



# **Final Contaminant Candidate List 3 Chemicals: Screening to a PCCL**

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## List of Acronyms and Abbreviations

<	Less than
≤	Less than or equal to
>	Greater than
≥	Greater than or equal to
μg/L	Micrograms per liter
CASRN	Chemical Abstract Services Registry Number
CCL	Contaminant Candidate List
CCL 1	EPA's first contaminant candidate list
CCL 3	EPA's third Contaminant Candidate List
CE	Clear evidence of carcinogenicity
CUS/IUR	Chemical Update System/Inventory Update Rule
DBPs	Disinfection By-Products
DBP-CAN	Disinfection By-Product with Carcinogenicity Estimates
DSS-Tox	Distributed Structure-Searchable Toxicity
DWEL	Drinking water equivalent level
E	Equivocal
EE	Equivocal evidence of carcinogenicity
EPA	United States Environmental Protection Agency
FDA	United States Food and Drug Administration
FW/AW	Finished Water/Ambient Water
H	High probability of causing cancer
HM	High moderate probability of causing cancer
IRIS	Integrated Risk Information System (EPA)
kg	Kilogram
L	Liter
L	Low probability of causing cancer
LD <sub>50</sub>	Lethal dose 50; an estimate of a single dose that is expected to cause the death of 50 percent of the exposed animals; it is derived from experimental data.

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lbs	Pounds
LM	Low moderate probability of causing cancer
LOAEL	Lowest observed adverse effect level
M	Moderate probability of causing cancer
Mar	Marginal probability of causing cancer
MCLG	Maximum contaminant level goal
MRDD	Maximum recommended daily dose
mg/kg	Milligrams per kilogram body weight
mg/kg/day	Milligrams per kilogram body weight per day
N	Negative
NAWQA	National Water Quality Assessment Program (USGS)
NCFAP	National Center for Food and Agricultural Policy
NCI	National Cancer Institute
NDWAC	National Drinking Water Advisory Council
NE	No evidence of carcinogenicity
NOAEL	No observed adverse effect level
NPDWR	National Primary Drinking Water Regulations
NREC	National Reconnaissance of Emerging Contaminants
NTP	National Toxicology Program
NTPMSR	National Toxicology Program multi-species results
P	Positive
PCCL	Preliminary CCL
PPMP	Pesticide Pilot Monitoring Program
RfD	Reference dose
QSAR	Quantitative Structure Activity Relationship
RfD-eq	Reference Dose -equivalent
SE	Some evidence of carcinogenicity
TD <sub>50</sub>	Tumorigenic dose 50; The dose-rate which if administered chronically for the standard life-span of the species will have a 50% probability of causing tumors at some point during that period.

TRI	Toxics Release Inventory
TS	Test Set of chemicals
U	Universe
USGS	United States Geological Survey
yr	Year

## 1.0 Introduction

Every five years the United States Environmental Protection Agency (EPA) is required to publish a list of contaminants (1) that are currently unregulated, (2) that are known or anticipated to occur in public water systems, and (3) which may require regulations under the Safe Drinking Water Act (SDWA). This list is known as the Contaminant Candidate List or CCL. SDWA section 1412(b)(1) requires that in the development of the CCL, EPA consider specific data sources and include the scientific community. EPA must evaluate substances identified in section 101(14) of the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) of 1980 and substances registered as pesticides under the Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA). SDWA also requires the Agency to consider the National Contaminant Occurrence Database established under section 1445(g) of SDWA. SDWA directs the Agency to consult with the scientific community, including the Science Advisory Board (SAB). In addition, it directs the Agency to consider the health effects and occurrence information for unregulated contaminants to identify those contaminants that present the greatest public health concern related to exposure from drinking water.

EPA interprets the criterion that contaminants are known or anticipated to occur in public water systems broadly. In evaluating this criterion, EPA considers not only public water system monitoring data, but also data on concentrations in ambient surface and ground waters, releases to the environment (e.g., Toxics Release Inventory), and production. While such data may not establish conclusively that contaminants are known to occur in public water systems, EPA believes these data are sufficient to anticipate that contaminants may occur in public water systems and support their inclusion on the CCL. The Agency considered adverse health effects that may pose a greater risk to life stages and other sensitive groups which represent a meaningful portion of the population. Adverse health effects associated with infants, children, pregnant women, the elderly, and individuals with a history of serious illness were evaluated. In selecting contaminants for the CCL 3, each of the above requirements was met.

SDWA section 1412(b)(1) also requires EPA to determine whether to regulate at least five contaminants from the CCL every five years. SDWA specifies that EPA shall regulate a contaminant if the Administrator determines that:

- The contaminant may have an adverse effect on the health of persons;
- The contaminant is known to occur, or there is a substantial likelihood that the contaminant will occur in public water systems with a frequency and at levels of public health concern; and
- In the sole judgment of the Administrator, regulation of such contaminant presents a meaningful opportunity for health risk reduction for persons served by public water systems.

Once contaminants have been placed on the CCL, EPA identifies if there are any additional data needs or if there are sufficient information to make a regulatory determination. EPA interprets these criteria for regulatory determination as more rigorous than what is used to place contaminants on the CCL.



EPA developed a multi-step process, based on available data, to characterize occurrence and adverse health risks a contaminant may pose to consumers of public water systems for inclusion on the Contaminant Candidate Lists (CCL). The steps involve:

- 1) Building a broad CCL Universe of potential drinking water contaminants for consideration (see “*Final Contaminant Candidate List 3 Chemicals: Identifying the Universe*” (USEPA, 2009a));
- 2) Using straightforward screening criteria related to a contaminant’s potential to occur in drinking water and potential for public health concern to narrow the Universe to a Preliminary CCL (PCCL), and;
- 3) Using a structured classification approach (e.g., a classification model) as a tool, along with expert judgment, to develop a proposed CCL from the PCCL (see “*Final Contaminant Candidate List 3 Chemicals: Classification of the PCCL to the CCL*” (USEPA, 2009b)).
- 4) Providing opportunities for public comment and contaminant nomination (see “*Summary of Nominations for the Third Contaminant Candidate List*” (USEPA, 2009c)).

This report focuses on the second step, in which EPA uses an approach to screen chemicals to a PCCL using the data available from a set of data sources that EPA evaluated for health effects and occurrence information to compile the CCL 3 Universe.

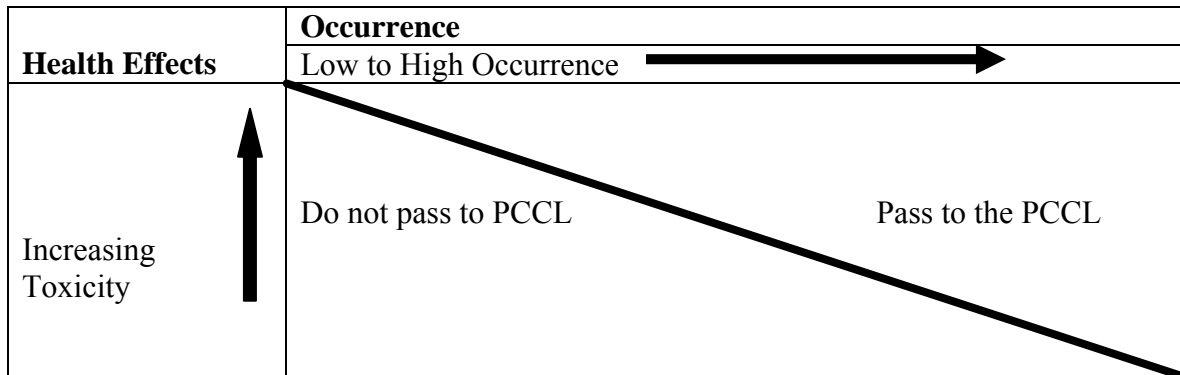
These data sources have yielded over 6,000 chemicals which populate the CCL 3 Chemical Universe. Along with the names and identifying characteristics of these chemicals the Universe is the repository for the health-related and occurrence-related information. This information was used to screen individual contaminants to determine if they should advance from the Universe to the PCCL. In the case of health effects, the Universe includes both quantitative and qualitative information on the hazard and/or dose-response properties of the contaminants. For occurrence, the Universe includes both quantitative and qualitative information on occurrence in water, releases to the environment, and amount produced. The process for the selection of data sources and Universe chemicals is detailed in the document entitled, “*Contaminant Candidate List 3 Chemicals: Identifying the Universe*” (USEPA, 2009a).

EPA based the screening approach, in part, on the National Drinking Water Advisory Council (NDWAC) recommendation that screening the Universe of chemicals for selection of the PCCL should be based on widely available data elements that represent important health effects and occurrence properties (NDWAC, 2004). NDWAC also recommended that the screening be versatile, yet as simple as possible, and facilitate the identification of those contaminants most in need of further consideration through the PCCL to CCL process. EPA considered this an important goal when establishing the screening criteria.

The basic framework developed by EPA for use in screening is shown in Exhibit 1. Applying this framework to the CCL 3 Universe groups contaminants categorized by their toxicity along the vertical axis and by their occurrence on the horizontal axis. It arrays the data in a way that will allow for a separation of chemicals into those that move to the PCCL based on their toxicity and occurrence properties (e.g., upper right in Exhibit 1) and those that are not further evaluated

and remain in the CCL chemical universe (e.g., lower left in Exhibit 1). The type of available data determines which chemicals move to the PCCL and those that remain in the universe.

**Exhibit 1: Partition for Screening the Universe**



To adequately represent the broad spectrum of health effects data elements at the screening level, the toxicity categories must accommodate both dose-response and descriptive data. The occurrence screening categories must also accommodate a variety of occurrence data elements such as water concentration, environmental release, or production data.

The challenge in screening is to group the chemicals into categories for health effects and occurrence using the variety of data elements available in the Universe in a generally equivalent manner. Section 2.0 describes the approach that was used for grouping the health effects data elements into the separate toxicity-based categories. Section 3.0 describes the approach that is used to group the occurrence data elements. The application of the screening framework as a tool, and the results from screening are discussed in Section 4.0. Appendix 1 summarizes the screening criteria for each type of data considered. Appendix 2 shows the contaminants and the data EPA used that moved them to the PCCL for additional consideration in the CCL 3 process.

## 2.0 Health Effects Data Elements

The toxicity information and health effects data extracted from the data sources are quite varied (USEPA, 2009a and b). The health data elements that provide toxicity information to populate Exhibit 1 fall into two major categories:

- Data elements that provide dose-response information (potency)
- Categorical data elements on hazard (mostly related to carcinogenic potential).

Some chemicals come from data sources that provide dose-response data in the form of Lowest Observable Adverse Effects Level (LOAELs), Lethal Dose 50 (LD<sub>50</sub>), or Reference Doses and their equivalents (RfDs and RfD-eq). Some data sources only include descriptive data such as the positive, negative, or equivocal results from National Toxicology Program (NTP) studies or International Agency for Research on Cancer (IARC) carcinogen classifications. Still other

chemicals are in the Universe by virtue of their being on a list, such as the State of California list of reproductive or developmental toxicants (“Proposition 65”) which does not have any accompanying toxicological data. For this reason, it is important that the screening process for deriving the PCCL be able to accommodate a variety of health effects data inputs.

After examining the breadth of available health effects data, EPA established five categories for screening. The five categories are as follows:

- Toxicity Category 1
- Toxicity Category 2
- Toxicity Category 3 (the central tendency grouping)
- Toxicity Category 4
- Toxicity Category 5

The toxicity of the grouping decreases as the number for the grouping increases, with Toxicity Category 1 being the most toxic grouping and Toxicity Category 5 the least toxic grouping. Within each Toxicity Category, the partitioning criteria vary depending on the data element used. The partitioning criteria that place a LOAEL in Toxicity Category 1 differ from the criteria used for LD<sub>50</sub> values that place it in the same category. Both criteria are intended to identify contaminants of approximately equivalent toxicity. The following sections provide information on the data elements available in the Universe that reflect the dose-response properties and categorical or descriptive information for the chemicals in the Universe.

## **2.1 Dose-Response Data Elements**

The NDWAC recommended that screening be based on data elements that demonstrate toxic effects (i.e., LOAELs, LD<sub>50</sub>s, Cancer Slope Factors, etc.) rather than on data elements that are based on no effects (i.e., No observed adverse effect level (NOAELs) or that include uncertainty factors in their derivation (i.e., RfD-eq). However, because of the limitations on the types of data available for many of the contaminants, it is not possible to be this restrictive. Of the chemicals in the universe, about 500 had LOAEL data and about 2,000 had LD<sub>50</sub> data. The remainder were lacking the endpoints recommended by the NDWAC, so EPA used other data elements that provide quantitative information on dose-response that can be partitioned into the five toxicity groupings. Major endpoints that fall in this category, in addition to LOAELs and LD<sub>50</sub>s, are as follows:

- RfDs and RfD-equivalents: RfDs, Minimal Risk Levels from the Agency for Toxic Substance and Disease Registry, Tolerable Daily Intakes from the World Health Organization (WHO), Acceptable Daily Intakes from WHO and the Food and Drug Administration (FDA), Public Health Goals from California EPA, and Tolerable Upper Intake Levels from the Institute of Medicine.
- NOAELs - No Observed Adverse Effect Levels.

- TD<sub>50S</sub> - The dose-rate which if administered chronically for the standard life-span of the species will have a 50% probability of causing tumors throughout that period. Chemicals with TD<sub>50</sub> data have positive cancer results in at least one study.
- Maximum Recommended Daily Dose (MRDD) - Recommendations for the maximum adult daily therapeutic doses for pharmaceuticals (FDA).

Including the measures of toxic potency listed above in the health effects screening framework expands the number of chemicals from the Universe that can be screened on the basis of their dose-response for possible inclusion in the PCCL. The approach used to partition each of these toxicity measures for screening is described in Section 2.3.

## **2.2 Categorical Data Elements**

There are three groups of categorical data elements and health effects information in the Universe. These groups categorize chemicals according to their carcinogenic potential, mutagenicity information, or classification as a developmental or reproductive toxicant. Categorical data sets in the Universe include the following:

- U.S. EPA Cancer Groupings
- IARC Cancer Groupings
- NTP weight-of-evidence findings from cancer bioassays
- National Cancer Institute (NCI) weight-of-evidence findings from cancer bioassays
- California EPA list of chemicals suspected of causing cancer
- EPA Water Disinfection By-Products with Carcinogenicity Estimates (DBP-CAN) groupings based on carcinogenic potential derived from Quantitative Structure Activity Relationship (QSAR) projections and expert judgment
- California list of chemicals suspected of being developmental or reproductive toxicants
- U.S. EPA groupings of disinfection by-products (DBPs) based on QSAR predictions of their ability to cause developmental or reproductive toxicity.

Even with the expansion of the types of dose-response data suitable for screening described in Section 2.1, many chemicals in the Universe lack dose-response data elements making it important to use the categorical information at this screening stage.

The categorical cancer information is amenable to the screening approach illustrated in Exhibit 1 because, in most cases, it includes subcategories related to the strength of the cancer data and its applicability to humans.

The second group of categorical data elements provides information on genotoxicity and mutagenicity. This group is considered categorical because results are classified as positive, negative, or equivocal. However, it is common to have multiple genotoxicity assays for any given chemical, and it is unusual for all assays of a given chemical to have the same result.

Accordingly, there is a need to integrate all of the genotoxicity results and determine a categorical weight-of-evidence if the data are to be useful for screening. However, the Universe contained few weight-of-evidence findings on genotoxicity, and, when such results are available, they are usually tied to cancer assessments with dose-response measures. Accordingly, the use of the categorical cancer information along with TD<sub>50</sub> dose-response data reduces the importance of including genotoxicity as a screening criterion. The genotoxicity data remain available as a supplemental health effects element that can be applied in the evaluation of the PCCL and in making decisions for chemicals that fall close to the screening barrier that separates the chemicals that will move to the PCCL from those that will remain in the Universe.

The third type of categorical information in the database comes from the State of California's list of reproductive and developmental toxicants or other similar lists. These lists are groupings that are based on a single toxicological property, but not partitioned by the degree of hazard. In this respect the lists are different from the cancer information that includes subdivisions based on the hazard weight-of-evidence and supported by quantitative cancer slope factors and/or TD<sub>50</sub> values. For this reason, the California list of developmental and reproductive toxicants and the California list of carcinogens are not used for the screening framework but they are retained as supplemental information that may be useful in the evaluation of the initial PCCL screening results.

## **2.3 Calibration of the Data for Partitioning into Toxicity Categories**

### **2.3.1 Dose-Response Data**

As mentioned in the previous section, the health effects information found in the Universe is diverse. Accordingly, the challenge in screening is to be able to partition each type of data element into the five toxicity-based categories in a reproducible and logical manner. The main data elements proposed for screening (RfD-eq, NOAEL, and LOAEL values) have been used by EPA in establishing Maximum Contaminant Level Goals (MCLGs) or Lifetime Health Advisories. Accordingly, it was possible to compile a set of test chemicals (TS) found in drinking water that had multiple data elements from the set of toxicity data (i.e., RfD-eq, NOAEL, LOAEL, LD<sub>50</sub>) and examine the range and distribution of values associated with each dose-response data element. Distributions were also determined for the other measures of dose-response found in the Universe (U) at the time the screening process was developed (i.e., LOAELs, LD<sub>50</sub>s, MRDDs, TD<sub>50</sub>s). Each measure of toxicity covered a range of close to ten orders of magnitude and had a roughly normal distribution when arrayed according to their log<sub>10</sub> value rounded to a single significant figure (Exhibit 2). Each data set is skewed toward higher potency chemicals due to the difficulty in identifying conventional toxicity data for many chemicals that are slightly or practically nontoxic. The RfDs and NOAELs in the Universe were not initially compiled.

## Exhibit 2: Potency Distributions for the Health Effects Test Set and Universe Chemicals

Log	RfD-eq	NOAEL	LOAEL		MRDD	TD <sub>50</sub>	LD <sub>50</sub>	
	TS	TS	TS	U	U	U	TS	U
<-7	1							
-7								
-6	1							
-5	8				3			
-4	59		1	3	4	3		
-3	105	5	2	4	15	8		
-2	121	21	13	15	53	17	0	1
-1	63	45	28	52	183	53	0	1
0	11	92	63	83	271	184	9	10
1	4	106	121	120	453	266	11	26
2	3	29	85	139	223	272	45	239
3		13	28	73	12	139	75	1023
4			1	8		25	40	672
5						1	1	19
6								

TS = Test Set, U= Universe  
The TS for RfDs includes chemicals on the IRIS as well as those with MCLGs and/or Health Advisory values

A reference point for the potency of drinking water was established by converting the 2 L/day, 90 percentile drinking water intake (used by the Office of Water for risk analyses), into a NOAEL equivalent mg/kg/day dose for 70 Kg adults. This dose equivalent, for perspective, would occur in the Log 5 cell in the NOAEL health effects diagnostic set. Including this dose-response value for drinking water allows all other contaminants to be viewed in perspective as they relate to the CCL screening framework (in Exhibit 2).

EPA evaluated the distribution of the Test Set or the Universe dose-response parameters shown in Exhibit 2. EPA defined the modal grouping from the distribution for each type of toxicity parameter as Toxicity Category 3 for screening. The higher and lower screening toxicity categories were partitioned from the remainder of the distribution based on its shape and the numeric groupings of chemicals above and below the modal grouping. For most parameters other than the LD<sub>50</sub> values, partitioning was based on powers of 10 and a desire to be more inclusive rather than exclusive during the screening process, especially during initial testing.

There is a discrepancy between the modal LOAEL in the Universe and that from the Test Set. The data from the Universe have a modal value that is one log<sub>10</sub> unit less toxic than that for the Test Set (Exhibit 2). A decision was made by EPA to base Toxicity Category 3 LOAEL grouping on the Test Set rather than the universe because the combination of the Office of Water Health Advisory chemicals and those on Integrated Risk Information System (IRIS) that made

up that set is more representative of chemicals that EPA had found to be of environmental and/or regulatory concern than the Universe compilation.

The partitioning for the LD<sub>50</sub> values was treated differently from the RfD-eq, NOAEL, and LOAEL values because there has long been an accepted categorization of LD<sub>50</sub> values into six categories. The Hodge Sterner scale is shown in Exhibit 3 (Hodge Sterner, 1956). The six categories were reduced to the five screening categories by combining the two lowest toxicity categories from the Hodge Sterner Scale.

### Exhibit 3: Hodge Sterner Scale for Categorizing Chemicals Based on LD<sub>50</sub> Values (Health Canada, 2005)

Extremely Toxic	<1 mg/kg
Highly Toxic	1 - <50 mg/kg
Moderately Toxic	50 - <500 mg/kg
Slightly Toxic	500 - <5000 mg/kg
Practically nontoxic	5000 - <15000 mg/kg
Relatively harmless	≥15000 mg/kg

The MRDD values were partitioned as if they were LOAELs because the maximum therapeutic doses are established by balancing their benefit with their risk. Accordingly, although MRDD doses are safe for human consumption, some adverse effects are always possible, especially in sensitive populations. This situation justifies considering them as LOAELs rather than NOAELs.

The partitioning of the TD<sub>50</sub> values was unique in that they apply to the probability for tumor development. They were, accordingly, combined with the categorical data elements that are discussed in Section 2.3.2.

Exhibit 4 illustrates how the Universe dose-response data elements partition into their toxicity categories for screening. The partitioning considered both the distribution of the data for each of the health effects data elements and the number of contaminants that would fall in each of the toxicity categories. The testing of the partitioning for the third CCL (CCL 3) Universe at the time of protocol development suggested that the approach performed reasonably well. Its performance can be further evaluated and modified if needed for future CCLs.

### Exhibit 4: Potency Measures for Universe Data Element Partitioned Based on Toxicity (mg/kg/day or mg/kg)

	RfD	NOAEL	LOAEL	MRDD	LD <sub>50</sub>
Toxicity Category 1	<0.0001	<0.01	<0.01	<0.01	<1
Toxicity Category 2	0.0001 - <0.001	0.01 - < 1	0.01 - <1	0.01 - < 1	1 - <50
Toxicity Category 3	0.001 - <0.05	1 - <10	1 - <10	1 - <10	50 - <500
Toxicity Category 4	0.05 - <0.1	10 - < 1000	10 - <1000	10 - < 1000	500 - <5000
Toxicity Category 5	≥0.1	≥1000	≥1000	≥1000	≥5000

### 2.3.2 Categorical Data

As discussed in Section 2.0, the categorical data selected for screening were primarily those that applied to cancer and provided a weight-of-evidence evaluation for the probability that the agent was carcinogenic to humans. The data from the EPA include either an alpha-numeric grouping or a weight-of-evidence statement on carcinogenic potential and often a cancer slope factor. The alpha-numeric groupings (Exhibit 5) apply to the chemicals evaluated for their carcinogenicity under the Guidelines for Carcinogen Risk Assessment (USEPA, 1986).

### Exhibit 5: Cancer Grouping and Description under the U.S. EPA 1986 Guidelines

Group	Description
A	Human carcinogen
B <sub>1</sub>	Probable human carcinogen
B <sub>2</sub>	Limited evidence in animals and inadequate or no evidence in humans
C	Possible human carcinogen
D	Not classifiable as to human carcinogenicity
E	Evidence of noncarcinogenicity in humans

In 1996 and 1999 the U.S. EPA issued draft updated guidelines for evaluating carcinogenicity. EPA finalized the revised guidelines in 2005 (USEPA, 2005). Chemicals evaluated under the 2005 Guidelines and its drafts are grouped according to five weight-of-evidence descriptors as follows:

- Carcinogenic to humans
- Likely to be carcinogenic to humans
- Suggestive evidence for carcinogenicity
- Insufficient evidence to determine carcinogenicity
- Not likely to be carcinogenic

IARC uses a Numeric-Alpha grouping for carcinogens (ITER, 2006) that is similar to the 1986 U.S. EPA groupings. Exhibit 6 summarizes the IARC cancer groupings. The Health Canada groupings are derived from the IARC system but use Roman numerals I through V for the five IARC groupings (ITER, 2006).



**Exhibit 6: IARC Cancer Groupings (ITER, 2006)**

Group	Description
1	Carcinogenic to humans
2A	Probably carcinogenic to humans
2B	Possibly carcinogenic to humans
3	Not classifiable as to its carcinogenicity to humans
4	Probably not carcinogenic to humans

The data abstracted from the NTP database on cancer studies are those from studies conducted by both the NTP and the NCI. The NTP (2005) describes the results of the studies as:

- Clear evidence of carcinogenicity (CE)
- Some evidence of carcinogenicity (SE)
- Equivocal evidence of carcinogenicity (EE)
- No evidence of carcinogenicity (NE)

The NTP studies are conducted using groups of male and female rats and/or mice. The results in both species and both sexes have separate weight-of-evidence determinations. “Clear evidence” in both species and both sexes is stronger evidence that a chemical could be a potential human carcinogen than “clear evidence” in only two species-one sex, or in two sexes-one species. Clear evidence is stronger than some evidence and some evidence stronger than equivocal evidence. EPA took these distinctions into account when partitioning chemicals based on their NTP categorical cancer data.

The NCI was responsible for conducting cancer studies for the U.S. Public Health Service prior to the formation of the NTP. They used a simpler system (NTP, 2005) by reporting results from cancer bioassays as either positive (P), negative (N) or equivocal (E). The NCI findings are reported in the NTP database. NCI Studies were also conducted in both sexes for rats and mice. The studies with positive results in both species and both sexes are those that present the highest level of concern regarding the potential for human carcinogenicity.

The DBP-CAN data grouping within the EPA Distributed Structure-Searchable Toxicity (DSS-Tox) database is a compilation of projections on carcinogenic potential, of an assortment of unregulated DBPs, derived from QSAR modeling and expert judgment. The chemicals are categorized according to the estimated probability that they will cause cancer from high (H) to unlikely (L) with intermediary probabilities of high moderate (HM), moderate (M), low moderate (LM) and marginal (Mar).

EPA placed the qualitative and quantitative data for carcinogenicity of chemicals only in the upper three toxicity categories. Carcinogens are not generally considered as having low toxicity. The cancer screening criteria are based on USEPA, IARC, and NTP cancer groupings for screening rather than the cancer slope factors because many chemicals are categorized for cancer

but do not have cancer slope factors. Therefore use of the categorical data is more inclusive than use of slope-factor data.

An exception to using the categorical data for the screening for the cancer endpoint is the TD<sub>50</sub> data. The TD<sub>50</sub> data set includes quantitative estimates of cancer risk for some chemicals that are not in the other data sets, and thus they will be used in screening in cases where no categorical cancer data elements are available.

EPA partitioned the cancer-related data elements in the Universe as described in Exhibit 7. Quantitative measures of dose-response for carcinogenicity will be used in scoring the Potency attribute for potential carcinogens in the PCCL to CCL process (see the PCCL to CCL Report, USEPA, 2009b) but not in screening at the Universe level.

### Exhibit 7: Partitioning of Cancer Data Based on TD<sub>50</sub> Values and Weight of Evidence

	TD <sub>50</sub>	EPA	IARC /HC	NTP	NCI	DSS-Tox
Toxicity Category 1	<0.1	Group A; Human Carcinogen	Group 1	CE 2 species/2 sexes; or 2 species; or 2 sexes	P 2 species/2 sexes; or 2 species; or 2 sexes	H
Toxicity Category 2	0.1 - 100	Groups B1 and B2; likely carcinogens	Group 2A	Combinations of CE, SE, EE, and NE	Combinations of P, E and N	HM
Toxicity Category 3	>100	Group C; Suggestive evidence of carcinogenicity	Group 2B	Combinations of SE, EE, and NE	Combinations of E and N	M and LM

\*\* Cancer data placed chemicals in only the three highest Toxicity Categories  
CE = clear evidence, SE = some evidence, EE = equivocal evidence, NE = no evidence  
P= positive, N= Negative, E = equivocal  
H = high probability, HM= high to medium probability, M = medium probability, LM = medium to low probability

The U.S. EPA Groups D and E, “Insufficient Evidence” and “Not Likely” descriptors, as well as the IARC Group 3 and 4 or Health Canada Groups IV or V, are not used when partitioning the categorical data elements as described in Exhibit 7. The DSS-Tox, “unlikely” and TD<sub>50</sub>, “NP” field entries are also not used. EPA’s decision is based on the premise that low toxicity concerns related to low tumorigenic properties do not mean there is no systemic toxicity for a contaminant. In these cases, other non-cancer data were used for screening.

## 2.4 Combining the Data Elements for Screening

As discussed in this report, there are a variety of data elements available in the Universe that can be used to screen for adverse health effects. To avoid favoring chemicals with rich data sets, the EPA evaluated all available dose-response and categorical data elements for a given chemical in the screening process. When each of the data elements for a given chemical is placed in the screening framework, the most conservative health effects category is identified. Accordingly, if there is just one data element that places a chemical in Toxicity Category 1 it will be categorized as such even if some of the other data elements for that same chemical place it a lower toxicity category. For example, if a chemical is classified as a 2A carcinogen by IARC it will be placed in Toxicity Category 2 even if its LOAEL from a different study places it in Toxicity Category 3. Exhibit 8 includes several examples drawn from the Universe of chemicals that have either one or multiple available potency data elements. The data elements used to evaluate the chemicals are bolded.

**Exhibit 8: Examples of Potency Data Elements for the Selected Chemical Drawn from the Universe**

Chemical	Toxicity Category 1	Toxicity Category 2	Toxicity Category 3	Toxicity Category 4	Toxicity Category 5
4-Biphenylamine	<b>Group 1</b>	TD <sub>50</sub>			
Hexane				<b>LD<sub>50</sub></b>	RfD-eq
Methylazoxy-methanol acetate			<b>Group 2B</b>		
Molybdenum oxide			<b>NTP</b>		
3-hydroxycarbofuran		<b>LD<sub>50</sub></b>			
Methylenediphenol			LOAEL	LD <sub>50</sub>	
BMX-1		<b>DBP-CAN</b>			
Primiphos methyl		<b>NOAEL</b>	RfD-eq LOAEL	LD <sub>50</sub> LOAEL	

Four of the contaminants in Exhibit 8 have more than one health effects data element. Each health effects data element for a chemical will be used for the screening process but the one data element demonstrating the highest potency in combination with its measure of occurrence will determine if it is selected for the PCCL. For example, 4-biphenylamine falls in Toxicity Category 1 because it has an IARC Group 1 classification even though its TD<sub>50</sub> places it in Toxicity Category 2. Hexane falls in Toxicity Category 4 based on its LD<sub>50</sub> value even though its RfD-eq value would place it in Toxicity Category 5.

### **3.0 Occurrence Data Elements**

EPA found that data elements representing a chemical's potential to occur in drinking water vary greatly in terms of the occurrence factor they represent. The goal was to determine which data elements best represented the potential to occur in drinking water. EPA considered and evaluated data elements in the following categories:

- Finished Water – measures concentration and frequency of detections
- Ambient Water – measures concentration and frequency of detections
- Total Releases in the Environment – measures pounds per year and number of states
- Pesticide Application Rates – measures pounds per year and number of states
- Production volume – measures pounds per year

In addition to evaluating quantitative data elements, EPA also analyzed chemicals with descriptive data based upon their likelihood of occurring in drinking water. Examples of these types of chemicals include disinfection byproducts and drinking water treatment additives. The following sections describe the occurrence categories and how EPA utilized them in the development of the screening criteria.

To analyze the occurrence data and develop the screening criteria, EPA assembled a diagnostic test set of approximately 200 chemicals. Some of these chemicals were selected from past CCLs and National Primary Drinking Water Regulations (NPDWRs), and some were randomly pulled from the Universe of contaminants considered for the draft CCL 3. Most of them had data on concentrations in water, environmental release and production, and as such constituted a relatively complete set of occurrence data elements.

#### **3.1 Finished Water Data**

Using the Universe as a starting point, EPA considered data elements that are readily available for chemicals in finished water. The finished water data elements are from the National Contaminant Occurrence Database (unregulated contaminant monitoring) Rounds 1 and 2, the National Inorganic Radionuclides Survey, the Unregulated Contaminant Monitoring Regulation monitoring, the Information Collection Rule database for DBPs, U.S. Department of Agriculture Pesticide Data Program (PDP), and Pesticides Pilot Monitoring Program (PPMP) (USGS and USEPA).

The finished water data elements evaluated include:

- percent of samples with detections,
- percent of public water systems with detections,
- median concentration of detections,
- mean concentration of detections, and
- maximum concentration of detections.

The median, mean, and maximum concentration values are based on analytical detections only. Non-detections were not included in these concentration measure calculations. In both the data

sets for finished and ambient water (Section 3.2), some chemicals had no detections at any of the sites surveyed. Some data sets included mean, median, and maximum values whereas others included only one or two of the data elements.

For screening purposes, EPA determined that the concentration data were the most appropriate data elements because they have a more direct relationship with dose-response than the detection frequency. The concentration data ranged from <0.1 µg/L to >10,000 µg/L. The range was subdivided using powers of ten. Some chemicals had finished water data available from multiple sources; in those cases, the highest value was used for the purposes of screening.

Using the toxicity categories EPA arrayed 107 chemicals with finished water data based on their toxicity data elements and their median concentration in finished water as shown in Exhibit 9. This Exhibit illustrates the distribution of chemicals across the categories. EPA developed additional analyses that focused on the specific chemicals within the different occurrence categories to set the screening criteria.

### Exhibit 9: Number of Chemicals with Median Concentrations Distributed through the Screening Framework by Health Effects Category

Health Effects Categories	Occurrence - Finished Water - Median (µg/L)							Totals
	0- <0.1	0.1- <1	1- <10	10- <100	100- <1,000	1K- <10K	≥10K	
Toxicity Category 1	1	7	22	0	4	1	0	35
Toxicity Category 2	0	5	15	8	0	0	0	28
Toxicity Category 3	0	8	16	3	0	0	1	28
Toxicity Category 4	0	4	6	0	1	0	1	12
Toxicity Category 5	0	1	2	1	0	0	0	4
<b>Total</b>	1	25	61	12	5	1	2	107

Exhibit 9 shows that about 82% (87 of 107) of the chemicals with finished water data have median concentrations less than 10 µg/L, a concentration that is not of high concern for Toxicity Category 3 to Toxicity Category 5 chemicals. This grouping would have a maximum drinking water equivalent level (DWEL) of ≥ 40 µg/L based on an RfD of 0.001 (see Section 4.1 for additional information). However, these same concentrations for finished water are of greater concern for chemicals with Toxicity Category 1 and Toxicity Category 2 RfDs. These types of analyses helped EPA evaluate the effectiveness of the screening framework as a tool to separate chemicals of high concern from those of low concern, especially for chemicals with finished water data.

### **3.2 Ambient Water Data**

EPA obtained data on ambient water values from the United States Geological Survey (USGS) National Water Quality Assessment Program (NAWQA), the USGS National Reconnaissance of Emerging Contaminants (NREC), and the PPMP. The NAWQA data include all the nationwide data from Cycle 1 of NAWQA, which encompasses data collected from 1992 to 2001. The NREC's database includes occurrence data collected by the USGS Toxic Substances Hydrology Program from 1999 to 2001 in samples from 142 streams, 55 wells, and seven effluent samples from 36 states. The PPMP data includes pesticide concentrations in water, and the sampling methods include 178 different pesticides and degradation products.

The ambient water data elements analyzed include:

- percent of samples with detections,
- percent of sites with detections,
- median concentration of detections,
- mean concentration of detections, and
- maximum concentration of detections.

As was the case for finished water, the median, mean, and maximum values are based on analytical detections only. Non-detections were not included in the concentration datasets. The subdivisions for the data were developed by first determining the range of available ambient water concentration data, and then partitioning the range by powers of ten. In this case, the concentration data ranged from <0.01 µg/L (for all concentration data) to >10,000 µg/L. One of the data sources, NREC, did not contain mean or maximum concentration data, so it was only represented in the percent of samples, percent of sites, and median concentrations. EPA developed matrices similar to Exhibit 9 for all of the ambient water data elements using the set of 200 diagnostic chemicals.

### **3.3 Environmental Release Data**

The environmental release data are those reported for 2002 from the Toxics Release Inventory (TRI) and the National Pesticide Use Database, as created by the National Center for Food and Agricultural Policy (NCFAP). The most recent version of the NCFAP database was released in 2000, and reflects pesticide use in 1997.

The environmental release data elements considered include:

- total releases to the environment (lbs/yr)
- number of states with total releases
- pesticide application (lbs/yr)
- number of states with pesticide application

As was the case for the finished and ambient water data, EPA chose to use the data on the pounds per year released to the environment for screening rather than the number of states with releases. The subdivisions used for release data were developed by first determining the range of

release values represented by the data, and then partitioning the range based on powers of ten. In this case, the release data ranged from less than 10 pounds per year to greater than 10 million pounds per year. EPA developed matrices similar to Exhibit 9 for all of the environmental release data elements.

### **3.4 Production Data**

The data used to assess production volume are the Toxic Substances Control Act chemical production volume ranges reported under the Chemical Update System/Inventory Update Rule (CUS/IUR). EPA used the most recent year of data available for each particular chemical. Every chemical on EPA's High Production Volume list is also in the CUS/IUR data source. Therefore, CUS/IUR is the primary source for production data.

CUS/IUR reports chemical production data as ranges rather than as exact values. Therefore, EPA chose to use those ranges as the subdivisions for the production occurrence data. The production data ranges from less than 10,000 lbs/yr to greater than 1 billion lbs/yr. EPA developed matrices similar to Exhibit 9 for all of the production data on the test set chemicals.

### **3.5 Disinfection Byproducts (DBPs) and Drinking Water Treatment Chemicals**

EPA recognized that two groupings of chemicals have water occurrence even in cases where quantitative data were not available: the DBPs from the DSS-Tox data source and the treatment chemicals from NSF Standard 60. In many cases there were finished water data or production data for some of these chemicals, but some of the chemicals lacked quantitative data. Among the Universe of chemicals that lacked the preferred data elements, both the DBPs and treatment chemicals have a strong potential to be present in drinking water. Accordingly, EPA is moving chemicals in these two categories forward to the PCCL for further evaluation, even when limited health effects or occurrence information are available.

### **3.6 Combining the Data Elements for Screening**

EPA selected the occurrence data elements for screening based upon their presence in the universe and their suitability as a screening tool. Analyses were performed to see if the occurrence could be correlated across the various data elements. The diagnostic chemicals were used for the correlation analysis since most had data for the following data elements: mean, median, or maximum concentrations in finished and/or ambient water, amount released to the environment, and production volume. The analyses with the diagnostic chemicals demonstrated a limited correlation across the data elements. A chemical with a high release to the environment did not necessarily occur in finished or ambient water at a high concentration or even have a high frequency of detections. As a result, EPA decided to apply the occurrence screening data elements in a hierarchical manner.

Chemicals known to occur in finished or ambient water occupy the highest position in the hierarchy and are most representative of a chemical's potential to occur in drinking water.

Environmental releases and production are less reflective of a chemical's potential to occur in drinking water. Accordingly, EPA selected the following hierarchy:

**Finished Water = Ambient Water > Environmental Release Data > Production Data.**

EPA also decided that when multiple values exist for the chemicals within a given component of the hierarchy, the most conservative would be used as the occurrence screening element. For example, in the case of a chemical that has finished water data and ambient water data, the highest available numerical concentration value would be selected as the occurrence screening data element.

## **4.0 Criteria for Selecting a PCCL**

The last step in the screening process was to use the intersections between health effects and occurrence data elements to establish the criteria for moving chemicals from the Universe to a PCCL. EPA grouped the Universe of chemicals that had values for health effects and occurrence data elements using the screening framework described in Section 1.0. Because the chemicals would be evaluated using a hierarchical approach for their occurrence elements, separate criteria were developed for each of the occurrence elements.

To test the criteria, EPA used the set of 200 diagnostic chemicals. As stated in Section 3.0, the set of diagnostic contaminants included some chemicals regulated through NPDWRs, some from past CCLs, and a few drawn from the Universe because they had fairly complete data for all of the occurrence data elements. The selected regulated chemicals represented the characteristics of chemicals that the screening process should move to the PCCL. Accordingly, the locations of these chemicals in the completed screening framework were used to assist in placing the barrier separating those chemical contaminants that would move to the PCCL from those that would not be further evaluated. The series of criteria are described in the following sections and summarized in Appendix 1.

### **4.1 Finished and Ambient Water Concentration Data**

As mentioned earlier, the finished and ambient water data are those most representative of contaminants likely to be found in drinking water. For this reason EPA scrutinized these data elements more closely than the other occurrence data elements. Initially, the placement of the bold black line on Exhibit 10 was positioned so that it would move the regulated chemicals and most of the past CCL chemicals to the PCCL. Past CCL contaminants that remained in the Universe and did not pass on to the PCCL (fell to the gray side of the black line) were ones proven to be poor candidates for regulation.

The second tool used to evaluate the position of the black line was the DWEL. The DWEL is calculated by multiplying the RfD in mg/kg/day by an adult body weight of 70 kg and dividing by a drinking water intake of 2 L/day (rounded to one significant figure). The RfD is a dose that is estimated to be without adverse effects for even sensitive populations. It includes a margin of safety in the form of a composite uncertainty factor. Most often, the uncertainty factor is a value of 100, 300, 1000 or 3000. For this exercise, the DWEL was derived from the lower RfD value



in each Toxicity Category (See Exhibit 4) and then positioned in the appropriate toxicity and occurrence cell of the framework.

Since all Toxicity Category 1 contaminants are moved to the PCCL, it is the DWELs for the Toxicity Category 2 to Toxicity Category 5 groupings that are of interest for this analysis. The calculated DWELs for the four toxicity categories of interest are as follows:

- Toxicity Category 2 – 4 µg/L
- Toxicity Category 3 – 40 µg/L
- Toxicity Category 4 – 2,000 µg/L
- Toxicity Category 5 – 4,000 µg/L

As shown in Exhibit 10 by the asterisk in the cells, three of the four DWELs fall in the drinking water concentration range of the first cell that moves to the PCCL. The DWEL for the Toxicity Category 4 grouping is one unit above the divider. This analysis combined with the positions of the chemicals in the occurrence test set of chemicals provided support for the position of the PCCL selection line for finished and ambient water.

### Exhibit 10: Criteria for Screening Health Effects and Water Categories

Screening Health Effects Categories	Occurrence – Finished Water – Concentration (µg/L)						
	0-<0.1	0.1-<1	1-<10	10-<100	100-<1,000	1K-<10K	≥10K
Toxicity Category 1							
Toxicity Category 2			*				
Toxicity Category 3				*			
Toxicity Category 4						*	
Toxicity Category 5						*	

#### 4.2 Environmental Release Data

EPA used total releases to the environment (TRI) and pesticide application rate data to develop the criteria for this category. To aid in setting the limits for the release category, EPA started with criteria used to develop the first CCL (CCL 1): that a chemical had to be released in quantities greater than 400,000 lbs/yr to surface waters. EPA found that this CCL 1 criterion was too stringent and only a few chemicals would have moved to the PCCL. Accordingly EPA used the positions of the test set chemicals to position the Universe to PCCL barrier. The criterion for moving a chemical with environmental release data to the PCCL is displayed in Exhibit 11. Chemicals with environmental releases above the non-shaded area move to the PCCL. Chemicals in the shaded area stay in the Universe.

### Exhibit 11: Criteria for Screening Health Effects and Environmental Release Categories

Screening Health Effects Categories	Occurrence – Environmental Release Category – Total Environmental Releases (lbs/year)							
	0 - <10	10 - <100	100 - <1K	1K - <10K	10K - <100K	100K <1M	1M - <10M	≥10M
Toxicity Category 1								
Toxicity Category 2								
Toxicity Category 3								
Toxicity Category 4								
Toxicity Category 5								

#### 4.3 Production Data

Similar to the release category, EPA started with the criteria used to develop CCL 1 that a chemical be produced in quantities greater than 1 billion lbs/yr. EPA decided that the CCL 1 guideline was too restrictive and proposed criteria that are less stringent for screening at this stage of the process. The criterion for moving a chemical, with production data, to the PCCL is displayed in Exhibit 12. Chemicals above the line move to the PCCL. Chemicals in the shaded areas remain in the CCL Universe.

### Exhibit 12: Criteria for Screening Health Effects and Production Categories

Screening Health Effects Categories	Occurrence - Production Category (lbs/year)								
	<10K	10K-500K	>500K-1M	>1M-10M	>10M-50M	>50M-100M	>100M-500M	>500M-1B	>1B
Toxicity Category 1									
Toxicity Category 2									
Toxicity Category 3									
Toxicity Category 4									
Toxicity Category 5									

#### **4.4 DBPS and Drinking Water Additives**

The DBPs and drinking water additives that lacked quantitative occurrence data but fell in the Toxicity Category 1 or Toxicity Category 2 groupings based on their toxicity were added to the PCCL because of their high probability for being present in disinfected and treated drinking water.

### **5.0 Efficacy of the Framework as a Screening Tool**

The proposed screening approach provides a data-driven, objective, and transparent process for selecting the PCCL from the Universe. Chemicals are screened based on their data elements and not based on their names or CAS numbers for the initial PCCL screen. All Toxicity Category 1 chemicals are captured no matter what the occurrence data element. The occurrence threshold required for the PCCL selection become less inclusive as the contaminant toxicity decreases. Once the initial screening is complete, the names of the PCCL chemicals are apparent. After the initial screen, quality assurance measures were applied. EPA then conducted a detailed examination of decisions that placed chemicals close to the borderline.

The screening approach on the CCL 3 Universe selected 561 chemical contaminants from the approximately 6,000 chemicals in the CCL 3 Universe that were screened. (This includes contaminant information that was compiled as part of EPA's nominations and surveillance process and submitted in the public comments on the draft CCL 3.) Appendix 2 shows the contaminants that moved to the PCCL for additional consideration and the data used in their screening.

## 6.0 References

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USEPA. 2009c. Summary of Nominations for the Third Contaminant Candidate List. EPA-815-R-09-011. August 2009.

## 7.0 Appendices

### **Appendix 1. Criteria for Selecting the PCCL**

Contains the series of criteria used to select the PCCL from the CCL Chemical Universe.  
This criterion is based upon the following hierarchy: Concentrations in Water > Releases to the Environment > Production

#### **Concentrations in Water**

- Toxicity Category 1 chemicals with any concentration
- Toxicity Category 2 chemicals with concentrations  $\geq 1 \mu\text{g/l}$
- Toxicity Category 3 chemicals with concentrations  $\geq 10 \mu\text{g/l}$
- Toxicity Category 4 chemicals with concentrations  $\geq 100 \mu\text{g/l}$
- Toxicity Category 5 chemicals with concentrations  $\geq 1000 \mu\text{g/l}$

#### **Releases to the Environment**

- Toxicity Category 1 chemicals with any amount released
- Toxicity Category 2 chemicals with releases/application  $\geq 10,000 \text{ lbs/yr}$
- Toxicity Category 3 chemicals with releases/application  $\geq 100,000 \text{ lbs/yr}$
- Toxicity Category 4 chemicals with releases/application  $\geq 1 \text{ M lbs/yr}$
- Toxicity Category 5 chemicals with releases/application  $\geq 10 \text{ M lbs/yr}$

#### **Production**

- Toxicity Category 1 chemicals with any amount produced
- Toxicity Category 2 chemicals production volumes  $> 500,000 \text{ lbs/yr}$
- Toxicity Category 3 chemicals with production volumes  $> 10 \text{ M lbs/yr}$
- Toxicity Category 4 chemicals with production volumes  $> 50 \text{ M lbs/yr}$
- Toxicity Category 5 chemicals with production volumes  $> 100 \text{ M lbs/yr}$

## ***Appendix 2. Chemicals Passing Screening to the PCCL***

The following table in Appendix 2 presents the CASRN, names of the contaminants listed on the PCCL, and the health effects and occurrence data elements that were used in their screening. The data elements are described in the text of this report.

For the Health Effects Data Element, Cancer Studies NTP, the Value is shown as the National Toxicology Program multi-species results (NTPMSR), representing the more detailed criteria and data used to derive the Toxicity Screening Category. They are described in detail in the text. For the Occurrence data elements, the Release data may be either national TRI data or pesticide application data. The notation “FW/AW” indicates the data are finished or ambient water data. Also noted, for some pesticide degradates, data from the parent compound were used for screening; for some contaminants supplemental data, compiled in the nominations and surveillance process were also used.

Further data and information for the contaminants are available on the Contaminant Information Sheets available in the CCL 3 water docket.

## Appendix 2

CASRN	Common Name	Health Effect/Toxicity Data Element Used For Screening			Toxicity Screening Category	Occurrence Data Element Used For Screening	
		Health Effect Data Element	Value	Units		Occurrence Data Element	Value
5989275	(d)-Limonene	Cancer Studies, NTP	NTPMSR		Toxicity Category 2	FW/AW-Median Value (ug/L)	1.0
100641	(Hydroxyimino)cyclohexane	Lowest Observed Adverse Effect Level (LOAEL)	17.9	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
630206	1,1,1,2-Tetrachloroethane	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	FW/AW-Max Value (ug/L)	18
918003	1,1,1-Trichloropropanone	Cancer Class	LM		Toxicity Category 3	FW/AW-Max Value (ug/L)	16.97
79345	1,1,2,2-Tetrachloroethane	Reference Dose (RfD)	0.00005	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	200
75343	1,1-Dichloroethane	Cancer Classification, EPA	C		Toxicity Category 3	FW/AW-Max Value (ug/L)	500
119642	1,2,3,4-Tetrahydronaphthalene	Lethal Dose 50 (LD50)	2,860	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
87616	1,2,3-Trichlorobenzene	Tolerable Daily Intake (TDI)	0.0015	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	15
96184	1,2,3-Trichloropropane	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	FW/AW-Max Value (ug/L)	3,000
95943	1,2,4,5-Tetrachlorobenzene	Reference Dose (RfD)	0.0003	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
95636	1,2,4-Trimethylbenzene	TD50	4,350	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	260
122667	1,2-Diphenylhydrazine	Risk Specific Dose (RSD)	0.00001	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	0
106876	1,2-Epoxy-4-(epoxyethyl)cyclohexane	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
106990	1,3-Butadiene	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	1,964,956
542927	1,3-Cyclopentadiene	Lethal Dose 50 (LD50)	113	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
77485	1,3-Dibromo-5,5-dimethylhydantoin	Lowest Observed Adverse Effect Level (LOAEL)	0.44	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>500K - 1M
542756	1,3-Dichloropropene	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	FW/AW-Max Value (ug/L)	39
99627	1,3-Diisopropylbenzene	Lowest Observed Adverse Effect Level (LOAEL)	0.25	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
99650	1,3-Dinitrobenzene	Reference Dose (RfD)	0.0001	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	528,962
105113	1,4-Benzoquinone dioxime	Cancer Studies, NTP	NTPMSR		Toxicity Category 2	Production Volume (lbs/year)	>500K - 1M
110634	1,4-Butanediol	No Observed Effect Level (NOEL)	200	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>500M - 1B
110656	1,4-Butynediol	Lowest Observed Adverse Effect Level (LOAEL)	2	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>100M - 500M
105088	1,4-Cyclohexanedimethanol	Lethal Dose 50 (LD50)	1,600	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
123911	1,4-Dioxane	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	821,067
4904614	1,5,9-Cyclododecatriene	Lethal Dose 50 (LD50)	1,780	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
2432997	11-Aminoundecanoic acid	Cancer Studies, NTP	NTPMSR		Toxicity Category 2	Production Volume (lbs/year)	>10M - 50M
57910	17alpha-estradiol	Acceptable Daily Intake (ADI)	0.00005	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	0.074
81492	1-Amino-2,4-dibromoanthraquinone	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
71363	1-Butanol	Lowest Observed Adverse Effect Level (LOAEL)	0.2	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	17,648,846
112301	1-Decanol	Lethal Dose 50 (LD50)	4,720	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
112538	1-Dodecanol	Lethal Dose 50 (LD50)	1,170	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
111706	1-Heptanol	Lowest Observed Adverse Effect Level (LOAEL)	0.0251	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>500K - 1M
592416	1-Hexene	Lowest Observed Adverse Effect Level (LOAEL)	1,000	mg/kg-day	Toxicity Category 5	Production Volume (lbs/year)	>500M - 1B
71410	1-Pentanol	Lethal Dose 50 (LD50)	200	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
71238	1-Propanol	Lowest Observed Adverse Effect Level (LOAEL)	600	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
2439352	2-(Dimethylamino)ethyl acrylate	No Observed Effect Level (NOEL)	4	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
96139	2,3-Dibromopropanol	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
95954	2,4,5-Trichlorophenol	No Observed Adverse Effect Level (NOAEL)	0.3	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	18,879
88062	2,4,6-Trichlorophenol	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	FW/AW-Max Value (ug/L)	0
105679	2,4-Dimethylphenol	Reference Dose (RfD)	0.02	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	168,992
51285	2,4-Dinitrophenol	Lowest Observed Adverse Effect Level (LOAEL)	0.0006	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	0.0
121142	2,4-Dinitrotoluene	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	FW/AW-Max Value (ug/L)	333
95807	2,4-Toluenediamine	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	11,834
95874	2,5-Xylenol	Lethal Dose 50 (LD50)	383	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
576261	2,6-Dimethylphenol	Reference Dose (RfD)	0.0006	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>100M - 500M
87627	2,6-Xylidine	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	5,256
96297	2-Butanone oxime	No Observed Effect Level (NOEL)	4	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
78897	2-Chloro-1-propanol	Lethal Dose 50 (LD50)	100	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>500M - 1B

## Appendix 2

CASRN	Common Name	Health Effect/Toxicity Data Element Used For Screening			Toxicity Screening Category	Occurrence Data Element Used For Screening	
		Health Effect Data Element	Value	Units		Occurrence Data Element	Value
645625	2-Ethyl-3-propylacrolein	Lethal Dose 50 (LD50)	3,000	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
123057	2-Ethylhexanal	Lethal Dose 50 (LD50)	2,600	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
149575	2-Ethylhexanoic acid	Lowest Observed Adverse Effect Level (LOAEL)	885	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
104767	2-Ethylhexanol	Lethal Dose 50 (LD50)	2,053	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>500M - 1B
26266682	2-Ethylhexenal	Lethal Dose 50 (LD50)	2,005	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
103117	2-Ethylhexyl acrylate	Lowest Observed Adverse Effect Level (LOAEL)	3	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>100M - 500M
7659861	2-Ethylhexyl thioglycolate	Lethal Dose 50 (LD50)	303	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
818611	2-Hydroxyethyl acrylate	Lethal Dose 50 (LD50)	300	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
149304	2-Mercaptobenzothiazole	TD50	344	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	644,590
109864	2-Methoxyethanol	Reference Dose (RfD)	0.001	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	153,774
78784	2-Methylbutane	Lowest Observed Adverse Effect Level (LOAEL)	357.1	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	> 1B
109068	2-Methylpyridine	Lowest Observed Adverse Effect Level (LOAEL)	0.0099	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	27,839
91598	2-Naphthalenamine	Cancer Classification, IARC	1		Toxicity Category 1	Release (lbs/yr)	5
135193	2-Naphthalenol	Lowest Observed Adverse Effect Level (LOAEL)	0.437	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
79469	2-Nitropropane	Cancer Classification, EPA	B2		Toxicity Category 2	Release (lbs/yr)	25,344
127060	2-Propanone oxime	TD50	12.1	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
107186	2-Propen-1-ol	Lowest Observed Adverse Effect Level (LOAEL)	0.05	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	604,872
616455	2-Pyrrolidone	Lethal Dose 50 (LD50)	328	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
1948330	2-tert-Butylhydroquinone	Maximum Recommended Daily Dose (MRDD)	0.2	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
91941	3,3'-Dichlorobenzidine	Risk Specific Dose (RSD)	0.00022	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	2
612828	3,3'-Dimethylbenzidine dihydrochloride	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
760236	3,4-Dichloro-1-butene	No Observed Effect Level (NOEL)	2	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>100M - 500M
3401807	3,6-Dichlorosalicylic acid	Lowest Observed Adverse Effect Level (LOAEL)	3	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
132059531	3-Bromo-4-(dibromomethyl)-5-hydroxy-2(5H)-furanone (BMX-3)	Cancer class only	HM		Toxicity Category 2	FW/AW-Max Value (ug/L)	0.04
563473	3-Chloro-2-methyl-1-propene	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	6,635
132059519	3-Chloro-4-(bromochloromethyl)-5-hydroxy-2(5H)-furanone (BMX-1)	Cancer class only	HM		Toxicity Category 2	FW/AW-Max Value (ug/L)	0.17
132059520	3-Chloro-4-(dibromomethyl)-5-hydroxy-2(5H)-furanone (BMX-2)	Cancer class only	HM		Toxicity Category 2	FW/AW-Max Value (ug/L)	0.03
16655826	3-Hydroxycarbofuran	Lethal Dose 50 (LD50)	7	mg/kg	Toxicity Category 2	FW/AW-Max Value (ug/L)	66.3
108996	3-Methylpyridine	Lethal Dose 50 (LD50)	400	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
100549	3-Pyridinecarbonitrile	No Observed Effect Level (NOEL)	5	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
553264	4,4'-Bipyridine	Lethal Dose 50 (LD50)	172	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
101804	4,4'-Diaminodiphenyl ether	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	985
80079	4,4'-Dichlorodiphenyl sulfone	Reference Dose (RfD)	0.005	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
101611	4,4'-Methylenebis(N,N-dimethyl)benzenamine	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
101688	4,4'-Methylenedi(phenyl isocyanate)	Lethal Dose 50 (LD50)	2,200	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
101779	4,4'-Methylenedianiline	Lowest Observed Adverse Effect Level (LOAEL)	4.3	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	168,919
92671	4-Aminobiphenyl	Cancer Classification, IARC	1		Toxicity Category 1	Release (lbs/yr)	1
101542	4-Aminodiphenylamine	Lowest Observed Adverse Effect Level (LOAEL)	150	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
95830	4-Chloro-1,2-diaminobenzene	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
5216251	4-Chlorobenzotrifluoride	Cancer Classification, EPA	B2		Toxicity Category 2	Production Volume (lbs/year)	>10M - 50M
123422	4-Hydroxy-4-methyl-2-pentanone	No Observed Effect Level (NOEL)	30	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
108112	4-Methyl-2-pentanol	Lethal Dose 50 (LD50)	2,600	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
6610293	4-Methyl-3-thiosemicarbazide	Lethal Dose 50 (LD50)	14	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M



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CASRN	Common Name	Health Effect/Toxicity Data Element Used For Screening			Toxicity Screening Category	Occurrence Data Element Used For Screening	
		Health Effect Data Element	Value	Units		Occurrence Data Element	Value
98533	4-tert-Butylcyclohexanone	Lethal Dose 50 (LD50)	5,000	mg/kg	Toxicity Category 5	Production Volume (lbs/year)	>500M - 1B
100403	4-Vinylcyclohexene	Cancer Studies, NTP	NTPMSR		Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
95794	5-Chloro-o-toluidine	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
16219753	5-Ethylidene-2-norbornene	No Observed Effect Level (NOEL)	4	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
99592	5-Nitro-o-anisidine	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
99558	5-Nitro-o-toluidine	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	255
71751412	Abamectin	Lethal Dose 50 (LD50)	2	mg/kg	Toxicity Category 2	Release (lbs/yr)	14,965
30560191	Acephate	Lowest Observed Effect Level (LOEL)	0.12	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	2,467,744
75070	Acetaldehyde	Cancer Classification, EPA	B2		Toxicity Category 2	Release (lbs/yr)	14,683,890
79027	Acetaldehyde, dichloro-Dichloroacetaldehyde	Cancer Class	M		Toxicity Category 3	FW/AW-Max Value (ug/L)	14
60355	Acetamide	TD50	180	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	1,202,667
103902	Acetaminophen	TD50	495	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	10
64197	Acetic acid	Lowest Observed Adverse Effect Level (LOAEL)	1.47	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	> 1B
108247	Acetic anhydride	Lethal Dose 50 (LD50)	1,780	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	> 1B
34256821	Acetochlor	Reference Dose (RfD)	0.02	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	30.4
187022113	Acetochlor ethanesulfonic acid (ESA)	Reference Dose (RfD)	Parent data	mg/kg-day	Toxicity Category 3	FW/AW	Parent
184992444	Acetochlor oxanilic acid (OA)	Reference Dose (RfD)	Parent data	mg/kg-day	Toxicity Category 3	FW/AW	Parent
67641	Acetone	No Observed Effect Level (NOEL)	100	mg/kg-day	Toxicity Category 4	FW/AW-Max Value (ug/L)	1,806
75865	Acetone cyanohydrin	Reference Dose (RfD)	0.0008	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	106,961
75058	Acetonitrile	Reference Dose (RfD)	0.006	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	12,784,367
107028	Acrolein	Reference Dose (RfD)	0.0005	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	3.4
79107	Acrylic acid	No Observed Adverse Effect Level (NOAEL)	53	mg/kg-day	Toxicity Category 4	Release (lbs/yr)	6,817,569
107131	Acrylonitrile	Risk Specific Dose (RSD)	0.000019	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	7,925,644
124049	Adipic acid	Lowest Observed Adverse Effect Level (LOAEL)	4,000	mg/kg-day	Toxicity Category 5	Production Volume (lbs/year)	> 1B
111693	Adiponitrile	Lethal Dose 50 (LD50)	22	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	> 1B
142363539	Alachlor ethanesulfonic acid (ESA)	Reference Dose (RfD)	Parent data	mg/kg-day	Toxicity Category 2	FW/AW	Parent
171262172	Alachlor oxanilic acid (OA)	Reference Dose (RfD)	Parent data	mg/kg-day	Toxicity Category 2	FW/AW	Parent
309002	Aldrin	Reference Dose (RfD)	0.00003	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	4.4
96242	alpha-Chlorohydrin	Lethal Dose 50 (LD50)	26	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
319846	alpha-Hexachlorocyclohexane	Risk Specific Dose (RSD)	0.000002	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	0.21
98851	alpha-Methylbenzenemethanol	TD50	458	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	> 1B
98839	alpha-Methylstyrene	Reference Dose (RfD)	0.07	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
834128	Ametryn	Reference Dose (RfD)	0.009	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	446,546
33089611	Amitraz	No Observed Effect Level (NOEL)	0.25	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	137,397
7664417	Ammonia	Lowest Observed Adverse Effect Level (LOAEL)	6.2	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	34,000
1111780	Ammonium carbamate	Lethal Dose 50 (LD50)	681	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	> 1B
7783188	Ammonium thiosulfate	Lethal Dose 50 (LD50)	1,098	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
64285069	Anatoxin-a	Reference Dose (RfD)	0.0005	mg/kg-day	Toxicity Category 2	FW/AW	Supplemental
62533	Aniline	Cancer Classification, EPA	B2		Toxicity Category 2	Release (lbs/yr)	937,263
142041	Aniline hydrochloride	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
100663	Anisole	Lowest Observed Adverse Effect Level (LOAEL)	0.65	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>500K - 1M
50782	Aspirin	Lowest Observed Adverse Effect Level (LOAEL)	0.0021	mg/kg-day	Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
492808	Auramine	Cancer Classification, IARC	1		Toxicity Category 1	Release (lbs/yr)	0
86500	Azinphos-methyl	Lowest Observed Adverse Effect Level (LOAEL)	0.91	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	3.37
741582	Bensulide	Lethal Dose 50 (LD50)	271	mg/kg	Toxicity Category 3	Release (lbs/yr)	546,600

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CASRN	Common Name	Health Effect/Toxicity Data Element Used For Screening			Toxicity Screening Category	Occurrence Data Element Used For Screening	
		Health Effect Data Element	Value	Units		Occurrence Data Element	Value
25057890	Bentazon	Reference Dose (RfD)	0.03	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	11.46
100527	Benzaldehyde	TD50	1,490	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
92875	Benzidine	Risk Specific Dose (RSD)	0.00000043	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	83
271896	Benzofuran	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
65850	Benzoic acid	No Observed Adverse Effect Level (NOAEL)	34	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
95147	Benzotriazole	Lowest Observed Adverse Effect Level (LOAEL)	0.60	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
98077	Benzotrithloride	Risk Specific Dose (RSD)	0.0000008	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	745
100516	Benzyl alcohol	Maximum Recommended Daily Dose (MRDD)	5	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
100447	Benzyl chloride	Risk Specific Dose (RSD)	0.00006	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	18,750
108601	Bis(2-chloro-1-methylethyl) ether	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	883
111444	Bis(2-chloroethyl) ether	Risk Specific Dose (RSD)	0.0000091	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	478
577117	Bis(2-ethylhexyl) sodium sulfosuccinate	Lowest Observed Adverse Effect Level (LOAEL)	0.45	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>10M - 50M
542881	Bis(chloromethyl) ether	Risk Specific Dose (RSD)	0.00000045	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	0
80057	Bisphenol A -- BPA	Lowest Observed Adverse Effect Level (LOAEL)	2.5	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	12
7440428	Boron	Minimal Risk Level (MRL)	0.01	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	3,950
314409	Bromacil	Cancer Classification, EPA	C		Toxicity Category 3	FW/AW-Max Value (ug/L)	57
7726956	Bromine	Lethal Dose 50 (LD50)	440	mg/kg	Toxicity Category 3	Release (lbs/yr)	381,257
108861	Bromobenzene	Reference Dose (RfD)	0.02	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	40
83463621	Bromochloroacetonitrile (BCAN)	Cancer class only	M		Toxicity Category 3	FW/AW-Max Value (ug/L)	13.4
74964	Bromoethane	Cancer Studies, NTP	NTPMSR		Toxicity Category 2	Production Volume (lbs/year)	>500K - 1M
109740	Butanenitrile	Lethal Dose 50 (LD50)	28	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>500K - 1M
85687	Butyl benzyl phthalate	Cancer Studies, NTP	NTPMSR		Toxicity Category 2	Production Volume (lbs/year)	>50M - 100M
25013165	Butylated hydroxyanisole	Lowest Observed Adverse Effect Level (LOAEL)	0.25	mg/kg-day	Toxicity Category 2	FW/AW-Median Value (ug/L)	1.2
107926	Butyric acid	Lethal Dose 50 (LD50)	2,000	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
106310	Butyric anhydride	Lethal Dose 50 (LD50)	8,790	mg/kg	Toxicity Category 5	Production Volume (lbs/year)	>100M - 500M
6459945	C.I. Acid Red 114, disodium salt	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
2429745	C.I. Direct Blue 15	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	>500K - 1M
28407376	C.I. Direct Blue 218	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	2,609
2832408	C.I. Disperse Yellow 3	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	0
5160021	C.I. Pigment Red 53, barium salt (2:1)	Cancer Studies, NTP	NTPMSR		Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
842079	C.I. Solvent Yellow 14	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
471341	Calcium carbonate	Lowest Observed Adverse Effect Level (LOAEL)	60,000	mg/kg-day	Toxicity Category 5	Production Volume (lbs/year)	>100M - 500M
1305620	Calcium hydroxide	Lethal Dose 50 (LD50)	7,300	mg/kg	Toxicity Category 5	Production Volume (lbs/year)	>100M - 500M
1592230	Calcium octadecanoate	Lethal Dose 50 (LD50)	10,000	mg/kg	Toxicity Category 5	Production Volume (lbs/year)	>100M - 500M
105602	Caprolactam	No Observed Adverse Effect Level (NOAEL)	50	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	> 1B
133062	Captan	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	4,001,523
63252	Carbaryl	Lowest Observed Adverse Effect Level (LOAEL)	0.23	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	33.5
10605217	Carbendazim	Lowest Observed Adverse Effect Level (LOAEL)	0.59	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
75150	Carbon disulfide	Minimal Risk Level (MRL)	0.01	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	34
120809	Catechol	TD50	84.7	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	35,911
75694	CFC-11	Lowest Observed Adverse Effect Level (LOAEL)	349	mg/kg-day	Toxicity Category 4	FW/AW-Max Value (ug/L)	1,444
75718	CFC-12	No Observed Adverse Effect Level (NOAEL)	15	mg/kg-day	Toxicity Category 4	FW/AW-Max Value (ug/L)	404.9
302170	Chloral hydrate	TD50	106	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	92.2
14866683	Chlorate	Cancer Studies, NTP	NTPMSR		Toxicity Category 2	FW/AW-Max Value (ug/L)	2,234

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CASRN	Common Name	Health Effect/Toxicity Data Element Used For Screening			Toxicity Screening Category	Occurrence Data Element Used For Screening	
		Health Effect Data Element	Value	Units		Occurrence Data Element	Value
115286	Chlorendic acid	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	0
54593838	Chlorethoxyfos	Lowest Observed Adverse Effect Level (LOAEL)	0.05	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	253,345
107200	Chloroacetaldehyde	TD50	36.1	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	2.4
79049	Chloroacetyl chloride	Lethal Dose 50 (LD50)	208	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>100M - 500M
510156	Chlorobenzilate	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	5
75003	Chloroethane	Cancer Studies, NTP	NTPMSR		Toxicity Category 2	FW/AW-Max Value (ug/L)	288.2
74873	Chloromethane (Methyl chloride)	Reference Dose (RfD)	0.004	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	550
107302	Chloromethyl methyl ether	Cancer Classification, EPA	A		Toxicity Category 1	Release (lbs/yr)	1,085
25167800	Chlorophenol	No Observed Adverse Effect Level (NOAEL)	0.3	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	43,439
76062	Chloropicrin	Lowest Observed Adverse Effect Level (LOAEL)	32	mg/kg-day	Toxicity Category 4	Release (lbs/yr)	13,912,578
126998	Chloroprene	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	925,010
1897456	Chlorothalonil	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	FW/AW-Max Value (ug/L)	0.71
104552	Cinnamaldehyde	Lowest Observed Adverse Effect Level (LOAEL)	0.21	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
77929	Citric acid	Maximum Recommended Daily Dose (MRDD)	100	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
110429624	Clethodim	Acceptable Daily Intake (ADI)	0.01	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	672,189
81777891	Clomazone	Lethal Dose 50 (LD50)	1,369	mg/kg	Toxicity Category 4	Release (lbs/yr)	2,536,701
7440484	Cobalt	Lowest Observed Adverse Effect Level (LOAEL)	0.04	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	684
	Cobalt compounds	Lethal Dose 50 (LD50)	150	mg/kg	Toxicity Category 3	Release (lbs/yr)	6,910,811
91645	Coumarin	TD50	13.9	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
1319773	Cresol	Lowest Observed Adverse Effect Level (LOAEL)	177	mg/kg-day	Toxicity Category 4	Release (lbs/yr)	1,475,929
15096523	Cryolite	Lowest Observed Adverse Effect Level (LOAEL)	23.1	mg/kg-day	Toxicity Category 4	Release (lbs/yr)	2,565,970
80159	Cumene hydroperoxide	Lethal Dose 50 (LD50)	382	mg/kg	Toxicity Category 3	Release (lbs/yr)	443,722
135206	Cupferron	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	0
13752517	Cure-Rite 18	TD50	90.8	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
21725462	Cyanazine	Lowest Observed Adverse Effect Level (LOAEL)	0.98	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	160
506774	Cyanogen chloride	Reference Dose (RfD)	0.05	mg/kg-day	Toxicity Category 4	FW/AW-Max Value (ug/L)	20.6
108805	Cyanuric acid	No Observed Effect Level (NOEL)	600	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
108770	Cyanuric chloride	Lethal Dose 50 (LD50)	350	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>100M - 500M
113136779	Cyclanilide	Lethal Dose 50 (LD50)	208	mg/kg	Toxicity Category 3	Release (lbs/yr)	177,474
110827	Cyclohexane	Lethal Dose 50 (LD50)	813	mg/kg	Toxicity Category 4	Release (lbs/yr)	4,761,999
108930	Cyclohexanol	Lethal Dose 50 (LD50)	1,400	mg/kg	Toxicity Category 4	Release (lbs/yr)	4,538,466
108941	Cyclohexanone	No Observed Adverse Effect Level (NOAEL)	462	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	> 1B
108918	Cyclohexylamine	Lethal Dose 50 (LD50)	11	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>10M - 50M
68359375	Cyfluthrin	Reference Dose (RfD)	0.025	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	178,171
143545908	Cylindrospermopsin	Reference Dose (RfD)	0.00003	mg/kg-day	Toxicity Category 1	FW/AW	Supplemental
52315078	Cypermethrin	Lethal Dose 50 (LD50)	24.6	mg/kg	Toxicity Category 2	Release (lbs/yr)	188,403
66215278	Cyromazine	No Observed Effect Level (NOEL)	0.75	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	14,328
1861321	Dacthal	Reference Dose (RfD)	0.01	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	100
	Dacthal mono/di-acid degradate	Reference Dose (RfD)	Parent data	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	190
1163195	Decabromodiphenyl ether	Reference Dose (RfD)	0.01	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	953,472
541026	Decamethylcyclopentasiloxane	Lethal Dose 50 (LD50)	24,134	mg/kg	Toxicity Category 5	Production Volume (lbs/year)	>100M - 500M
6190654	Desethylatrazine	Reference Dose (RfD)	Parent data	mg/kg-day	Toxicity Category 2	FW/AW	Parent
1007289	Desisopropylatrazine	Reference Dose (RfD)	Parent data	mg/kg-day	Toxicity Category 2	FW/AW	Parent
50997	D-Glucose	Maximum Recommended Daily Dose (MRDD)	100	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>500M - 1B

## Appendix 2

CASRN	Common Name	Health Effect/Toxicity Data Element Used For Screening			Toxicity Screening Category	Occurrence Data Element Used For Screening	
		Health Effect Data Element	Value	Units		Occurrence Data Element	Value
142223	Diallyl glycol carbonate	Lethal Dose 50 (LD50)	279	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
7398698	Diallyldimethylammonium chloride	Lowest Observed Adverse Effect Level (LOAEL)	1,000	mg/kg-day	Toxicity Category 5	Production Volume (lbs/year)	>100M - 500M
333415	Diazinon	Reference Dose (RfD)	0.00009	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	19
	Diazinon oxygen analog	Reference Dose (RfD)	Parent data	mg/kg-day	Toxicity Category 2	FW/AW	Parent
3252435	Dibromoacetone (DBAN)	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	FW/AW-Max Value (ug/L)	24
74953	Dibromomethane	Reference Dose (RfD)	0.01	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	21.1
683181	Dibutyltin dichloride	Lethal Dose 50 (LD50)	0.05	mg/kg	Toxicity Category 1	Production Volume (lbs/year)	>1M - 10M
818086	Dibutyltin oxide	Lowest Observed Adverse Effect Level (LOAEL)	0.17	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
99309	Dichloran	Acceptable Daily Intake (ADI)	0.01	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	189,096
3018120	Dichloroacetone (DCAN)	Cancer Class	LM		Toxicity Category 3	FW/AW-Max Value (ug/L)	24.6
594047	Dichloriodomethane	Cancer Class	M		Toxicity Category 3	FW/AW-Max Value (ug/L)	11
62737	Dichlorvos	Risk Specific Dose (RSD)	0.00003	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	264
115322	Dicofol	TD50	32.9	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	788,527
141662	Dicrotophos	Reference Dose (RfD)	0.0001	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	360,513
77736	Dicyclopentadiene	Reference Dose (RfD)	0.03	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	392,668
60571	Dieldrin	Reference Dose (RfD)	0.00005	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	5.6
111422	Diethanolamine	No Observed Adverse Effect Level (NOAEL)	20	mg/kg-day	Toxicity Category 4	Release (lbs/yr)	1,396,761
64675	Diethyl sulfate	Cancer Classification, IARC	2A		Toxicity Category 2	Release (lbs/yr)	10,644
25340174	Diethylbenzene	Lowest Observed Adverse Effect Level (LOAEL)	0.64	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>10M - 50M
111466	Diethylene glycol	TD50	1,660	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>500M - 1B
112345	Diethylene glycol monobutyl ether	Reference Dose (RfD)	0.01	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>100M - 500M
111400	Diethylenetriamine	Lowest Observed Adverse Effect Level (LOAEL)	10	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
68479981	Diethyltoluenediamine	Lethal Dose 50 (LD50)	472	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
43222486	Difenoquat methyl sulfate	Lethal Dose 50 (LD50)	206	mg/kg	Toxicity Category 3	Release (lbs/yr)	347,066
101906	Diglycidyl resorcinol ether	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	1
55290647	Dimethipin	Reference Dose (RfD)	0.02	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	283,076
60515	Dimethoate	Reference Dose (RfD)	0.0002	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	1,896,947
868859	Dimethyl hydrogen phosphite	Cancer Studies, NTP	NTPMSR		Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
112185	Dimethyl laurylamine	Lethal Dose 50 (LD50)	740	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
77781	Dimethyl sulfate	Cancer Classification, IARC	2A		Toxicity Category 2	Release (lbs/yr)	10,221
120616	Dimethyl terephthalate	Cancer Studies, NTP	NTPMSR		Toxicity Category 3	Production Volume (lbs/year)	> 1B
124403	Dimethylamine	Lowest Observed Adverse Effect Level (LOAEL)	0.347	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	618,880
75785	Dimethyldichlorosilane	Lethal Dose 50 (LD50)	800	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>500M - 1B
753731	Dimethyltin dichloride	Lethal Dose 50 (LD50)	73.9	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
25321146	Dinitrotoluene	Risk Specific Dose (RSD)	0.00001	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	6,802
122394	Diphenylamine	Lowest Observed Adverse Effect Level (LOAEL)	0.83	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	414,131
142847	Dipropylamine	Lowest Observed Adverse Effect Level (LOAEL)	5	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
25265718	Dipropylene glycol	Lethal Dose 50 (LD50)	14,850	mg/kg	Toxicity Category 5	Production Volume (lbs/year)	>100M - 500M
2764729	Diquat	Lethal Dose 50 (LD50)	30	mg/kg	Toxicity Category 2	Release (lbs/yr)	267,442
928723	Disodium iminodiacetate	Lethal Dose 50 (LD50)	8,070	mg/kg	Toxicity Category 5	Production Volume (lbs/year)	>500M - 1B
298044	Disulfoton	Reference Dose (RfD)	0.00004	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	3.81
330541	Diuron	No Observed Effect Level (NOEL)	0.63	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	23.3
27176870	Dodecylbenzenesulfonic acid	Lethal Dose 50 (LD50)	650	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
2439103	Dodine	Reference Dose (RfD)	0.004	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	151,870
115297	Endosulfan	No Observed Adverse Effect Level (NOAEL)	0.7	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	1,604,700

## Appendix 2

CASRN	Common Name	Health Effect/Toxicity Data Element Used For Screening			Toxicity Screening Category	Occurrence Data Element Used For Screening	
		Health Effect Data Element	Value	Units		Occurrence Data Element	Value
759944	EPTC	Reference Dose (RfD)	0.025	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	40
517099	equilenin	Acceptable Daily Intake (ADI)	0.00005	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	0.278
474862	equilin	Acceptable Daily Intake (ADI)	0.00005	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	0.147
114078	Erythromycin	Maximum Recommended Daily Dose (MRDD)	66.7	mg/kg-day	Toxicity Category 4	Supp	
66230044	Esfenvalerate	Lethal Dose 50 (LD50)	325	mg/kg	Toxicity Category 3	Release (lbs/yr)	229,386
50282	Estradiol (17-beta estradiol)	Acceptable Daily Intake (ADI)	0.00005	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	0.2
140670	Estragole	TD50	51.8	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
50271	Estrinol	Acceptable Daily Intake (ADI)	0.00005	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	0.051
53167	Estrone	Acceptable Daily Intake (ADI)	0.00005	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	0.12
64175	Ethanol	Lowest Observed Adverse Effect Level (LOAEL)	1.43	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	> 1B
16672870	Ethephon	Lowest Observed Effect Level (LOEL)	0.5	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	5,419,825
57636	Ethinyl Estradiol (17-alpha ethynyl estradiol)	Maximum Recommended Daily Dose (MRDD)	0.0005	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	0.831
563122	Ethion	Reference Dose (RfD)	0.0005	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	505,639
13194484	Ethoprop	Acceptable Daily Intake (ADI)	0.0004	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	1.95
141786	Ethyl acetate	Maximum Recommended Daily Dose (MRDD)	25	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
140885	Ethyl acrylate	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	152,024
75047	Ethylamine	Lethal Dose 50 (LD50)	400	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
107211	Ethylene glycol	Tolerable Daily Intake (TDI)	0.05	mg/kg-day	Toxicity Category 4	Release (lbs/yr)	10,076,483
111762	Ethylene glycol monobutyl ether	Lowest Observed Adverse Effect Level (LOAEL)	5.1	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>100M - 500M
75218	Ethylene oxide	Cancer Classification, IARC	1		Toxicity Category 1	Release (lbs/yr)	374,110
96457	Ethylene thiourea	Reference Dose (RfD)	0.00008	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	299
107153	Ethylenediamine	Reference Dose (RfD)	0.09	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
60004	Ethylenediaminetetraacetic acid	Lethal Dose 50 (LD50)	30	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>10M - 50M
22224926	Fenamiphos	Reference Dose (RfD)	0.00025	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	728,266
13356086	Fenbutatin oxide	Acceptable Daily Intake (ADI)	0.03	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	265,856
14484641	Ferbam	Acceptable Daily Intake (ADI)	0.003	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	317,819
2164172	Fluometuron	Reference Dose (RfD)	0.01	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	37.8
144490	Fluoroacetic acid	Lethal Dose 50 (LD50)	0.47	mg/kg	Toxicity Category 1	Production Volume (lbs/year)	>1M - 10M
72178020	Fomesafen	Risk Specific Dose (RSD)	0.00005	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	1,102,750
944229	Fonofos	No Observed Effect Level (NOEL)	0.2	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	1.2
50000	Formaldehyde	TD50	2.19	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	26,992,234
23422539	Formetanate hydrochloride	Lethal Dose 50 (LD50)	18	mg/kg	Toxicity Category 2	Release (lbs/yr)	134,821
64186	Formic acid	Lowest Observed Adverse Effect Level (LOAEL)	360	mg/kg-day	Toxicity Category 4	Release (lbs/yr)	10,144,003
110009	Furan	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	>10M - 50M
98011	Furfural	Cancer Studies, NTP	NTPMSR		Toxicity Category 2	Production Volume (lbs/year)	>10M - 50M
96480	gamma-Butyrolactone	Lowest Observed Adverse Effect Level (LOAEL)	160.7	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
7440564	Germanium	Lowest Observed Adverse Effect Level (LOAEL)	0.32	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	225.1
111308	Glutaraldehyde	Lowest Observed Adverse Effect Level (LOAEL)	0.3	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>10M - 50M
56815	Glycerine	Maximum Recommended Daily Dose (MRDD)	999	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
556525	Glycidol	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
107222	Glyoxal	Lethal Dose 50 (LD50)	200	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
74975	Halon 1011	Reference Dose (RfD)	0.01	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	210
75887	HCFC-133a	TD50	87.3	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	56,253
75456	HCFC-22	Lowest Observed Adverse Effect Level (LOAEL)	13.5	mg/kg-day	Toxicity Category 4	Release (lbs/yr)	7,075,769
142825	Heptane	Lowest Observed Adverse Effect Level (LOAEL)	2,857	mg/kg-day	Toxicity Category 5	Production Volume (lbs/year)	>100M - 500M

## Appendix 2

CASRN	Common Name	Health Effect/Toxicity Data Element Used For Screening			Toxicity Screening Category	Occurrence Data Element Used For Screening	
		Health Effect Data Element	Value	Units		Occurrence Data Element	Value
87683	Hexachlorobutadiene	Reference Dose (RfD)	0.0002	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	10
67721	Hexachloroethane	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	1,015
4719044	Hexahydro-1,3,5-tris(2-hydroxyethyl)-s-triazine	Lethal Dose 50 (LD50)	1.99	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>10M - 50M
111499	Hexahydroazepine	Lethal Dose 50 (LD50)	20.7	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
822060	Hexamethylene-1,6-diisocyanate	Lethal Dose 50 (LD50)	350	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>50M - 100M
124094	Hexamethylenediamine	Lethal Dose 50 (LD50)	750	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	> 1B
100970	Hexamethylenetetramine	Lethal Dose 50 (LD50)	569	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
110543	Hexane	Reference Dose (RfD)	0.06	mg/kg-day	Toxicity Category 4	Release (lbs/yr)	39,844,882
2691410	HMX	Lowest Observed Adverse Effect Level (LOAEL)	0.99	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>500K - 1M
302012	Hydrazine	Risk Specific Dose (RSD)	0.0000033	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	165,485
7647010	Hydrochloric acid	Lethal Dose 50 (LD50)	900	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	> 1B
6386385	Hydrocinnamic acid, 3,5-di-tert-butyl-4-hydroxy-, methyl ester	Lowest Observed Adverse Effect Level (LOAEL)	600	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
7783064	Hydrogen sulfide	Reference Dose (RfD)	0.003	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	> 1B
123319	Hydroquinone	TD50	82.8	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	574,933
868779	Hydroxyethyl methacrylate	Lowest Observed Adverse Effect Level (LOAEL)	2.50	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
13463406	Iron pentacarbonyl	Lethal Dose 50 (LD50)	12	mg/kg	Toxicity Category 2	Release (lbs/yr)	43,517
78831	Isobutanol	Lethal Dose 50 (LD50)	74.1	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>100M - 500M
115117	Isobutene	Cancer Studies, NTP	NTPMSR		Toxicity Category 3	Production Volume (lbs/year)	> 1B
110190	Isobutyl acetate	Lethal Dose 50 (LD50)	4,763	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
78820	Isobutyronitrile	Lethal Dose 50 (LD50)	25	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
29590429	Isooctyl acrylate	Lethal Dose 50 (LD50)	5,000	mg/kg	Toxicity Category 5	Production Volume (lbs/year)	>100M - 500M
121915	Isophthalic acid	Lethal Dose 50 (LD50)	10,400	mg/kg	Toxicity Category 5	Production Volume (lbs/year)	>100M - 500M
78795	Isoprene	Cancer Studies, NTP	NTPMSR		Toxicity Category 2	Production Volume (lbs/year)	>100M - 500M
67630	Isopropanol	Lowest Observed Adverse Effect Level (LOAEL)	18	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	> 1B
625558	Isopropyl formate	Lethal Dose 50 (LD50)	1.4	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
75310	Isopropylamine	Lethal Dose 50 (LD50)	111	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>100M - 500M
6846500	Kodaflex txib	No Observed Effect Level (NOEL)	30	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
77501634	Lactofen	Reference Dose (RfD)	0.002	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	390,240
78977	Lactonitrile	Lethal Dose 50 (LD50)	31	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>10M - 50M
91465086	lambda-Cyhalothrin	Lethal Dose 50 (LD50)	56	mg/kg	Toxicity Category 3	Release (lbs/yr)	321,987
1335326	Lead acetate	Cancer Classification, EPA	B		Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
330552	Linuron	Lowest Observed Effect Level (LOEL)	0.63	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	1.4
554132	Lithium carbonate	Lowest Observed Adverse Effect Level (LOAEL)	0.017	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	211,661
7447418	Lithium chloride	Lowest Observed Adverse Effect Level (LOAEL)	0.009	mg/kg-day	Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
121755	Malathion	No Observed Effect Level (NOEL)	0.23	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	9.58
108316	Maleic anhydride	Lethal Dose 50 (LD50)	390	mg/kg	Toxicity Category 3	Release (lbs/yr)	769,446
123331	Maleic hydrazide	Lowest Observed Effect Level (LOEL)	500	mg/kg-day	Toxicity Category 4	Release (lbs/yr)	2,147,846
109773	Malononitrile	Reference Dose (RfD)	0.0001	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	854,039
12427382	Maneb	Reference Dose (RfD)	0.005	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	3,046,585
94746	MCPA	Reference Dose (RfD)	0.0005	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	18.6
108394	m-Cresol	Cancer Classification, EPA	C		Toxicity Category 3	Release (lbs/yr)	374,903
541731	m-Dichlorobenzene	Minimal Risk Level (MRL)	0.03	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	22.4
108781	Melamine	Cancer Studies, NTP	NTPMSR		Toxicity Category 2	Production Volume (lbs/year)	>100M - 500M
24307264	Mepiquat chloride	Reference Dose (RfD)	0.03	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	182,976

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CASRN	Common Name	Health Effect/Toxicity Data Element Used For Screening			Toxicity Screening Category	Occurrence Data Element Used For Screening	
		Health Effect Data Element	Value	Units		Occurrence Data Element	Value
68111	Mercaptoacetic acid	Lethal Dose 50 (LD50)	114	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
150505	Merphos	Reference Dose (RfD)	0.00003	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	12
72333	Mestranol	Maximum Recommended Daily Dose (MRDD)	0.00083	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	0.407
79390	Methacrylamide	Lethal Dose 50 (LD50)	451	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>50M - 100M
79414	Methacrylic acid	Lowest Observed Adverse Effect Level (LOAEL)	5	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>100M - 500M
126987	Methacrylonitrile	Reference Dose (RfD)	0.0001	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	89,330
10265926	Methamidophos	Reference Dose (RfD)	0.00005	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	967,698
67561	Methanol	Lowest Observed Adverse Effect Level (LOAEL)	3.1	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	201,697,278
3268493	Methional	Lethal Dose 50 (LD50)	1.52	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>100M - 500M
16752775	Methomyl	Lowest Observed Adverse Effect Level (LOAEL)	0.1	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	3
59052	Methotrexate	Lowest Observed Adverse Effect Level (LOAEL)	0.00435	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	ND
79209	Methyl acetate	Lethal Dose 50 (LD50)	3,705	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	> 1B
96333	Methyl acrylate	Reference Dose (RfD)	0.03	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	206,487
74839	Methyl bromide (Bromomethane)	Reference Dose (RfD)	0.001	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	43
598550	Methyl carbamate	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	>1M - 10M
74931	Methyl mercaptan	Lethal Dose 50 (LD50)	61	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	> 1B
80626	Methyl methacrylate	Lowest Observed Adverse Effect Level (LOAEL)	0.36	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	3,657,567
1634044	Methyl tert-butyl ether	Tolerable Daily Intake (TDI)	0.01	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	23,000
74895	Methylamine	Lethal Dose 50 (LD50)	100	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>50M - 100M
12108133	Methylcyclopentadienyl manganese tricarbonyl	Lethal Dose 50 (LD50)	8	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
93152	Methyleugenol	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
4553622	Methylglutaronitrile	Lethal Dose 50 (LD50)	10	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>10M - 50M
75796	Methyltrichlorosilane	Lethal Dose 50 (LD50)	800	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
9006422	Metiram	Acceptable Daily Intake (ADI)	0.03	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	1,388,363
51218452	Metolachlor	Cancer Classification, EPA	C		Toxicity Category 3	FW/AW-Max Value (ug/L)	77.6
171118095	Metolachlor ethanesulfonic acid (ESA)	Reference Dose (RfD)	Parent data	mg/kg-day	Toxicity Category 3	FW/AW	Parent
152019733	Metolachlor oxanilic acid (OA)	Reference Dose (RfD)	Parent data	mg/kg-day	Toxicity Category 3	FW/AW	Parent
21087649	Metribuzin	Lowest Observed Adverse Effect Level (LOAEL)	0.62	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	6.61
101043372	Microcystin-LR	Reference Dose (RfD)	0.000003	mg/kg-day	Toxicity Category 1	FW/AW	Supplemental
2212671	Molinate	No Observed Effect Level (NOEL)	0.2	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	200
7439987	Molybdenum	Lowest Observed Adverse Effect Level (LOAEL)	0.14	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	4,733
1313275	Molybdenum trioxide	Cancer Studies, NTP	NTPMSR		Toxicity Category 3	Release (lbs/yr)	2,102,324
105555	N,N'-Diethylthiourea	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
127195	N,N-Dimethylacetamide	Maximum Recommended Daily Dose (MRDD)	0.58	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>10M - 50M
108010	N,N-Dimethylethanolamine	Maximum Recommended Daily Dose (MRDD)	15	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
300765	Naled	No Observed Effect Level (NOEL)	0.2	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	606,781
91203	Naphthalene	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	FW/AW-Max Value (ug/L)	906
123864	n-Butyl acetate	Lethal Dose 50 (LD50)	14,000	mg/kg	Toxicity Category 5	Production Volume (lbs/year)	>100M - 500M
97881	N-Butyl methacrylate	Lowest Observed Adverse Effect Level (LOAEL)	3.57	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
126307	Neopentyl glycol	No Observed Effect Level (NOEL)	100	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
7440020	Nickel	Cancer Classification, IARC	1		Toxicity Category 1	FW/AW-Max Value (ug/L)	666
	Nickel compounds	Cancer Classification, IARC	1		Toxicity Category 1	Release (lbs/yr)	34,676,669
7440031	Niobium	Cancer Classification, EPA	A		Toxicity Category 1	Production Volume (lbs/year)	>1M - 10M
139139	Nitrioltriacetic acid	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	30,679
98953	Nitrobenzene	Reference Dose (RfD)	0.0005	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	100

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CASRN	Common Name	Health Effect/Toxicity Data Element Used For Screening			Toxicity Screening Category	Occurrence Data Element Used For Screening	
		Health Effect Data Element	Value	Units		Occurrence Data Element	Value
1836755	Nitrofen	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	25,300
55630	Nitroglycerin	Lowest Observed Adverse Effect Level (LOAEL)	0.008	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	55,979
75525	Nitromethane	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	>10M - 50M
872504	N-Methyl-2-pyrrolidone	Lowest Observed Adverse Effect Level (LOAEL)	120	mg/kg-day	Toxicity Category 4	Release (lbs/yr)	6,311,503
924425	N-Methylolacrylamide	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	12,306
55185	N-Nitrosodiethylamine (NDEA)	Risk Specific Dose (RSD)	0.00000007	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	1,000
62759	N-nitrosodimethylamine (NDMA)	Reference Dose (RfD)	0.000008	mg/kg-day	Toxicity Category 1	FW/AW	DBP
924163	N-Nitroso-di-n-butylamine (NDBA)	Risk Specific Dose (RSD)	0.000002	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	5
621647	N-Nitroso-di-n-propylamine (NDPA)	Risk Specific Dose (RSD)	0.000001	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	506
86306	N-Nitrosodiphenylamine	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	14
10595956	N-Nitrosomethylethylamine (NMEA)	Risk Specific Dose (RSD)	0.0000004	mg/kg-day	Toxicity Category 1	FW/AW	DBP
684935	N-Nitroso-N-methylurea	TD50	0.093	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	5
930552	N-nitrosopyrrolidine (NPYR)	Risk Specific Dose (RSD)	0.000005	mg/kg-day	Toxicity Category 1	FW/AW	DBP
68224	Norethindrone (19-Norethisterone)	Maximum Recommended Daily Dose (MRDD)	0.0167	mg/kg-day	Toxicity Category 2	Fails screen	
27314132	Norflurazon	Reference Dose (RfD)	0.04	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	44.0
103651	n-Propylbenzene	Lowest Observed Adverse Effect Level (LOAEL)	2.5	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	47
88733	o-Chloronitrobenzene	Reference Dose (RfD)	0.001	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
95498	o-Chlorotoluene	Reference Dose (RfD)	0.02	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	52.4
556672	Octamethylcyclotetrasiloxane	Lethal Dose 50 (LD50)	1,540	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
20325400	o-Dianisidine dihydrochloride	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	46
528290	o-Dinitrobenzene	Reference Dose (RfD)	0.0001	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	105,280
88722	o-Nitrotoluene	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	>10M - 50M
95534	o-Toluidine	Cancer Classification, IARC	2A		Toxicity Category 2	Release (lbs/yr)	10,774
636215	o-Toluidine hydrochloride	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	22
19666309	Oxadiazon	No Observed Effect Level (NOEL)	0.5	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	28,822
75569	Oxirane, methyl-	Risk Specific Dose (RSD)	0.000042	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	433,536
301122	Oxydemeton-methyl	Lethal Dose 50 (LD50)	10	mg/kg	Toxicity Category 2	Release (lbs/yr)	154,565
42874033	Oxyfluorfen	No Observed Effect Level (NOEL)	0.3	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	706,799
10028156	Ozone	TD50	1.9	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	715,830
72559	p,p'-DDE	Risk Specific Dose (RSD)	0.000029	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	0.062
4685147	Paraquat	Lowest Observed Adverse Effect Level (LOAEL)	0.93	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	6,899,701
100005	p-Chloronitrobenzene	TD50	473	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
106434	p-Chlorotoluene	Reference Dose (RfD)	0.02	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	22.5
120718	p-Cresidine	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	0
100254	p-Dinitrobenzene	Reference Dose (RfD)	0.0001	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	28,711
32534819	Pentabromodiphenyl ethers	Reference Dose (RfD)	0.002	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
76017	Pentachloroethane	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	865
115775	Pentaerythritol	No Observed Effect Level (NOEL)	100	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
3296900	Pentaerythritol dibromide	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	>1M - 10M
110623	Pentanal	Lethal Dose 50 (LD50)	5.66	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>50M - 100M
14797730	Perchlorate	No Observed Effect Level (NOEL)	0.007	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	420
52645531	Permethrin	No Observed Effect Level (NOEL)	5	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	1,068,390
335671	Perfluorooctanoic acid (PFOA)	Lowest Observed Adverse Effect Level (LOAEL)	1.0	mg/kg-day	Toxicity Category 2	FW/AW	Supplemental
1763231	Perfluorooctane sulfonic acid (PFOS)	Lethal Dose 50 (LD50)	251.0	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	10K - 500K
77098	Phenolphthalein	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
101848	Phenyl ether	Lethal Dose 50 (LD50)	2,450	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M



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CASRN	Common Name	Health Effect/Toxicity Data Element Used For Screening			Toxicity Screening Category	Occurrence Data Element Used For Screening	
		Health Effect Data Element	Value	Units		Occurrence Data Element	Value
62384	Phenylmercury acetate	Reference Dose (RfD)	0.00008	mg/kg-day	Toxicity Category 1	Production Volume (lbs/year)	>1M - 10M
57410	Phenytoin	TD50	59.1	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	15,981
732116	Phosmet	Lethal Dose 50 (LD50)	26	mg/kg	Toxicity Category 2	Release (lbs/yr)	1,336,387
7723140	Phosphorus	Reference Dose (RfD)	0.00002	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	52,750
88993	Phthalic acid	Lowest Observed Adverse Effect Level (LOAEL)	0.56	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
110894	Piperidine	Lethal Dose 50 (LD50)	22.4	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
156105	p-Nitrosodiphenylamine	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	0
99990	p-Nitrotoluene	Reference Dose (RfD)	0.01	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
26062793	Poly(dimethyl diallyl ammonium chloride)	Lowest Observed Adverse Effect Level (LOAEL)	290	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
7440097	Potassium	Lowest Observed Adverse Effect Level (LOAEL)	0.94	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	23,955
156434	p-Phenetidine	Lowest Observed Adverse Effect Level (LOAEL)	0.24	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
41198087	Profenofos	Lowest Observed Adverse Effect Level (LOAEL)	0.05	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	881,702
1610180	Prometon	Reference Dose (RfD)	0.015	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	40
107120	Propanenitrile	Lethal Dose 50 (LD50)	35.8	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>10M - 50M
2312358	Propargite	Reference Dose (RfD)	0.02	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	20
107197	Propargyl alcohol	Lethal Dose 50 (LD50)	20	mg/kg	Toxicity Category 2	Release (lbs/yr)	64,096
123386	Propionaldehyde	Cancer Classification, DSSTOX	LM		Toxicity Category 3	Release (lbs/yr)	699,803
79094	Propionic acid	Lethal Dose 50 (LD50)	1,640	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
1639607	Propoxyphene hydrochloride	Lowest Observed Adverse Effect Level (LOAEL)	0.0013	mg/kg-day	Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
57556	Propylene glycol	Lowest Observed Adverse Effect Level (LOAEL)	5	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	> 1B
107982	Propylene glycol 1-methyl ether	Reference Dose (RfD)	0.7	mg/kg-day	Toxicity Category 5	Production Volume (lbs/year)	>100M - 500M
108656	Propylene glycol monomethyl ether acetate	No Observed Effect Level (NOEL)	300	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
57018527	Propylene glycol mono-t-butyl ether	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	>1M - 10M
1698608	Pyrazon	Lethal Dose 50 (LD50)	493	mg/kg	Toxicity Category 3	Release (lbs/yr)	118,553
110861	Pyridine	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	1,302,842
2176627	Pyridine, pentachloro-	Lethal Dose 50 (LD50)	435	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
14808607	Quartz (SiO2)	Cancer Classification, IARC	1		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
91225	Quinoline	Risk Specific Dose (RSD)	0.0000033	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	28,629
76578126	Quizalofop	Reference Dose (RfD)	Surrogate data	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	341,564
121824	RDX (Hexahydro-1,3,5-trinitro-1,3,5-triazine)	Risk Specific Dose (RSD)	0.00009	mg/kg-day	Toxicity Category 1	Production Volume (lbs/year)	>1M - 10M
793248	Santoflex 13	No Observed Effect Level (NOEL)	6	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>50M - 100M
135988	sec-Butylbenzene	Lowest Observed Adverse Effect Level (LOAEL)	4.42	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	22
74051802	Sethoxydim	No Observed Effect Level (NOEL)	8.9	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	1,721,030
7440213	Silicon	Lethal Dose 50 (LD50)	3,160	mg/kg	Toxicity Category 4	FW/AW-Max Value (ug/L)	98,916
7440235	Sodium	Lowest Observed Adverse Effect Level (LOAEL)	9.4	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	1,541,000
26628228	Sodium azide	Lowest Observed Adverse Effect Level (LOAEL)	0.25	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	66,425
532321	Sodium benzoate	Lethal Dose 50 (LD50)	1,600	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
7647156	Sodium bromide	Lowest Observed Adverse Effect Level (LOAEL)	0.13	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
7775099	Sodium chlorate	Lowest Observed Adverse Effect Level (LOAEL)	1.4	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	7,277,453
3926623	Sodium chloroacetate	Lethal Dose 50 (LD50)	95	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
128041	Sodium dimethyldithiocarbamate	Lethal Dose 50 (LD50)	300	mg/kg	Toxicity Category 3	Release (lbs/yr)	129,318
25155300	Sodium dodecylbenzenesulfonate	Lethal Dose 50 (LD50)	438	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>50M - 100M
62748	Sodium fluoroacetate	Reference Dose (RfD)	0.00002	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	0

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CASRN	Common Name	Health Effect/Toxicity Data Element Used For Screening			Toxicity Screening Category	Occurrence Data Element Used For Screening	
		Health Effect Data Element	Value	Units		Occurrence Data Element	Value
7681529	Sodium hypochlorite	Lowest Observed Adverse Effect Level (LOAEL)	2.2	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
137428	Sodium methylthiocarbamate	Lethal Dose 50 (LD50)	50	mg/kg	Toxicity Category 3	Release (lbs/yr)	60,154,489
1313822	Sodium sulfide	Lethal Dose 50 (LD50)	205	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>100M - 500M
13718268	Sodium vanadate	Lowest Observed Adverse Effect Level (LOAEL)	0.62	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
50704	Sorbitol	Maximum Recommended Daily Dose (MRDD)	833	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
131929607	Spinosyn A	Acceptable Daily Intake (ADI)	0.02	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	117,572
57114	Stearic acid	Lowest Observed Adverse Effect Level (LOAEL)	1,490.5	mg/kg-day	Toxicity Category 5	Production Volume (lbs/year)	>100M - 500M
7440246	Strontium	No Observed Adverse Effect Level (NOAEL)	190	mg/kg-day	Toxicity Category 4	FW/AW-Max Value (ug/L)	43,550
7782992	Sulfurous acid	Lowest Observed Adverse Effect Level (LOAEL)	0.5	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
2699798	Sulfuryl fluoride	Lethal Dose 50 (LD50)	100	mg/kg	Toxicity Category 3	Release (lbs/yr)	142,720
35400432	Sulprofos	Lowest Observed Adverse Effect Level (LOAEL)	0.6	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	308,713
1934210	Tartrazine	Lowest Observed Adverse Effect Level (LOAEL)	0.014	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
107534963	Tebuconazole	Acceptable Daily Intake (ADI)	0.03	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	479,616
112410238	Tebufenozide	Acceptable Daily Intake (ADI)	0.02	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	104,642
34014181	Tebuthiuron	No Observed Effect Level (NOEL)	7	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	17.3
13494809	Tellurium	Lethal Dose 50 (LD50)	20	mg/kg	Toxicity Category 2	FW/AW-Max Value (ug/L)	365.4
13071799	Terbufos	Reference Dose (RfD)	0.000025	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	0.56
56070167	Terbufos sulfone	Reference Dose (RfD)	Parent data	mg/kg-day	Toxicity Category 1	FW/AW	Surrogate
56070156	Terbufos-O-analogue sulfone	Reference Dose (RfD)	Parent data	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	0.016
100210	Terephthalic acid	Lowest Observed Adverse Effect Level (LOAEL)	142.5	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	> 1B
75650	tert-Butanol	TD50	64.6	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	1,548,617
75912	tert-Butyl hydroperoxide	Lethal Dose 50 (LD50)	320	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
75649	tert-Butylamine	Lethal Dose 50 (LD50)	44	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>10M - 50M
98066	tert-Butylbenzene	Lowest Observed Adverse Effect Level (LOAEL)	4.42	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	77.5
78002	Tetraethyl lead	Reference Dose (RfD)	0.0000001	mg/kg-day	Toxicity Category 1	Production Volume (lbs/year)	>1M - 10M
116143	Tetrafluoroethene	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	>50M - 100M
109999	Tetrahydrofuran	Cancer Studies, NTP	NTPMSR		Toxicity Category 2	FW/AW-Max Value (ug/L)	1,430
75570	Tetramethylammonium chloride	Lethal Dose 50 (LD50)	50	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
75592	Tetramethylammonium hydroxide	Lethal Dose 50 (LD50)	34	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>10M - 50M
64028	Tetrasodium EDTA	Lethal Dose 50 (LD50)	2,000	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
25265774	Texanol	Lethal Dose 50 (LD50)	3,200	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
79277671	Thifensulfuron	Reference Dose (RfD)	Surrogate data	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	105,375
2231574	Thiocarbazide	Lethal Dose 50 (LD50)	6	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
59669260	Thiodicarb	Acceptable Daily Intake (ADI)	0.03	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	823,065
23564058	Thiophanate-methyl	No Observed Effect Level (NOEL)	8	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	454,785
108985	Thiophenol	Reference Dose (RfD)	0.00001	mg/kg-day	Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
137268	Thiram	Reference Dose (RfD)	0.005	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	180,203
7440291	Thorium-232	Cancer Classification, EPA	A		Toxicity Category 1	FW/AW-Max Value (ug/L)	61.7
26471625	Toluene diisocyanate	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	129,143
66841256	Tralometrin	No Observed Effect Level (NOEL)	0.75	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	23,819
75967	Tribromoacetic Acid (TBAA)	Cancer Class	LM		Toxicity Category 3	FW/AW-Max Value (ug/L)	19
78488	Tribufos	Reference Dose (RfD)	0.00003	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	4,929,032
1461229	Tributyltin chloride	Lethal Dose 50 (LD50)	0.03	mg/kg	Toxicity Category 1	Production Volume (lbs/year)	>1M - 10M
545062	Trichloroacetonitrile	Cancer Class	LM		Toxicity Category 3	FW/AW-Max Value (ug/L)	41.54

## Appendix 2

CASRN	Common Name	Health Effect/Toxicity Data Element Used For Screening			Toxicity Screening Category	Occurrence Data Element Used For Screening	
		Health Effect Data Element	Value	Units		Occurrence Data Element	Value
102716	Triethanolamine	TD50	100	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>100M - 500M
121448	Triethylamine	Lowest Observed Adverse Effect Level (LOAEL)	1	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	1,167,219
112276	Triethylene glycol	Lowest Observed Adverse Effect Level (LOAEL)	3.6	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>100M - 500M
1582098	Trifluralin	No Observed Effect Level (NOEL)	0.75	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	1.74
552307	Trimellitic anhydride	Lethal Dose 50 (LD50)	1,900	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
512561	Trimethyl phosphate	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
75503	Trimethylamine	Lethal Dose 50 (LD50)	397	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>50M - 100M
77996	Trimethylolpropane	Acceptable Daily Intake (ADI)	0.05	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
118967	Trinitrotoluene	Reference Dose (RfD)	0.0005	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
101020	Triphenyl phosphite	Lethal Dose 50 (LD50)	444	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
76879	Triphenyltin hydroxide (TPTH)	Acceptable Daily Intake (ADI)	0.0005	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	662,418
126727	Tris(2,3-dibromopropyl) phosphate	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	500
140089	Tris(2-chloroethyl) phosphite	Lethal Dose 50 (LD50)	100	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
115968	Tris(chloroethyl)phosphate	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	FW/AW-Median Value (ug/L)	0.20
1120214	Undecane	No Observed Effect Level (NOEL)	100	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
57136	Urea	Lowest Observed Adverse Effect Level (LOAEL)	200	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	> 1B
51796	Urethane	TD50	16.9	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	96,050
7440622	Vanadium	Reference Dose (RfD)	0.007	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	70.4
1314621	Vanadium pentoxide	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	>1M - 10M
1929777	Vernolate	Reference Dose (RfD)	0.001	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	182,187
50471448	Vinclozolin	Reference Dose (RfD)	0.025	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	122,226
108054	Vinyl acetate	TD50	341	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	3,068,589
75025	Vinyl fluoride	Cancer Classification, IARC	2A		Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
25013154	Vinyltoluene	Reference Dose (RfD)	0.006	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
137304	Ziram	TD50	10.7	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	1,996,914