

# **Methodology for Hazard-Based Prioritization Under ChAMP**

**Office of Pollution Prevention & Toxics  
U.S. Environmental Protection Agency**

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## Introduction

Screening-level hazard-based prioritizations (HBP) are important contributions to the work being done under EPA's [Chemical Assessment and Management Program \(ChAMP\)](#). HBPs summarize the potential hazards of a chemical or chemical cluster; identify additional information relevant to the Agency's assignment of a high, medium, or low priority for further attention. An HBP document for individual chemicals or chemical clusters include a prioritization decision as well as its underlying screening-level hazard characterization. This methodology document describes the approach and procedures used to develop the screening-level hazard characterization that supports the HBP. An overview of the chemical hazard characterization work flow and outputs is provided in this document and illustrated in Appendix 1. Each of the steps involved in the development of the hazard characterizations are described in subsequent sections of this document.

HBPs are developed primarily for MPV chemicals, which are those manufactured or imported at volumes greater than or equal to 25,000 and less than 1 million pounds per year. This is because most MPV chemicals were not included in requirements for the submission of processing or use information under the IUR, and are therefore less likely to have information available to develop exposure and risk characterizations to support a risk-based prioritization. Further, since most MPV chemicals were not part of the HPV Challenge Program, they are also less likely to have a complete set of basic screening-level hazard data available. Therefore, they may be clustered with chemicals of similar structure and toxicity, and EPA will use predictive methods in developing the screening-level hazard characterization. In some cases, HBPs may be developed for chemicals that are HPV on the 2006 IUR. This may occur for chemicals that were not part of HPV Challenge or OECD HPV programs and for which the hazard data that are used for developing an RBP (i.e., Screening Initial Data Set) are therefore not currently available. In these cases, the HBP would also include a summary of IUR production volume information, and if available (i.e. if chemical is produced at greater than 300,000 pounds per year), reported use information. Industry has sponsored some of these HPV chemicals for collection of the SIDS under the industry initiated, extended HPV Program (EHPV). When these data become available, it may be possible to develop a risk-based prioritization for these chemicals.

The screening-level hazard characterization is based on existing data available to EPA and developed according to established New Chemicals Program and HPV Challenge Program practices and guidelines and EPA risk assessment guidance. Existing data available to OPPT may include publicly available data on the subject chemical(s), data on analogous chemicals from the US and OECD High Production Volume (HPV) Programs, publicly available data on analogous non-HPV supporting chemicals and are described in the **Data Sources** section. For many MPV chemicals, the extent of the data available is limited. In such cases, EPA uses a number of predictive tools and methods to characterize properties and hazards in developing fate and hazard characterizations, as described in the **Data Sources** section. Professional judgment of OPPT scientists with experience in the New and Existing Chemicals Programs at EPA us also applied in developing the screening-level hazard characterizations.

## Structural Clustering

The purpose of this initial step is to organize HPV, MPV, and supporting analogous chemicals into general structural clusters and to identify those compounds within each cluster that have existing measured data. To begin this process, a master structure file containing all chemicals listed on the public Inventory Update Rule (IUR) from 1986 – 2006 is being compiled. This structure file will contain all chemicals subject to assessment under ChAMP, including HPV Challenge Program chemicals and substances reported in the 2006 IUR as MPVs, along with other supporting chemicals reported in prior IURs that have data that may be leveraged to help inform the hazard characterization of the subject chemicals.

To be included in this master structure file, each CAS Registry Number included must be associated with a single structural depiction of the discrete compound or in the case of isomeric or complex mixtures, a representative structure when appropriate. This structure file will be linked to secondary information to indicate which chemicals have been subject to review under the U.S. HPV Challenge Program, the OECD HPV Programme, and the Canadian Environmental Protection Act (CEPA) review (categorization).

The master structure file will serve as the database from which clusters of compounds with closely related structures will be developed using a simple structure-based clustering algorithm. The program analyzes each compound for the presence or absence of a set of 645 chemical fragments, ranging in size from a single atom to a large chemical “backbone.” The result of this initial clustering activity will be some number of clusters of structurally-related compounds containing analogous HPVs, MPVs and supporting chemicals. These results will then be evaluated by OPPT scientists to confirm appropriateness of the groupings and to refine the structural clusters as necessary based on professional judgment and other supporting information. The chemicals in these refined clusters will then be moved forward for evaluation as a group such that available data from the HPV cluster members and other supporting chemicals can be used to inform the hazard characterization of the MPV chemicals. It is also anticipated that some chemicals will not be associated with any cluster, and therefore will proceed to hazard characterization as a single chemical.

The rationale for using general structural similarity as a starting point for organizing groups of chemicals is to maximize the number of potential analogs within a group, thus maximizing the potential data available to inform the hazard characterizations. Organizing each chemical and associated data within a cluster will aid assessors in identifying trends in chemical properties and activities, detecting outlying estimates and measured data, performing read-across, formulating weight of evidence analyses and identifying appropriate sub-clustering. As existing measured data and model estimates for properties and activities are gathered for the chemicals in a cluster, it is anticipated that assessors will identify endpoint-specific sub-clusters of compounds with similar mechanistic or biological properties within the larger structural cluster. These sub-clusters, breakpoints, and trends will be described in the hazard characterizations or in some cases, may provide evidence for refining the structural clusters to better reflect more appropriate groupings and data extrapolation. An illustration of the clustering and data gathering process is provided in Appendix 1.

## Data Collation, Selection, and OPPT Expert Review

Data identified from the various sources (described below) are evaluated for adequacy in a manner consistent with the High Production Volume (HPV) Challenge Program guidance on determining data adequacy.

### *Measured Data Quality/Adequacy*

For each MPV chemical in a cluster, as well as for analogous compounds, experimental data located from the various sources are evaluated for adequacy and selected for use in the hazard characterization according to the following hierarchy:

- Tier 1: Studies conducted according to established test guidelines (e.g. U.S. EPA or OECD);
- Tier 2: Non-guideline studies that are conducted according to sound scientific principles and provide sufficient documentation to evaluate quality; essentially “equivalent” to guideline studies;
- Tier 3: Data derived from experiments with minimal supporting details. Expert judgment will be used on a case-by-case basis to determine if modeled data or read-across may be more reliable than this type of measured data.

### *Estimated Data – Filling Data Gaps*

The following approaches will be used to fill data gaps when measured data are not available:

- Calculate from empirical tools;
- Structure Activity Relationships (SAR) or Quantitative Structure Activity Relationship (QSAR) methods where approaches are available;
- Read-across from analogs

### *Weight-of-Evidence and Best Professional Judgment*

When Tier 1 and Tier 2 measured data are unavailable, the specific approach used to fill data gaps is determined using a weight-of-evidence approach and best professional judgment because the “best” approach will depend on the quality/reliability of the model and the available existing data within the context of the chemical and endpoint being evaluated.

Read-across of data from tested chemicals to untested chemicals will generally follow the practice and experience in the U.S. and OECD HPV Programs; according to the principles and practices outlined in the OECD *Guidance on Grouping of Chemicals* (OECD, 2007; ENV/JM/MONO(2007)28). However, ‘expert review teams’ composed of OPPT staff will provide case-by-case review of data summary sheets (having existing measured data entered) and determine the nature and extent to which measured data for tested cluster chemicals can/should be read-across to other cluster members. Information regarding sources and quality of measured and estimated data (i.e. the ‘meta data’ behind the data summary tables) will be provided to the review teams when they are conducting their reviews.

## Data Sources

### *Sources for Existing Measured Data*

For each chemical in a cluster, whether MPV, HPV or other analog, data are collected in a manner consistent with the High Production Volume (HPV) Chemical Challenge Program guidance on searching for existing information. The following publicly available/accessible sources are searched for measured (experimentally-derived) data for all chemicals:

### *Sources Searched for Any/All Endpoints:*

- OECD HPV Programme SIDS (posted on OECD or UNEP website) - SIDS endpoint data for HPV chemical analogs
- U.S. HPV Challenge Program Data (submitted Robust Summaries and completed HCs) - SIDS endpoint data for HPV chemical analogs
- EPA TSCA Section 4 Data
- EPA TSCATS - Section 8e Data
- NIH Hazardous Substances Data Bank (HSDB)
- Beilstein
- Ashford's Dictionary of Industrial Chemicals
- CRC Handbook of Chemistry and Physics
- CRC Handbook on Organic Compounds
- Aldrich Handbook of Fine Chemicals
- Hawley's Condensed Chemical Dictionary.
- Handbook of Data on Common Organic Compounds
- Sax's Dangerous Properties of Industrial Materials
- Chemical Dictionary Online
- Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation
- CHRIP Online
- ChemIDplus
- Kirk Othmer Encyclopedia of Chemical Technology
- Lang's Handbook of Chemistry
- Merck Index
- Ullmann's Encyclopedia of Industrial Chemistry
- ChemSpider Online
- Environmental Fate Database (EFDB) – environmental fate data
- Japan's Ministry of Economy, Trade, and Industry's MITI Biodegradation Database
- Arnot and Gobas BAF/BCF database (Arnot, JA & Gobas FAPC. 2006. Environ. Rev.14:257-297)
- EPA ECOTOX Database – ecotoxicity and BCF data
- EPA IRIS Toxicological Profiles
- CCRIS
- National Toxicology Program
- ATSDR Toxicological Profiles
- IARC Monographs
- Carcinogenic Potency Project Database

- US GENETOX Database
- Neurotoxicity of Industrial and Commercial Chemicals, V. I and II
- Canada DSL Reports

#### *Sources of Estimated Data*

The following publicly available/accessible predictive tools are used to fill data gaps and support hazard characterizations via weight-of-evidence:

- EPISuite™ v 3.20 (<http://epa.gov/oppt/exposure/pubs/episuite.htm>) – physical-chemical properties and environmental fate.
- SPARC v 4.2 (<http://ibmlc2.chem.uga.edu/sparc/>) – dissociation constant (pKa).
- ECOSAR™ v 1.00 (<http://www.epa.gov/oppt/newchems/tools/21ecosar.htm>) – ecotoxicity for fish, aquatic invertebrates (daphnia) and aquatic plants (algae).
- OncoLogic™ v. 6.0 (<http://www.epa.gov/oppt/newchems/tools/oncologic.htm>) – carcinogenic potential.

#### **Formulation of the Data Tables**

For each chemical/endpoint in a cluster, data located from the sources listed in section IV are collated, evaluated for adequacy and compiled into **Data Tables**. Separate Data Tables are compiled for Physical-Chemical Properties and Fate (Table A), Aquatic Toxicity (Table B), and Human Health Toxicity (Table C).

#### *Measured Data*

- Measured data from standard sources are compiled into the data tables.
- Measured data are entered in **bolded** text, to distinguish them from estimated data.
- Numerical values are entered for aquatic toxicity (LC50 or EC50), acute toxicity (LD50 or LC50), repeated-dose toxicity (NOAEL/LOAEL), reproductive toxicity (NOAEL/LOAEL) and development toxicity (NOAEL/LOAEL).
- Qualitative indicators, i.e. –, ±, + are entered for genotoxicity, cancer, neurotoxicity, immunotoxicity, irritation and sensitization.
- Data adequacy is indicated in the data summary tables as a symbol next to the quantitative or qualitative data value.
- The symbols are as follows:

#### **Experimental**

- Value from guideline study, clear weight of evidence, or evaluated database
- Value from non-guideline but reliable experimental study
- ◆ Value reported without supporting details

#### *Estimated Data*

- Estimated data, either from SAR/QSAR or Read-Across, are compiled into the data tables;
- Estimated data are entered in normal/grayed text, to distinguish them from measured data.

- Numerical values are entered for aquatic toxicity (LC50 or EC50), acute toxicity (LD50 or LC50), repeated-dose toxicity (NOAEL/LOAEL), reproductive toxicity (NOAEL/LOAEL) and development toxicity (NOAEL/LOAEL).
- Qualitative indicators, i.e. -, ±, + are entered for genotoxicity, cancer, neurotoxicity, immunotoxicity, irritation and sensitization.
- Data type is indicated in the data summary table as a symbol next to the quantitative or qualitative data value.
- The data type indicators distinguish between values derived from SAR/QSAR vs. Read-Across.
- The symbols are as follows:

**Estimated**

✦ Value from SAR/QSAR

○ Value obtained using read-across

The data tables provide a summary of the supporting chemical/endpoint information that will support the basis for the hazard characterizations in the *Overall Hazard Characterization Summary*.

### **Data Summary Expert Review & Decisions on Data Gap Filling/Read-Across**

Following collection and compilation of existing and estimated data, the *Data Tables* are critically reviewed by OPPT expert staff.

The purpose of the OPPT expert review is to review and integrate qualitative and quantitative data from experimental studies and model estimates, identify of hazard/fate trends and/or break points within the clusters, evaluate the nature and extent to which read-across is supported, and finally to draft the hazard characterization.

### **Formulation of the Overall Hazard Characterization Summary**

Information from the data tables and expert review are used to characterize hazards for *Persistence, Bioaccumulation, Aquatic Toxicity and Human Health* as High, Moderate or Low. This information will be provided in the Overall Hazard Characterization Summary (Table D).

#### ***Individual Endpoints***

- Quantitative data (numeric values) are compared to the hazard characterization criteria in Appendix 2 and assigned low, moderate or high hazard. Quantitative endpoints include persistence, bioaccumulation, acute and chronic aquatic toxicity and acute, repeated-dose, reproductive, and developmental mammalian toxicity.
- Qualitative indicators, i.e. -, ±, + are entered for genotoxicity, cancer, neurotoxicity, immunotoxicity, irritation and sensitization.
- When multiple adequate data/studies are available for an endpoint with quantitative data, the most conservative value is chosen for the overall hazard characterization.

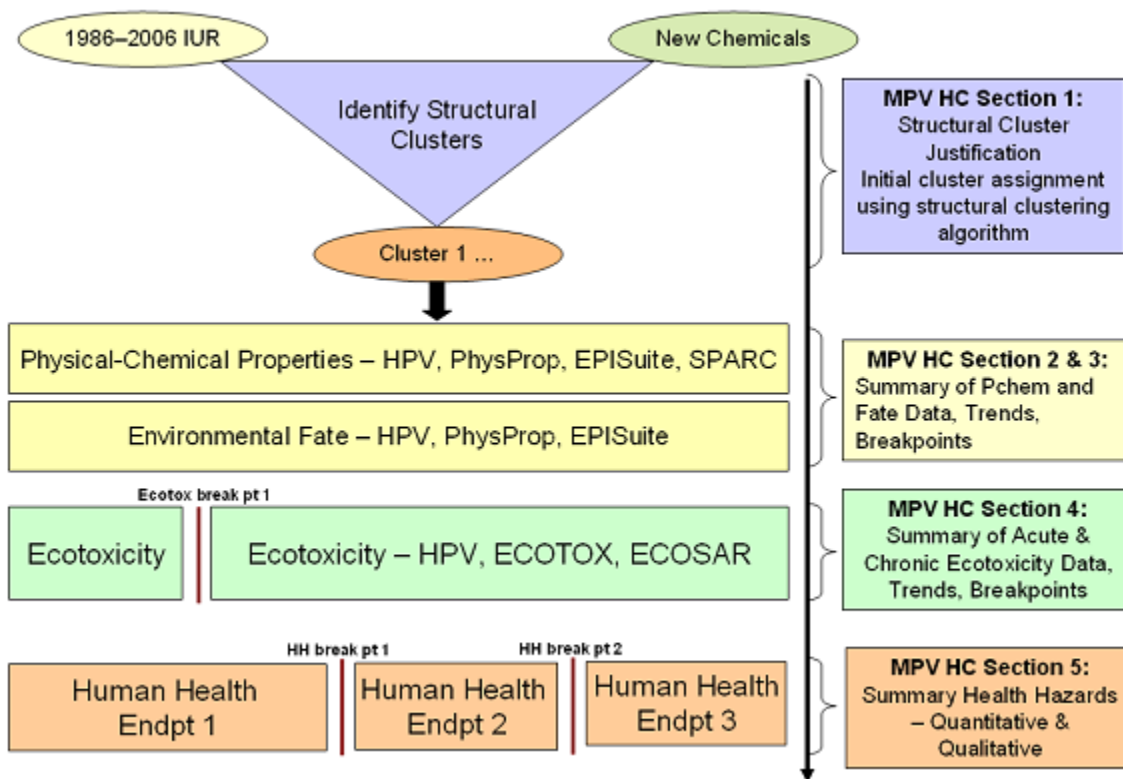
### ***Overall Hazard***

- An overall hazard call is provided for Persistence, Bioaccumulation, Aquatic Toxicity and Human Health.
- For Aquatic Toxicity, the overall hazard characterization is based on the highest hazard concern identified for any species, whether acute or chronic.
- For Human Health, the overall human health hazard characterization (i.e., H, M, L) is based on an integrative consideration of the quantitative endpoints (acute, repeated-dose, reproductive, and developmental mammalian toxicity) and qualitative endpoints (genotoxicity, cancer, neurotoxicity, immunotoxicity, irritation and sensitization), and study results and potential hazards will be described in section 1.5 of the hazard characterizations.
- In determining the overall hazard characterization for each endpoint, the data quality for the specific endpoint(s) that determine the call, as well as whether there is a clear weight-of-evidence from multiple studies and expert judgment will be used.

### **Hazard Characterization Report**

Following generation of the *Data Tables* and the *Overall Hazard Characterization Summary*, the screening-level hazard characterization document is written to include the sections outlined in Appendix 3.

### APPENDIX 1: Clustering Approach to Hazard Characterization



**APPENDIX 2: Hazard Characterization Criteria**

**Environmental Fate (Persistence and Bioaccumulation) Criteria**

**Table 1: Overall Persistence**

Persistence assessment includes evaluation of the potential half-life in air, water, soil, and sediment while considering the expected partitioning characteristics of the chemicals and all potential removal pathways based on standard physical-chemical properties and environmental fate parameters. The persistence characterization in the MPV HC is based on PBT criteria set forth in EPA’s policy statement on *Category for Persistent, Bioaccumulative, and Toxic New Chemical Substances* (Federal Register: November 4, 1999 (Volume 64, Number 213), pages 60194-60204; <http://www.epa.gov/oppt/newchems/pubs/pbtpolcy.htm>).

Persistence	Hazard Characterization		
	Not Persistent	Persistent	
	Low	Moderate	High
<b>Water, Soil, Sediment*</b>	<b>&lt; 60 days</b>	<b>≥ 60 days</b>	<b>&gt; 180 days</b>

\*For comparison purposes, calculations are based on 30 days in a month.

**Table 2: Bioconcentration and Bioaccumulation**

Bioaccumulation assessment includes evaluation of high quality bioaccumulation (measured or estimated BAF) data as the most preferred data for bioaccumulation assessment. When BAF data are not available, bioconcentration data (measured or estimated BCF) will be used to evaluate the potential for a chemical to bioaccumulate in organisms in the environment. The bioaccumulation characterization in the MPV HC is based on PBT criteria set forth in EPA’s policy statement on *Category for Persistent, Bioaccumulative, and Toxic New Chemical Substances* (Federal Register: November 4, 1999 (Volume 64, Number 213), pages 60194-60204; <http://www.epa.gov/oppt/newchems/pubs/pbtpolcy.htm>).

For BAF and BCF data, the criteria below will be applied to characterize bioaccumulation potential.

Bioaccumulation	Hazard Characterization		
	Not Bioaccumulative	Bioaccumulative	
	Low	Moderate	High
<b>BAF</b>	<b>&lt; 1000</b>	<b>≥ 1000</b>	<b>≥ 5000</b>
<b>BCF</b>	<b>&lt; 1000</b>	<b>≥ 1000</b>	<b>≥ 5000</b>

### Aquatic Toxicity Criteria

**Table 3: Acute and Chronic Toxicity**

For aquatic toxicity, whenever possible, a complete profile of acute and chronic values for fish, daphnid, and green algae will be derived for each MPV chemical and supporting analogs using either available measured data or predicted values from ECOSAR<sup>1</sup>. Criteria for characterization of acute toxicity are those used in the HPV Challenge Program, which are from the Globally Harmonized System (GHS) of Classification and Labeling<sup>2</sup>. For chronic toxicity, the GHS does not provide specific criteria for assigning hazard groupings. Therefore, criteria for evaluating chronic toxicity are those used in OPPT's New Chemical Program.

Endpoint	Hazard Characterization		
	High	Moderate	Low
Acute LC50 or EC50 (mg/L)	≤ 1	>1 – 10	> 10
Chronic (ChV or LOEC) (mg/L)	≤ 0.1	> 0.1 – 10	>10

### Human Health Criteria

**Table 4: Acute Toxicity**

When adequate acute toxicity data are identified, the following criteria will be used to characterize this hazard. These criteria are the same as those used in the HPV Challenge Program, which are criteria OPPT uses to determine reportability under TSCA Section 8(e).

Endpoint	Hazard Characterization		
	High	Moderate	Low
Oral LD50 (mg/kg)	≤ 50	> 50 – 500	> 500
Dermal LD50 (mg/kg)	≤ 200	> 200 – 2000	> 2000
Inhalation LC50 (ppm) – or – (mg/L)	≤ 200 ≤ 2	> 200 – 5000	> 5000 > 50

<sup>1</sup> U.S. EPA. 2000. ECOSAR: Ecological Structure-Activity Relationships. Office of Pollution Prevention and Toxics, Washington, DC. <http://www.epa.gov/oppt/newchems/tools/2/ecosar.htm>.

<sup>2</sup> United Nations. 2007. Globally Harmonized System of Classification and Labeling of Chemicals (GHS). Second Revised Edition. United Nations, New York and Geneva. [http://www.unece.org/trans/danger/publi/ghs/ghs\\_welcome\\_e.html](http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html).

**Table 5: Repeated-Dose & Systemic Parental Toxicity**

When adequate repeated-dose toxicity data are identified, the following criteria will be used to characterize this hazard. These criteria are the same as those used in the HPV Challenge Program, which are from the Globally Harmonized System (GHS) of Classification and Labeling<sup>3</sup>.

Endpoint	Hazard Characterization*		
	High	Moderate	Low
<b>Oral LOAEL (mg/kg-bw/day)</b>			
90-d / 13-wk	< 10	10 – 100	> 100
40-50-d	< 20	20 – 200	> 200
28-d / 4-wk	< 30	30 – 300	> 300
<b>Dermal LOAEL (mg/kg-bw/day)</b>			
90-d / 13-wk	< 20	20 – 200	> 200
40-50-d	< 40	40 – 400	> 400
28-d / 4-Wk	< 60	60 – 600	> 600
<b>Inhalation LOAEL (vapor) (mg/L/day)</b>			
90-d / 13-wk	< 0.2	0.2 – 1.0	> 1.0
40-50-d	< 0.4	0.4 – 2.0	> 2.0
28-d / 4-wk	< 0.6	0.6 – 3.0	> 3.0
<b>Inhalation LOAEL (dust) (mg/L/day)</b>			
90-d / 13-wk	< 0.02	0.02 – 0.2	> 0.2
40-50-d	< 0.04	0.04 – 0.4	> 0.4
28-d / 4-wk	< 0.06	0.06 – 0.6	> 0.6

\* If NOEAL values are only available from the study, NOAEL values will be provided in the data tables and use for the hazard characterization

<sup>3</sup> United Nations. 2007. Globally Harmonized System of Classification and Labeling of Chemicals (GHS). Second Revised Edition. United Nations, New York and Geneva.  
[http://www.unece.org/trans/danger/publi/ghs/ghs\\_welcome\\_e.html](http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html).

**Table 6: Reproductive & Developmental Toxicity**

When adequate reproductive and developmental toxicity data are identified, the following criteria will be used to characterize this hazard. These criteria are the same as those used in the HPV Challenge Program, which are criteria OPPT uses to determine reportability under TSCA Section 8(e).

Endpoint	Hazard Characterization *		
	High	Moderate	Low
Oral LOAEL (mg/kg/day)	< 50	50 – 250	> 250
Dermal LOAEL (mg/kg/day)	< 100	100 – 500	> 500
Inhalation LOAEL (vapor) (mg/L/day)	< 1.0	1 – 2.5	> 2.5
Inhalation LOAEL (dust/mist/fume) (mg/L/day)	< 0.1	0.1 – 0.5	> 0.5

\* If NOEAL values are only available from the study, NOAEL values will be provided in the data tables and use for the hazard characterization

**Table 7: Carcinogenicity**

When adequate carcinogenicity data are identified, the following qualitative criteria will be used to characterize this hazard. For chemicals with no measured data, but for which there is a suitable chemical class within the OncoLogic expert system, the estimated cancer potential will be qualitatively summarized by applying the following criteria for OncoLogic results. These qualitative criteria are those OPPT uses when evaluating chemicals under the New Chemicals Program.

Endpoint	Hazard Characterization		
	-	±	+
Carcinogenicity Potential From Measured Data	Negative Studies	Equivocal Studies	Positive Studies
Carcinogenicity Potential From OncoLogic Results	L	Marginal	LM/M/HM/H

**Table 8: Genotoxicity, Mutagenicity, Neurotoxicity, and Immunotoxicity**

When adequate genotoxicity, neurotoxicity, or immunotoxicity data are identified, the following criteria will be used to characterize these hazards. These qualitative criteria are those OPPT uses when evaluating chemicals under the New Chemicals Program.

Endpoint	Hazard Characterization		
	-	±	+
Genotoxicity, Neurotoxicity, Immunotoxicity	Negative Studies	Equivocal Studies	Positive Studies

**Table 9: Irritation**

When adequate irritation data are identified, the following criteria will be used to characterize these hazards. These qualitative criteria are those OPPT uses when evaluating chemicals under the New Chemicals Program.

Endpoint	Hazard Characterization		
	-	±	+
<b>Skin/Eye Irritation</b>	<b>Negative Studies</b>	<b>Equivocal Studies</b>	<b>Positive Studies</b>

**Table 10: Skin Sensitization**

When adequate sensitization data are identified, the following criteria will be used to characterize these hazards. These qualitative criteria are those OPPT uses when evaluating chemicals under the New Chemicals Program.

Endpoint	Hazard Characterization		
	-	±	+
<b>Skin Sensitization</b>	<b>Negative Studies</b>	<b>Equivocal Studies</b>	<b>Positive Studies</b>

## APPENDIX 3: Screening-Level Hazard Characterization and Prioritization Document

### TITLE PAGE

#### Chemical Cluster Name

List of Chemical Names & CAS Registry Numbers Included

Month / YEAR

Prepared By:

### Section 1. STRUCTURAL CLUSTER JUSTIFICATION

Description of structural features/rationale for assignment to chemical cluster

### Section 2. PHYSICAL-CHEMICAL PROPERTIES

Summary of physical-chemical properties; identification of trends and break-points where appropriate.

### Section 3. ENVIRONMENTAL FATE

Summary of environmental fate; identification of trends and break-points where appropriate.

### Section 4. AQUATIC ORGANISM TOXICITY

Summary of acute and chronic toxicity to fish, aquatic invertebrates and plants; identification of trends and break-points where appropriate.

### Section 5. HUMAN HEALTH TOXICITY

Summary of acute, repeated-dose, reproductive, developmental, genetic, neuro, immuno toxicity, irritation and sensitization and carcinogenic potential; identification of trends and break-points where appropriate.

### Section 6. OVERALL HAZARD CHARACTERIZATION SUMMARY

Qualitative (High/Moderate/Low or Positive/Negative) summary of persistence and bioaccumulation potential, aquatic toxicity and human health toxicity derived from the Hazard Characterization Summary Sheet

### Section 7. 2006 NON-CBI IUR INFORMATION

### Section 8. REGULATORY AND RELATED INFORMATION SUMMARY

### Section 9. INITIAL PRIORITIZATION DECISION FOR SUBJECT CHEMICAL(S)

Rationale and Uncertainties Considered in Prioritization Decision

Prioritization Decision for Chemical(s)

## APPENDIX 4: Standard Units for the Summary Data Tables

### P-Chem and Fate Endpoints:

Melting Point – Degrees Celcius (°C)  
Boiling Point – Degrees Celcius (°C)  
Vapor Pressure – hPa @ 25 °C  
Water Solubility – mg/L  
Log  $K_{ow}$  – unitless  
 $K_{oc}$  – unitless  
 $pK_A/pK_B$  – unitless  
Henry's Law Constant – atm-m<sup>3</sup>/mole  
Hydrolysis - %degraded/time  
Photolysis - %degraded/time  
Photooxidation half-life – days  
Readily Biodegradable – Qualitative (Yes/No) – unitless  
Rapid Biodegradation (probability) – Qualitative (Yes/No) – unitless  
Ultimate Biodegradation – Qualitative (Duration) – hours, hours-days, days, days-weeks, weeks, weeks-months, months, longer  
Aerobic Biodegradation - %degraded/time  
Anaerobic Biodegradation - %degraded/time  
Level 3 Fugacity Estimate – % in each media  
BCF – unitless  
BAF – unitless

### Aquatic Toxicity Endpoints:

Acute LC50 or EC50 – mg/L  
Chronic ChV or NOEC – mg/L

### Human Health Endpoints:

Acute Toxicity – Oral LD50 (mg/kg-bw), Dermal LD50 (mg/kg-bw), Inhalation LC50 (mg/L)  
Repeat Dose and Systemic Toxicity – Oral (mg/kg-bw/day), Dermal (mg/kg-bw/day), Inhalation (vapor) (mg/L/day), Inhalation (dust) (mg/L/day)  
Reproductive and Developmental Toxicity – Oral (mg/kg-bw/day), Dermal (mg/kg-bw/day), Inhalation (vapor) (mg/L/day), Inhalation (dust/mist/fume) (mg/L/day)  
Carcinogenicity, Genotoxicity, Mutagenicity, Neurotoxicity, and Immunotoxicity, Irritation, Skin Sensitization – Qualitative (– Negative, ± Equivocal, + Positive) – unitless