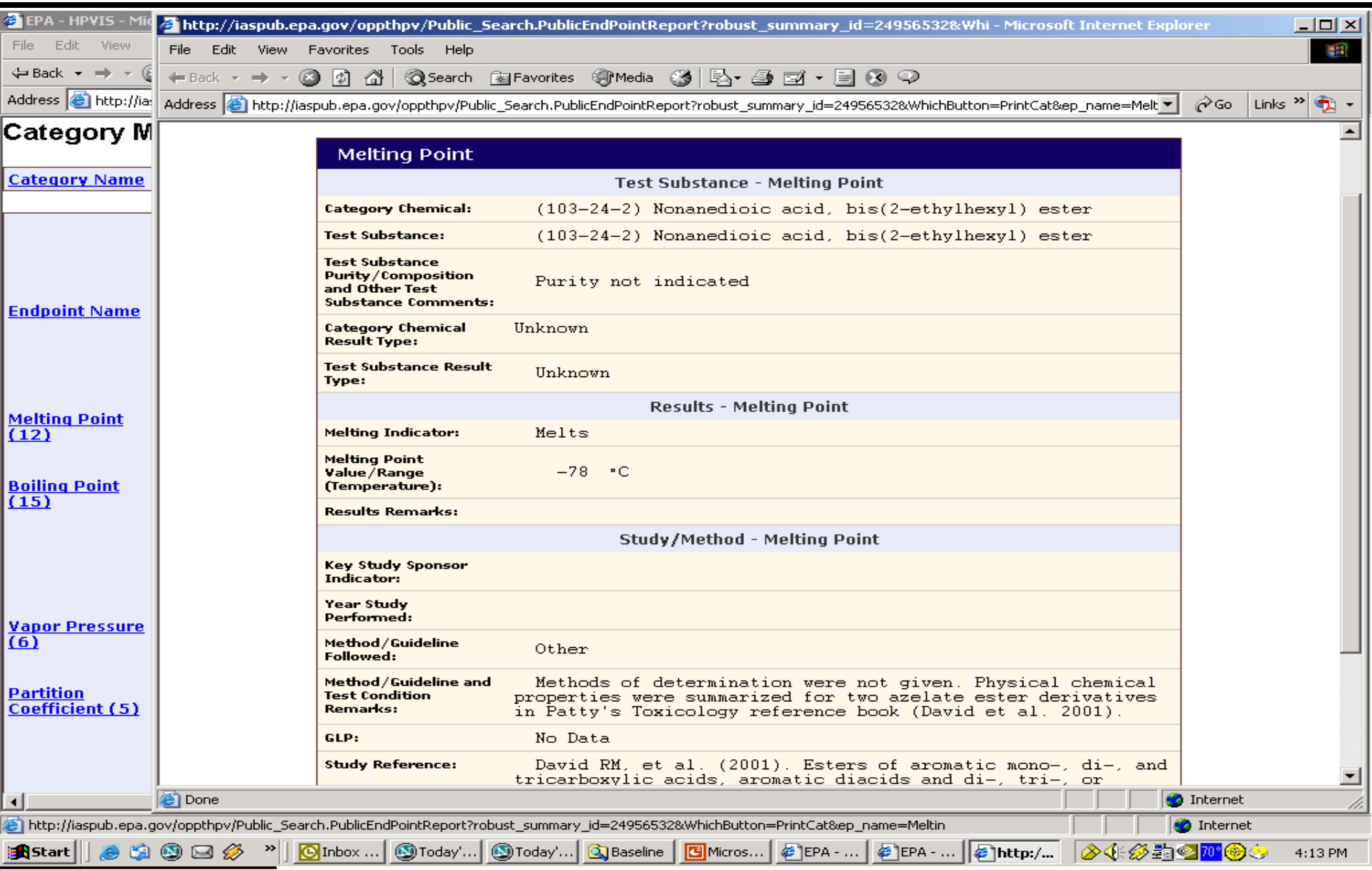
Category Matrix Report Example



Category Matrix Report Example (continued)



Category Matrix Report Example (continued)



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Category M

Category Name

Endpoint Name

Melting Point (12)

Boiling Point (15)

Vapor Pressure (6)

Partition Coefficient (5)

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

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

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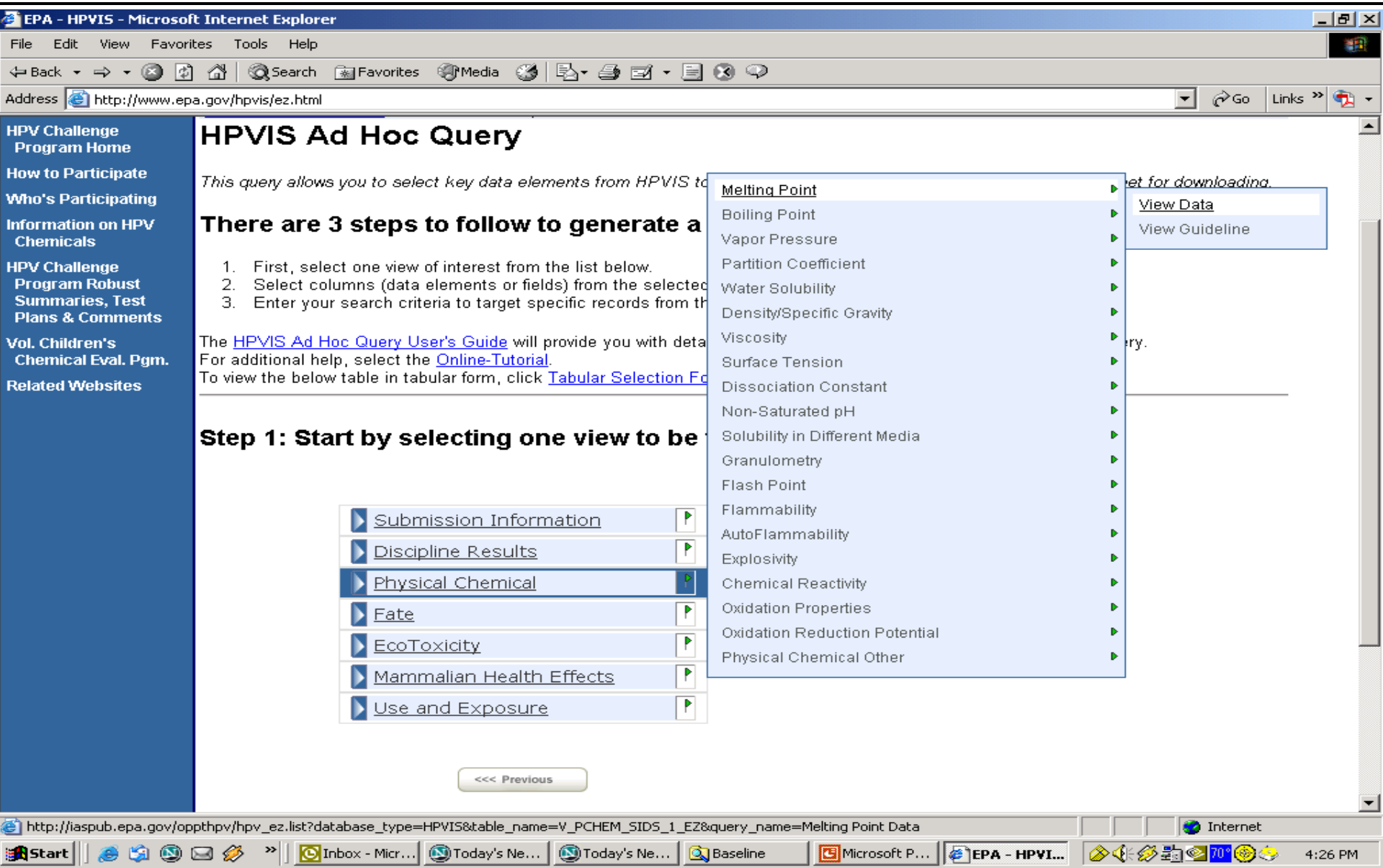
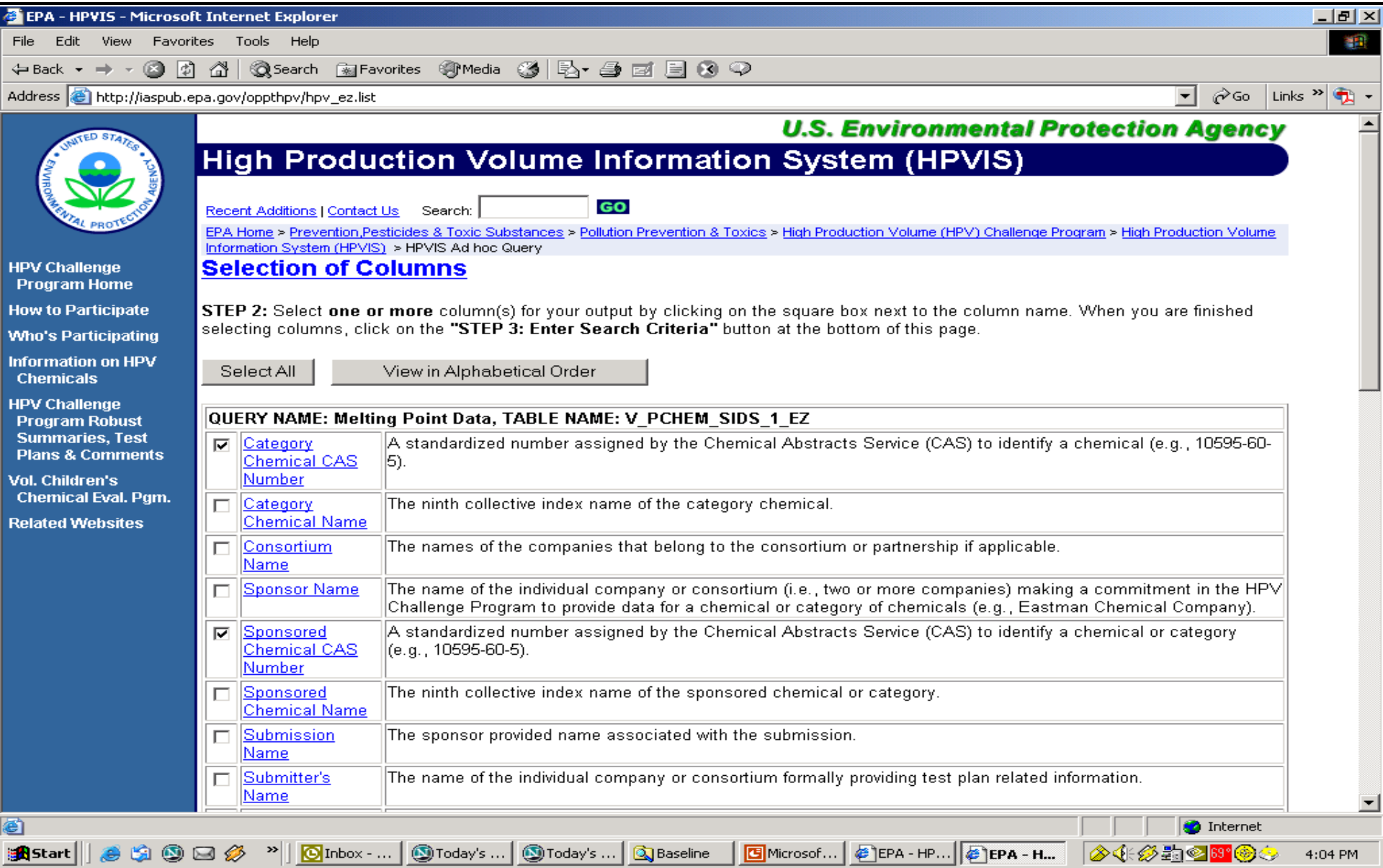
Ad hoc Query Example



Ad hoc Query Example (continued)



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U.S. Environmental Protection Agency

High Production Volume Information System (HPVIS)

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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

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

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

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

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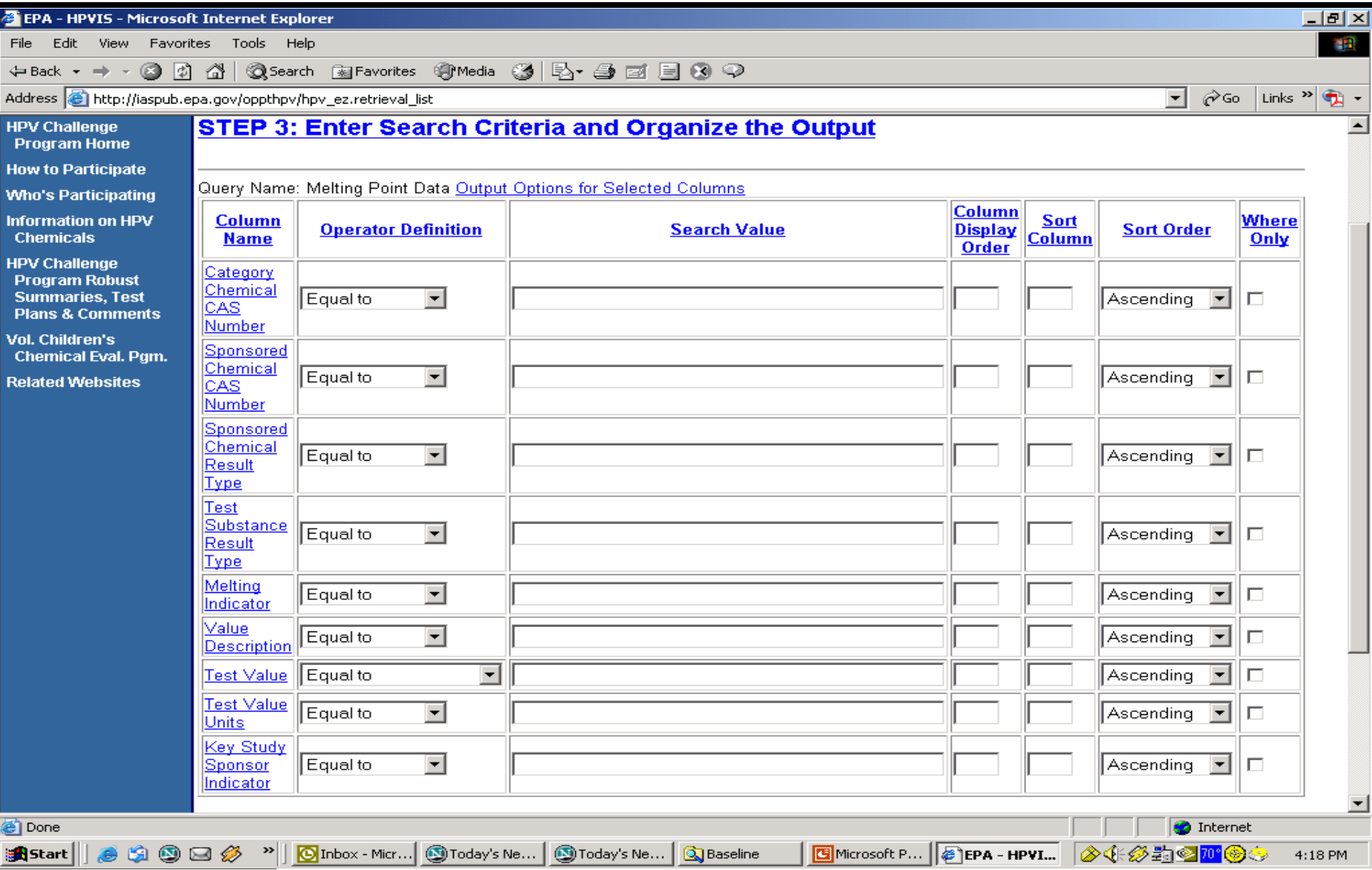
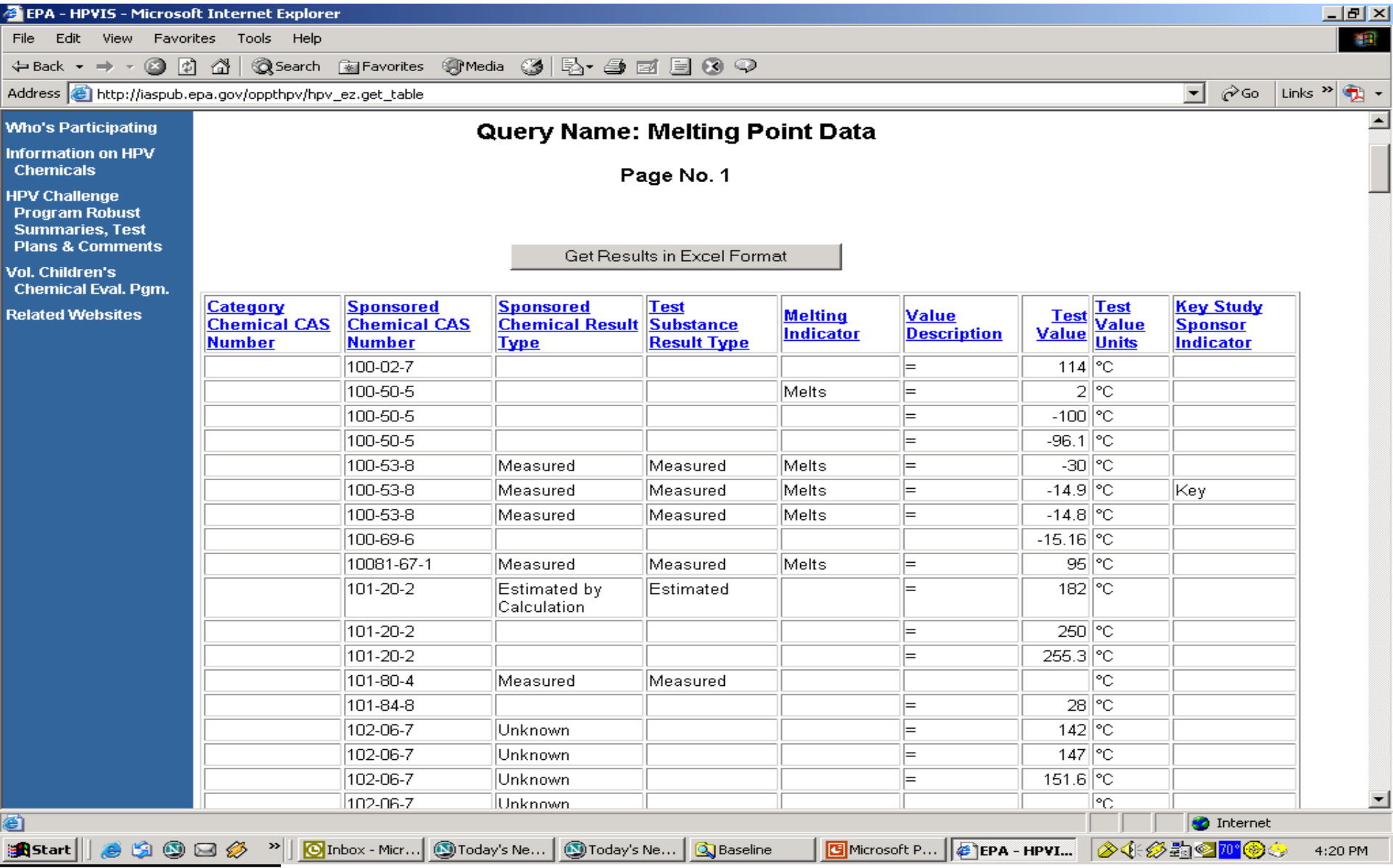
Ad hoc Query Example (continued)



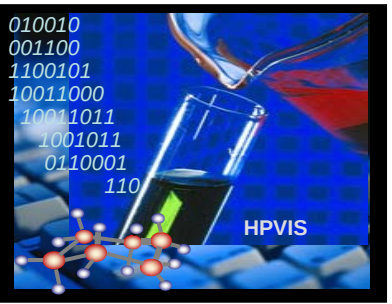
Ad hoc Query Example (continued)



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	

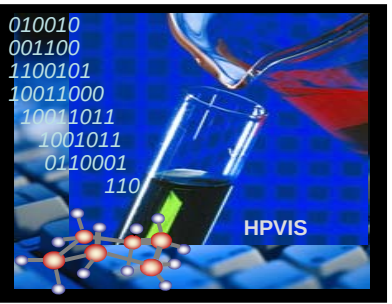
HPVIS Training/Demonstration

- 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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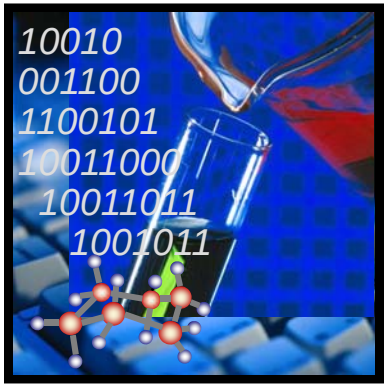
High Production Volume Information System (HPVIS)



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