



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 ₅₀	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.

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 ₅₀	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

The United States Environmental Protection Agency (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 (CCLs). The steps involve:

- 1) Building a broad CCL Universe of potential drinking water contaminants for consideration;
- 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.
- 4) Providing opportunities for public comment and contaminant nomination.

This report focuses on the second step, in which the 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.

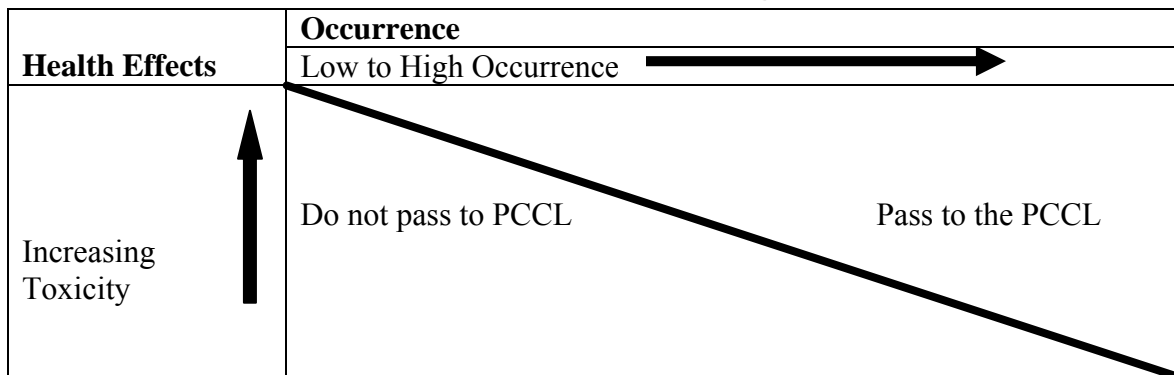
These data sources have yielded approximately 6,000 chemicals with which to populate the CCL Chemical Universe. Along with the names and identifying characteristics of these chemicals the Universe is the repository for the health-related and occurrence-related information. This information will be used 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, 2008a).

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 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 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 data considered. Appendix 2 shows the contaminants and the data EPA used that moved them to the PCCL for additional consideration.

2.0 Health Effects Data Elements

The toxicity information and health effects data extracted from the data sources are quite varied (USEPA, 2008a 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 (LD₅₀), 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 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 LD₅₀ 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, LD₅₀s, 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 LD₅₀ 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 LD₅₀s, are as follows:

- RfDs and RfD-eq: 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.
- TD₅₀s - 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 TD₅₀ 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.

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 TD₅₀ 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 TD₅₀ 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, LD₅₀) 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, LD₅₀s, MRDDs, TD₅₀s). 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 log₁₀ 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 ₅₀	LD ₅₀	
	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 LD₅₀ 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 log₁₀ 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 LD₅₀ values was treated differently from the RfD-eq, NOAEL, and LOAEL values because there has long been an accepted categorization of LD₅₀ 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 LD₅₀ 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 TD₅₀ 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 ₅₀
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 ₁	Probable human carcinogen
B ₂	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 DPB-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 TD₅₀ data. The TD₅₀ 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, EPA, 2008b) but not in screening at the Universe level.

Exhibit 7: Partitioning of Cancer Data Based on TD₅₀ Values and Weight of Evidence

	TD ₅₀	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 TD₅₀, “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	Group 1	TD ₅₀			
Hexane				LD₅₀	RfD-eq
Methylazoxy-methanol acetate			Group 2B		
Molybdenum oxide			NTP		
3-hydroxycarbofuran		LD₅₀			
Methylenediphenol			LOAEL	LD ₅₀	
BMX-1		DBP-CAN			
Primiphos methyl		NOAEL	RfD-eq LOAEL	LD ₅₀ 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 TD₅₀ places it in Toxicity Category 2. Hexane falls in Toxicity Category 4 based on its LD₅₀ 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 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).

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
Total	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 NRECs 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 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 it) were ones proven to be a 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 532 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.) 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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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 $\geq 500,000 \text{ lbs/yr}$
- Toxicity Category 3 chemicals with production volumes $\geq 10 \text{ M lbs/yr}$
- Toxicity Category 4 chemicals with production volumes $\geq 50 \text{ M lbs/yr}$
- Toxicity Category 5 chemicals with production volumes $\geq 100 \text{ M lbs/yr}$

Appendix 2. Chemicals Passing Screening to the PCCL

The following table in Appendix 2 presents the CASRN number, 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	Substance Name	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	Cyclohexene, 1-methyl-4-(1-methylethenyl)-, (4R)-	(d)-Limonene	Cancer Studies, NTP		NTPMSR	Toxicity Category 2	FW/AW-Median Value (ug/L)	1.0
100641	Cyclohexanone, oxime	(Hydroxyimino)cyclohexane	Lowest Observed Adverse Effect Level (LOAEL)	17.9	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
630206	Ethane, 1,1,1,2-tetrachloro-	1,1,1,2-Tetrachloroethane	Cancer Studies, NTP		NTPMSR	Toxicity Category 1	FW/AW-Max Value (ug/L)	18
79345	Ethane, 1,1,2,2-tetrachloro-	1,1,2,2-Tetrachloroethane	Reference Dose (RfD)	0.0005	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	200
75343	Ethane, 1,1-dichloro-	1,1-Dichloroethane	Cancer Classification, EPA		C	Toxicity Category 3	FW/AW-Max Value (ug/L)	500
119642	Naphthalene, 1,2,3,4-tetrahydro-	1,2,3,4-Tetrahydronaphthalene	Lethal Dose 50 (LD50)	2,860	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
87616	Benzene, 1,2,3-trichloro-	1,2,3-Trichlorobenzene	Tolerable Daily Intake (TDI)	0.0015	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	15
96184	Propane, 1,2,3-trichloro-	1,2,3-Trichloropropane	Cancer Studies, NTP		NTPMSR	Toxicity Category 1	FW/AW-Max Value (ug/L)	3,000
95943	Benzene, 1,2,4,5-tetrachloro-	1,2,4,5-Tetrachlorobenzene	Reference Dose (RfD)	0.0003	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
95636	Benzene, 1,2,4-trimethyl-	1,2,4-Trimethylbenzene	TD50	4,350	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	260
122667	Hydrazine, 1,2-diphenyl-	1,2-Diphenylhydrazine	Risk Specific Dose (RSD)	0.00001	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	0
106876	7-Oxabicyclo[4.1.0]heptane, 3-oxiranyl-	1,2-Epoxy-4-(epoxyethyl)cyclohexane	Cancer Studies, NTP		NTPMSR	Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
106990	1,3-Butadiene	1,3-Butadiene	Cancer Studies, NTP		NTPMSR	Toxicity Category 1	Release (lbs/yr)	1,964,956
542927	1,3-Cyclopentadiene	1,3-Cyclopentadiene	Lethal Dose 50 (LD50)	113	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
77485	2,4-Imidazolidinedione, 1,3-dibromo-5,5-dimethyl-	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-Propene, 1,3-dichloro-	1,3-Dichloropropene	Cancer Studies, NTP		NTPMSR	Toxicity Category 1	FW/AW-Max Value (ug/L)	39
99627	Benzene, 1,3-bis(1-methylethyl)-	1,3-Diisopropylbenzene	Lowest Observed Adverse Effect Level (LOAEL)	0.25	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
99650	Benzene, 1,3-dinitro-	1,3-Dinitrobenzene	Reference Dose (RfD)	0.0001	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	528,962
105113	2,5-Cyclohexadiene-1,4-dione, dioxime	1,4-Benzoquinone dioxime	Cancer Studies, NTP		NTPMSR	Toxicity Category 2	Production Volume (lbs/year)	>500K - 1M
110634	1,4-Butanediol	1,4-Butanediol	No Observed Effect Level (NOEL)	200	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>500M - 1B
110656	2-Butyne-1,4-diol	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	1,4-Cyclohexanedimethanol	Lethal Dose 50 (LD50)	1,600	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
123911	1,4-Dioxane	1,4-Dioxane	Cancer Studies, NTP		NTPMSR	Toxicity Category 1	Release (lbs/yr)	821,067
4904614	1,5,9-Cyclododecatriene	1,5,9-Cyclododecatriene	Lethal Dose 50 (LD50)	1,780	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
2432997	Undecanoic acid, 11-amino-	11-Aminoundecanoic acid	Cancer Studies, NTP		NTPMSR	Toxicity Category 2	Production Volume (lbs/year)	>10M - 50M
81492	9,10-Anthracenedione, 1-amino-2,4-dibromo-	1-Amino-2,4-dibromoanthraquinone	Cancer Studies, NTP		NTPMSR	Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
71363	1-Butanol	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	1-Decanol	Lethal Dose 50 (LD50)	4,720	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
112538	1-Dodecanol	1-Dodecanol	Lethal Dose 50 (LD50)	1,170	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
111706	1-Heptanol	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	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	1-Pentanol	Lethal Dose 50 (LD50)	200	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
71238	1-Propanol	1-Propanol	Lowest Observed Adverse Effect Level (LOAEL)	600	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
2439352	2-Propenoic acid, 2-(dimethylamino)ethyl ester	2-(Dimethylamino)ethyl acrylate	No Observed Effect Level (NOEL)	4	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
96139	1-Propanol, 2,3-dibromo-	2,3-Dibromopropanol	Cancer Studies, NTP		NTPMSR	Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
95954	Phenol, 2,4,5-trichloro-	2,4,5-Trichlorophenol	No Observed Adverse Effect Level (NOAEL)	0.3	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	18,879
88062	Phenol, 2,4,6-trichloro-	2,4,6-Trichlorophenol	Cancer Studies, NTP		NTPMSR	Toxicity Category 1	FW/AW-Max Value (ug/L)	0
105679	Phenol, 2,4-dimethyl-	2,4-Dimethylphenol	Reference Dose (RfD)	0.02	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	168,992
51285	Phenol, 2,4-dinitro-	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	Benzene, 1-methyl-2,4-dinitro-	2,4-Dinitrotoluene	Cancer Studies, NTP		NTPMSR	Toxicity Category 1	FW/AW-Max Value (ug/L)	333
95807	1,3-Benzenediamine, 4-methyl-	2,4-Toluenediamine	Cancer Studies, NTP		NTPMSR	Toxicity Category 1	Release (lbs/yr)	11,834
95874	Phenol, 2,5-dimethyl-	2,5-Xylenol	Lethal Dose 50 (LD50)	383	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
576261	Phenol, 2,6-dimethyl-	2,6-Dimethylphenol	Reference Dose (RfD)	0.0006	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>100M - 500M
87627	Benzenamine, 2,6-dimethyl-	2,6-Xylidine	Cancer Studies, NTP		NTPMSR	Toxicity Category 1	Release (lbs/yr)	5,256
96297	2-Butanone, oxime	2-Butanone oxime	No Observed Effect Level (NOEL)	4	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
78897	1-Propanol, 2-chloro-	2-Chloro-1-propanol	Lethal Dose 50 (LD50)	100	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>500M - 1B
645625	2-Hexenal, 2-ethyl-	2-Ethyl-3-propylacrolein	Lethal Dose 50 (LD50)	3,000	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
123057	Hexanal, 2-ethyl-	2-Ethylhexanal	Lethal Dose 50 (LD50)	2,600	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
149575	Hexanoic acid, 2-ethyl-	2-Ethylhexanoic acid	Lowest Observed Adverse Effect Level (LOAEL)	885	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
104767	1-Hexanol, 2-ethyl-	2-Ethylhexanol	Lethal Dose 50 (LD50)	2,053	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>500M - 1B
2626682	Hexenal, 2-ethyl-	2-Ethylhexenal	Lethal Dose 50 (LD50)	2,005	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
103117	2-Propenoic acid, 2-ethylhexyl ester	2-Ethylhexyl acrylate	Lowest Observed Adverse Effect Level (LOAEL)	3	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>100M - 500M
7659861	Acetic acid, mercapto-, 2-ethylhexyl ester	2-Ethylhexyl thioglycolate	Lethal Dose 50 (LD50)	303	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
818611	2-Propenoic acid, 2-hydroxyethyl ester	2-Hydroxyethyl acrylate	Lethal Dose 50 (LD50)	300	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M

Appendix 2

CASRN	Substance Name	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	
149304	2(3H)-Benzothiazolethione	2-Mercaptobenzothiazole	TD50		344	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	644,590
109864	Ethanol, 2-methoxy-	2-Methoxyethanol	Reference Dose (RfD)		0.001	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	153,774
78784	Butane, 2-methyl-	2-Methylbutane	Lowest Observed Adverse Effect Level (LOAEL)		357.1	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	> 1B
109068	Pyridine, 2-methyl-	2-Methylpyridine	Lowest Observed Adverse Effect Level (LOAEL)		0.0099	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	27,839
91598	2-Naphthalenamine	2-Naphthalenamine	Cancer Classification, IARC		1		Toxicity Category 1	Release (lbs/yr)	5
135193	2-Naphthalenol	2-Naphthalenol	Lowest Observed Adverse Effect Level (LOAEL)		0.437	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
79469	Propane, 2-nitro-	2-Nitropropane	Cancer Classification, EPA		B2		Toxicity Category 2	Release (lbs/yr)	25,344
127060	2-Propanone, oxime	2-Propanone oxime	TD50		12.1	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
107186	2-Propen-1-ol	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-Pyrrolidinone	2-Pyrrolidone	Lethal Dose 50 (LD50)		328	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
1948330	1,4-Benzenediol, 2-(1,1-dimethylethyl)-	2-tert-Butylhydroquinone	Maximum Recommended Daily Dose (MRDD)		0.2	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
91941	[1,1'-Biphenyl]-4,4'-diamine, 3,3'-dichloro-	3,3'-Dichlorobenzidine	Risk Specific Dose (RSD)		0.000022	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	2
612828	[1,1'-Biphenyl]-4,4'-diamine, 3,3'-dimethyl-, dihydrochloride	3,3'-Dimethylbenzidine dihydrochloride	Cancer Studies, NTP		NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
760236	1-Butene, 3,4-dichloro-	3,4-Dichloro-1-butene	No Observed Effect Level (NOEL)		2	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>100M - 500M
3401807	Benzoic acid, 3,6-dichloro-2-hydroxy-	3,6-Dichlorosalicylic acid	Lowest Observed Adverse Effect Level (LOAEL)		3	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
563473	1-Propene, 3-chloro-2-methyl-	3-Chloro-2-methyl-1-propene	Cancer Studies, NTP		NTPMSR		Toxicity Category 1	Release (lbs/yr)	6,635
16655826	3,7-Benzofurandiyl, 2,3-dihydro-2,2-dimethyl-, 7-(methylcarbamate)	3-Hydroxycarbofuran	Lethal Dose 50 (LD50)		7	mg/kg	Toxicity Category 2	FW/AW-Max Value (ug/L)	66.3
108996	Pyridine, 3-methyl-	3-Methylpyridine	Lethal Dose 50 (LD50)		400	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
100549	3-Pyridinecarbonitrile	3-Pyridinecarbonitrile	No Observed Effect Level (NOEL)		5	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
553264	4,4'-Bipyridine	4,4'-Bipyridine	Lethal Dose 50 (LD50)		172	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
101804	Benzenamine, 4,4'-oxybis-	4,4'-Diaminodiphenyl ether	Cancer Studies, NTP		NTPMSR		Toxicity Category 1	Release (lbs/yr)	985
80079	Benzene, 1,1'-sulfonylbis[4-chloro-	4,4'-Dichlorodiphenyl sulfone	Reference Dose (RfD)		0.005	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
101611	Benzenamine, 4,4'-methylenebis[N,N-dimethyl-	4,4'-Methylenebis(N,N-dimethyl)benzenamine	Cancer Studies, NTP		NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
101688	Benzene, 1,1'-methylenebis[4-isocyanato-	4,4'-Methylenedi(phenyl isocyanate)	Lethal Dose 50 (LD50)		2,200	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
101779	Benzenamine, 4,4'-methylenebis-	4,4'-Methylenedianiline	Lowest Observed Adverse Effect Level (LOAEL)		4.3	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	168,919
92671	[1,1'-Biphenyl]-4-amine	4-Aminobiphenyl	Cancer Classification, IARC		1		Toxicity Category 1	Release (lbs/yr)	1
101542	1,4-Benzenediamine, N-phenyl-	4-Aminodiphenylamine	Lowest Observed Adverse Effect Level (LOAEL)		150	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
95830	1,2-Benzenediamine, 4-chloro-	4-Chloro-1,2-diaminobenzene	Cancer Studies, NTP		NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
5216251	Benzene, 1-chloro-4-(trichloromethyl)-	4-Chlorobenzotrichloride	Cancer Classification, EPA		B2		Toxicity Category 2	Production Volume (lbs/year)	>10M - 50M
123422	2-Pentanone, 4-hydroxy-4-methyl-	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	2-Pentanol, 4-methyl-	4-Methyl-2-pentanol	Lethal Dose 50 (LD50)		2,600	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
6610293	Hydrazinecarbothioamide, N-methyl-	4-Methyl-3-thiosemicarbazide	Lethal Dose 50 (LD50)		14	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
98533	Cyclohexanone, 4-(1,1-dimethylethyl)-	4-tert-Butylcyclohexanone	Lethal Dose 50 (LD50)		5,000	mg/kg	Toxicity Category 5	Production Volume (lbs/year)	>500M - 1B
100403	Cyclohexene, 4-ethenyl-	4-Vinylcyclohexene	Cancer Studies, NTP		NTPMSR		Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
95794	Benzenamine, 5-chloro-2-methyl-	5-Chloro-o-toluidine	Cancer Studies, NTP		NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
16219753	Bicyclo[2.2.1]hept-2-ene, 5-ethylidene-	5-Ethylidene-2-norbornene	No Observed Effect Level (NOEL)		4	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
99592	Benzenamine, 2-methoxy-5-nitro-	5-Nitro-o-anisidine	Cancer Studies, NTP		NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
99558	Benzenamine, 2-methyl-5-nitro-	5-Nitro-o-toluidine	Cancer Studies, NTP		NTPMSR		Toxicity Category 1	Release (lbs/yr)	255
71751412	Avermectin B1	Abamectin	Lethal Dose 50 (LD50)		2	mg/kg	Toxicity Category 2	Release (lbs/yr)	14,965
30560191	Phosphoramidothioic acid, acetyl-, O,S-dimethyl ester	Acephate	Lowest Observed Effect Level (LOEL)		0.12	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	2,467,744
75070	Acetaldehyde	Acetaldehyde	Cancer Classification, EPA		B2		Toxicity Category 2	Release (lbs/yr)	14,683,890
60355	Acetamide	Acetamide	TD50		180	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	1,202,667
64197	Acetic acid	Acetic acid	Lowest Observed Adverse Effect Level (LOAEL)		1.47	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	> 1B
108247	Acetic acid, anhydride	Acetic anhydride	Lethal Dose 50 (LD50)		1,780	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	> 1B
34256821	Acetamide, 2-chloro-N-(ethoxymethyl)-N-(2-ethyl-6-methylphenyl)-	Acetochlor	Reference Dose (RfD)		0.02	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	30.4
187022113	Acetochlor ethanesulfonic acid	Acetochlor ethanesulfonic acid (ESA)	Reference Dose (RfD)		Parent data	mg/kg-day	Toxicity Category 3	FW/AW	Parent
184992444	Acetochlor oxanilic acid	Acetochlor oxanilic acid (OA)	Reference Dose (RfD)		Parent data	mg/kg-day	Toxicity Category 3	FW/AW	Parent
67641	2-Propanone	Acetone	No Observed Effect Level (NOEL)		100	mg/kg-day	Toxicity Category 4	FW/AW-Max Value (ug/L)	1,806
75865	Propanenitrile, 2-hydroxy-2-methyl-	Acetone cyanohydrin	Reference Dose (RfD)		0.0008	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	106,961
75058	Acetonitrile	Acetonitrile	Reference Dose (RfD)		0.006	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	12,784,367
107028	2-Propenal	Acrolein	Reference Dose (RfD)		0.0005	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	3.4
79107	2-Propenoic acid	Acrylic acid	No Observed Adverse Effect Level (NOAEL)		53	mg/kg-day	Toxicity Category 4	Release (lbs/yr)	6,817,569

Appendix 2

CASRN	Substance Name	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
107131	2-Propenenitrile	Acrylonitrile	Risk Specific Dose (RSD)	0.000019	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	7,925,644
124049	Hexanedioic acid	Adipic acid	Lowest Observed Adverse Effect Level (LOAEL)	4,000	mg/kg-day	Toxicity Category 5	Production Volume (lbs/year)	> 1B
111693	Hexanedinitrile	Adiponitrile	Lethal Dose 50 (LD50)	22	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	> 1B
142363539	Ethanesulfonic acid, 2-[(2,6-diethylphenyl)(methoxymethyl)amino]-2-oxo-	Alachlor ethanesulfonic acid (ESA)	Reference Dose (RfD)	Parent data	mg/kg-day	Toxicity Category 2	FW/AW	Parent
171262172	Alachlor oxanilic acid	Alachlor oxanilic acid (OA)	Reference Dose (RfD)	Parent data	mg/kg-day	Toxicity Category 2	FW/AW	Parent
309002	1,4:5,8-Dimethanonaphthalene, 1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-, (1.alpha.,4.alpha.,4a.beta.,5.alpha.,8.alpha.,8a.beta.)-	Aldrin	Reference Dose (RfD)	0.00003	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	4.4
96242	1,2-Propanediol, 3-chloro-	alpha-Chlorohydrin	Lethal Dose 50 (LD50)	26	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
319846	Cyclohexane, 1,2,3,4,5,6-hexachloro-, (1.alpha.,2.alpha.,3.beta.,4.alpha.,5.beta.,6.beta.)-	alpha-Hexachlorocyclohexane	Risk Specific Dose (RSD)	0.000002	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	0.21
98851	Benzenemethanol, .alpha.-methyl-	alpha-Methylbenzenemethanol	TD50	458	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	> 1B
98839	Benzene, (1-methylethenyl)-	alpha-Methylstyrene	Reference Dose (RfD)	0.07	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
834128	1,3,5-Triazine-2,4-diamine, N-ethyl-N'-(1-methylethyl)-6-(methylthio)-	Ametryn	Reference Dose (RfD)	0.009	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	446,546
33089611	Methanimidamide, N'-[(2,4-dimethylphenyl)-N-[[[(2,4-dimethylphenyl)imino]methyl]-N-methyl	Amitraz	No Observed Effect Level (NOEL)	0.25	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	137,397
7664417	Ammonia	Ammonia	Lowest Observed Adverse Effect Level (LOAEL)	6.2	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	34,000
1111780	Carbamic acid, monoammonium salt	Ammonium carbamate	Lethal Dose 50 (LD50)	681	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	> 1B
7783188	Thiosulfuric acid (H2S2O3), diammonium salt	Ammonium thiosulfate	Lethal Dose 50 (LD50)	1,098	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
62533	Benzenamine	Aniline	Cancer Classification, EPA	B2		Toxicity Category 2	Release (lbs/yr)	937,263
142041	Benzenamine, hydrochloride	Aniline hydrochloride	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
100663	Benzene, methoxy-	Anisole	Lowest Observed Adverse Effect Level (LOAEL)	0.65	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>500K - 1M
50782	Benzoic acid, 2-(acetyloxy)-	Aspirin	Lowest Observed Adverse Effect Level (LOAEL)	0.0021	mg/kg-day	Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
492808	Benzenamine, 4,4'-carbonimidoylbis[N,N-dimethyl-	Auramine	Cancer Classification, IARC	1		Toxicity Category 1	Release (lbs/yr)	0
86500	Phosphorodithioic acid, O,O-dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] ester	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	Phosphorodithioic acid, O,O-bis(1-methylethyl) S-[2-[(phenylsulfonyl)amino]ethyl] ester	Bensulide	Lethal Dose 50 (LD50)	271	mg/kg	Toxicity Category 3	Release (lbs/yr)	546,600
25057890	1H-2,1,3-Benzothiadiazin-4(3H)-one, 3-(1-methylethyl)-, 2,2-dioxide	Bentazon	Reference Dose (RfD)	0.03	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	11.46
100527	Benzaldehyde	Benzaldehyde	TD50	1,490	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
92875	[1,1'-Biphenyl]-4,4'-diamine	Benzidine	Risk Specific Dose (RSD)	0.00000043	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	83
271896	Benzofuran	Benzofuran	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
65850	Benzoic acid	Benzoic acid	No Observed Adverse Effect Level (NOAEL)	34	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
95147	1H-Benzotriazole	Benzotriazole	Lowest Observed Adverse Effect Level (LOAEL)	0.60	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
98077	Benzene, (trichloromethyl)-	Benzotrifluoride	Risk Specific Dose (RSD)	0.0000008	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	745
100516	Benzenemethanol	Benzyl alcohol	Maximum Recommended Daily Dose (MRDD)	5	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
100447	Benzene, (chloromethyl)-	Benzyl chloride	Risk Specific Dose (RSD)	0.00006	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	18,750
108601	Propane, 2,2'-oxybis[1-chloro-	Bis(2-chloro-1-methylethyl) ether	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	883
111444	Ethane, 1,1'-oxybis[2-chloro-	Bis(2-chloroethyl) ether	Risk Specific Dose (RSD)	0.0000091	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	478
577117	Butanedioic acid, sulfo-, 1,4-bis(2-ethylhexyl) ester, sodium salt	Bis(2-ethylhexyl) sodium sulfosuccinate ester, sodium salt	Lowest Observed Adverse Effect Level (LOAEL)	0.5	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>10M - 50M
542881	Methane, oxybis(chloro-	Bis(chloromethyl) ether	Risk Specific Dose (RSD)	0.000000045	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	0
7440428	Boron	Boron	Minimal Risk Level (MRL)	0.01	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	3,950
314409	2,4-(1H,3H)-Pyrimidinedione, 5-bromo-6-methyl-3-(1-methylpropyl)-	Bromacil	Cancer Classification, EPA	C		Toxicity Category 3	FW/AW-Max Value (ug/L)	57
7726956	Bromine	Bromine	Lethal Dose 50 (LD50)	440	mg/kg	Toxicity Category 3	Release (lbs/yr)	381,257
108861	Benzene, bromo-	Bromobenzene	Reference Dose (RfD)	0.02	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	40

Appendix 2

CASRN	Substance Name	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
74964	Ethane, bromo-	Bromoethane	Cancer Studies, NTP	NTPMSR		Toxicity Category 2	Production Volume (lbs/year)	>500K - 1M
109740	Butanenitrile	Butanenitrile	Lethal Dose 50 (LD50)	28	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>500K - 1M
85687	1,2-Benzenedicarboxylic acid, butyl phenylmethyl ester	Butyl benzyl phthalate	Cancer Studies, NTP	NTPMSR		Toxicity Category 2	Production Volume (lbs/year)	>50M - 100M
25013165	Phenol, (1,1-dimethylethyl)-4-methoxy-	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	Butanoic acid	Butyric acid	Lethal Dose 50 (LD50)	2,000	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
106310	Butanoic acid, anhydride	Butyric anhydride	Lethal Dose 50 (LD50)	8,790	mg/kg	Toxicity Category 5	Production Volume (lbs/year)	>100M - 500M
6459945	1,3-Naphthalenedisulfonic acid, 8-[[3,3'-dimethyl-4'-[[4-[[4-methylphenyl)sulfonyl]oxy]phenyl]azo][1,1'-biphenyl]-4-yl]azo]-7-hydroxy-, disodium salt	C.I. Acid Red 114, disodium salt	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
2429745	2,7-Naphthalenedisulfonic acid, 3,3'-[(3,3'-dimethoxy[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[5-amino-4-hydroxy-, tetrasodium salt	C.I. Direct Blue 15	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	>500K - 1M
28407376	Cuprate(4-), [mu.-[[3,3'-[[3,3'-di(hydroxy-.kappa.O)][1,1'-biphenyl]-4,4'-diyl]bis(azo-.kappa.N1)]bis[5-amino-4-(hydroxy-.kappa.O)-2,7-naphthalenedisulfonato]](8-)]di-, tetrasodium	C.I. Direct Blue 218	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	2,609
2832408	Acetamide, N-[4-[(2-hydroxy-5-methylphenyl)azo]phenyl]-	C.I. Disperse Yellow 3	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	0
5160021	Benzenesulfonic acid, 5-chloro-2-[(2-hydroxy-1-naphthalenyl)azo]-4-methyl-, barium salt (2:1)	C.I. Pigment Red 53, barium salt (2:1)	Cancer Studies, NTP	NTPMSR		Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
842079	2-Naphthalenol, 1-(phenylazo)-	C.I. Solvent Yellow 14	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
471341	Carbonic acid calcium salt (1:1)	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 (Ca(OH)2)	Calcium hydroxide	Lethal Dose 50 (LD50)	7,300	mg/kg	Toxicity Category 5	Production Volume (lbs/year)	>100M - 500M
1592230	Octadecanoic acid, calcium salt	Calcium octadecanoate	Lethal Dose 50 (LD50)	10,000	mg/kg	Toxicity Category 5	Production Volume (lbs/year)	>100M - 500M
105602	2H-Azepin-2-one, hexahydro-	Caprolactam	No Observed Adverse Effect Level (NOAEL)	50	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	> 1B
133062	1H-Isoidole-1,3(2H)-dione, 3a,4,7,7a-tetrahydro-2-[(trichloromethyl)thio]-	Captan	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	4,001,523
63252	1-Naphthalenol, methylcarbamate	Carbaryl	Lowest Observed Adverse Effect Level (LOAEL)	0.23	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	33.5
10605217	Carbamic acid, 1H-benzimidazol-2-yl-, methyl ester	Carbendazim	Lowest Observed Adverse Effect Level (LOAEL)	0.59	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
75150	Carbon disulfide	Carbon disulfide	Minimal Risk Level (MRL)	0.01	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	34
120809	1,2-Benzenediol	Catechol	TD50	84.7	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	35,911
75694	Methane, trichlorofluoro-	CFC-11	Lowest Observed Adverse Effect Level (LOAEL)	349	mg/kg-day	Toxicity Category 4	FW/AW-Max Value (ug/L)	1,444
75718	Methane, dichlorodifluoro-	CFC-12	No Observed Adverse Effect Level (NOAEL)	15	mg/kg-day	Toxicity Category 4	FW/AW-Max Value (ug/L)	404.9
115286	Bicyclo[2.2.1]hept-5-ene-2,3-dicarboxylic acid, 1,4,5,6,7,7-hexachloro-	Chlorendic acid	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	0
54593838	Phosphorothioic acid, O,O-diethyl O-(1,2,2,2-tetrachloroethyl) ester	Chlorethoxyfos	Lowest Observed Adverse Effect Level (LOAEL)	0.05	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	253,345
79049	Acetyl chloride, chloro-	Chloroacetyl chloride	Lethal Dose 50 (LD50)	208	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>100M - 500M
510156	Benzenecacetic acid, 4-chloro-.alpha.-(4-chlorophenyl)-.alpha.-hydroxy-, ethyl ester	Chlorobenzilate	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	5
75003	Ethane, chloro-	Chloroethane	Cancer Studies, NTP	NTPMSR		Toxicity Category 2	FW/AW-Max Value (ug/L)	288.2
74873	Methane, chloro-	Chloromethane (Methyl chloride)	Reference Dose (RfD)	0.004	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	550
107302	Methane, chloromethoxy-	Chloromethyl methyl ether	Cancer Classification, EPA	A		Toxicity Category 1	Release (lbs/yr)	1,085
25167800	Phenol, chloro-	Chlorophenol	No Observed Adverse Effect Level (NOAEL)	0.3	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	43,439
76062	Methane, trichloronitro-	Chloropicrin	Lowest Observed Adverse Effect Level (LOAEL)	32	mg/kg-day	Toxicity Category 4	Release (lbs/yr)	13,912,578
126998	1,3-Butadiene, 2-chloro-	Chloroprene	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	925,010
1897456	1,3-Benzenedicarbonitrile, 2,4,5,6-tetrachloro-	Chlorothalonil	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	FW/AW-Max Value (ug/L)	0.71
104552	2-Propenal, 3-phenyl-	Cinnamaldehyde	Lowest Observed Adverse Effect Level (LOAEL)	0.21	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M

Appendix 2

CASRN	Substance Name	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
77929	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	Citric acid	Maximum Recommended Daily Dose (MRDD)	100	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
110429624	Clethodim	Clethodim	Acceptable Daily Intake (ADI)	0.01	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	672,189
81777891	3-Isoxazolidinone, 2-[(2-chlorophenyl)methyl]-4,4-dimethyl-	Clomazone	Lethal Dose 50 (LD50)	1,369	mg/kg	Toxicity Category 4	Release (lbs/yr)	2,536,701
7440484	Cobalt	Cobalt	Lowest Observed Adverse Effect Level (LOAEL)	0.04	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	684
	Cobalt compounds	Cobalt compounds	Lethal Dose 50 (LD50)	150	mg/kg	Toxicity Category 3	Release (lbs/yr)	6,910,811
91645	2H-1-Benzopyran-2-one	Coumarin	TD50	13.9	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
1319773	Phenol, methyl-	Cresol	Lowest Observed Adverse Effect Level (LOAEL)	177	mg/kg-day	Toxicity Category 4	Release (lbs/yr)	1,475,929
15096523	Cryolite (Na3(AIF6))	Cryolite	Lowest Observed Adverse Effect Level (LOAEL)	23.1	mg/kg-day	Toxicity Category 4	Release (lbs/yr)	2,565,970
80159	Hydroperoxide, 1-methyl-1-phenylethyl	Cumene hydroperoxide	Lethal Dose 50 (LD50)	382	mg/kg	Toxicity Category 3	Release (lbs/yr)	443,722
135206	Benzenamine, N-hydroxy-N-nitroso-, ammonium salt	Cupferron	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	0
13752517	Morpholine, 4-[(4-morpholinylthio)thiomethyl]-	Cure-Rite 18	TD50	90.8	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
21725462	Propanenitrile, 2-[[4-chloro-6-(ethylamino)-1,3,5-triazin-2-yl]amino]-2-methyl-	Cyanazine	Lowest Observed Adverse Effect Level (LOAEL)	0.98	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	160
108805	1,3,5-Triazine-2,4,6-(1H,3H,5H)-trione	Cyanuric acid	No Observed Effect Level (NOEL)	600	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
108770	1,3,5-Triazine, 2,4,6-trichloro-	Cyanuric chloride	Lethal Dose 50 (LD50)	350	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>100M - 500M
113136779	Cyclopropanecarboxylic acid, 1-[[[2,4-dichlorophenyl]amino]carbonyl]-	Cyclanilide	Lethal Dose 50 (LD50)	208	mg/kg	Toxicity Category 3	Release (lbs/yr)	177,474
110827	Cyclohexane	Cyclohexane	Lethal Dose 50 (LD50)	813	mg/kg	Toxicity Category 4	Release (lbs/yr)	4,761,999
108930	Cyclohexanol	Cyclohexanol	Lethal Dose 50 (LD50)	1,400	mg/kg	Toxicity Category 4	Release (lbs/yr)	4,538,466
108941	Cyclohexanone	Cyclohexanone	No Observed Adverse Effect Level (NOAEL)	462	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	> 1B
108918	Cyclohexanamine	Cyclohexylamine	Lethal Dose 50 (LD50)	11	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>10M - 50M
68359375	Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, cyano(4-fluoro-3-phenoxyphenyl)methyl ester	Cyfluthrin	Reference Dose (RD)	0.025	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	178,171
52315078	Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester	Cypermethrin	Lethal Dose 50 (LD50)	24.6	mg/kg	Toxicity Category 2	Release (lbs/yr)	188,403
66215278	1,3,5-Triazine-2,4,6-triamine, N-cyclopropyl-	Cyromazine	No Observed Effect Level (NOEL)	0.75	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	14,328
1861321	1,4-Benzenedicarboxylic acid, 2,3,5,6-tetrachloro-, dimethyl ester	Dacthal	Reference Dose (RD)	0.01	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	100
	DCPA mono/di-acid degradate	Dacthal mono/di-acid degradate	Reference Dose (RD)	Parent data	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	190
1163195	Benzene, 1,1'-oxybis[2,3,4,5,6-pentabromo-	Decabromodiphenyl ether	Reference Dose (RD)	0.01	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	953,472
541026	Cyclopentasiloxane, decamethyl-	Decamethylcyclopentasiloxane	Lethal Dose 50 (LD50)	24,134	mg/kg	Toxicity Category 5	Production Volume (lbs/year)	>100M - 500M
6190654	1,3,5-Triazine-2,4-diamine, 6-chloro-N-(1-methylethyl)-	Desethylatrazine	Reference Dose (RD)	Parent data	mg/kg-day	Toxicity Category 2	FW/AW	Parent
1007289	1,3,5-Triazine-2,4-diamine, 6-chloro-N-ethyl-	Desisopropylatrazine	Reference Dose (RD)	Parent data	mg/kg-day	Toxicity Category 2	FW/AW	Parent
50997	D-Glucose	D-Glucose	Maximum Recommended Daily Dose (MRDD)	100	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>500M - 1B
142223	2,5,8,10-Tetraoxatridec-12-enoic acid, 9-oxo-, 2-propenyl ester	Diallyl glycol carbonate	Lethal Dose 50 (LD50)	279	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
7398698	2-Propen-1-aminium, N,N-dimethyl-N-2-propenyl-, chloride	Diallyldimethylammonium chloride	Lowest Observed Adverse Effect Level (LOAEL)	1,000	mg/kg-day	Toxicity Category 5	Production Volume (lbs/year)	>100M - 500M
333415	Phosphorothioic acid, O,O-diethyl O-[6-methyl-2-(1-methylethyl)-4-pyrimidinyl] ester	Diazinon	Reference Dose (RD)	0.00009	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	19
	Diazinon oxygen analog	Diazinon oxygen analog	Reference Dose (RD)	Parent data	mg/kg-day	Toxicity Category 2	FW/AW	Parent
74953	Methane, dibromo-	Dibromomethane	Reference Dose (RD)	0.01	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	21.1
683181	Stannane, dibutylidichloro-	Dibutyltin dichloride	Lethal Dose 50 (LD50)	0.05	mg/kg	Toxicity Category 1	Production Volume (lbs/year)	>1M - 10M
818086	Stannane, dibutylloxo-	Dibutyltin oxide	Lowest Observed Adverse Effect Level (LOAEL)	0.17	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
99309	Benzenamine, 2,6-dichloro-4-nitro-	Dichloran	Acceptable Daily Intake (ADI)	0.01	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	189,096

Appendix 2

CASRN	Substance Name	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
62737	Phosphoric acid, 2,2-dichloroethyl dimethyl ester	Dichlorvos	Risk Specific Dose (RSD)	0.00003 mg/kg-day	Toxicity Category 1	Release (lbs/yr)	264
115322	Benzenemethanol, 4-chloro-.alpha.-(4-chlorophenyl)-.alpha.-(trichloromethyl)-	Dicofol	TD50	32.9 mg/kg-day	Toxicity Category 2	Release (lbs/yr)	788,527
141662	Phosphoric acid, 3-(dimethylamino)-1-methyl-3-oxo-1-propenyl dimethyl ester, (E)-	Dicrotophos	Reference Dose (RfD)	0.0001 mg/kg-day	Toxicity Category 2	Release (lbs/yr)	360,513
77736	4,7-Methano-1H-indene, 3a,4,7,7a-tetrahydro-	Dicyclopentadiene	Reference Dose (RfD)	0.03 mg/kg-day	Toxicity Category 3	Release (lbs/yr)	392,668
60571	2,7:3,6-Dimethanonaphth(2,3-b)oxirene, 3,4,5,6,9,9-hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-, (1a.alpha.,2.beta.,2a.alpha.,3.beta.,6.beta.,6a.alpha.,7.beta.,7a.alpha.)-	Dieldrin	Reference Dose (RfD)	0.00005 mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	5.6
111422	Ethanol, 2,2'-iminobis-	Diethanolamine	No Observed Adverse Effect Level (NOAEL)	20 mg/kg-day	Toxicity Category 4	Release (lbs/yr)	1,396,761
64675	Sulfuric acid, diethyl ester	Diethyl sulfate	Cancer Classification, IARC	2A	Toxicity Category 2	Release (lbs/yr)	10,644
25340174	Benzene, diethyl-	Diethylbenzene	Lowest Observed Adverse Effect Level (LOAEL)	0.64 mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>10M - 50M
111466	Ethanol, 2,2'-oxybis-	Diethylene glycol	TD50	1,660 mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>500M - 1B
112345	Ethanol, 2-(2-butoxyethoxy)-	Diethylene glycol monobutyl ether	Reference Dose (RfD)	0.01 mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>100M - 500M
111400	1,2-Ethanediamine, N-(2-aminoethyl)-	Diethylenetriamine	Lowest Observed Adverse Effect Level (LOAEL)	10 mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
68479981	Benzenediamine, ar,ar-diethyl-ar-methyl-	Diethyltoluenediamine	Lethal Dose 50 (LD50)	472 mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
43222486	1H-Pyrazolium, 1,2-dimethyl-3,5-diphenyl-, methyl sulfate	Difenzoquat methyl sulfate	Lethal Dose 50 (LD50)	206 mg/kg	Toxicity Category 3	Release (lbs/yr)	347,066
101906	Oxirane, 2,2'-[1,3-phenylenebis(oxy)methylene]bis-	Diglycidyl resorcinol ether	Cancer Studies, NTP	NTPMSR	Toxicity Category 1	Release (lbs/yr)	1
55290647	1,4-Dithiin, 2,3-dihydro-5,6-dimethyl-, 1,1,4,4-tetraoxide	Dimethipin	Reference Dose (RfD)	0.02 mg/kg-day	Toxicity Category 3	Release (lbs/yr)	283,076
60515	Phosphorodithioic acid, O,O-dimethyl S-[2-(methylamino)-2-oxoethyl] ester	Dimethoate	Reference Dose (RfD)	0.0002 mg/kg-day	Toxicity Category 2	Release (lbs/yr)	1,896,947
868859	Phosphonic acid, dimethyl ester	Dimethyl hydrogen phosphite	Cancer Studies, NTP	NTPMSR	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
112185	1-Dodecanamine, N,N-dimethyl-	Dimethyl laurylamine	Lethal Dose 50 (LD50)	740 mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
77781	Sulfuric acid, dimethyl ester	Dimethyl sulfate	Cancer Classification, IARC	2A	Toxicity Category 2	Release (lbs/yr)	10,221
120616	1,4-Benzenedicarboxylic acid, dimethyl ester	Dimethyl terephthalate	Cancer Studies, NTP	NTPMSR	Toxicity Category 3	Production Volume (lbs/year)	> 1B
124403	Methanamine, N-methyl-	Dimethylamine	Lowest Observed Adverse Effect Level (LOAEL)	0.347 mg/kg-day	Toxicity Category 2	Release (lbs/yr)	618,880
75785	Silane, dichlorodimethyl-	Dimethyldichlorosilane	Lethal Dose 50 (LD50)	800 mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>500M - 1B
753731	Stannane, dichlorodimethyl-	Dimethyltin dichloride	Lethal Dose 50 (LD50)	73.9 mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
25321146	Benzene, methylidinitro-	Dinitrotoluene	Risk Specific Dose (RSD)	0.00001 mg/kg-day	Toxicity Category 1	Release (lbs/yr)	6,802
122394	Benzenamine, N-phenyl-	Diphenylamine	Lowest Observed Adverse Effect Level (LOAEL)	0.83 mg/kg-day	Toxicity Category 2	Release (lbs/yr)	414,131
142847	1-Propanamine, N-propyl-	Dipropylamine	Lowest Observed Adverse Effect Level (LOAEL)	5 mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
25265718	Propanol, oxybis-	Dipropylene glycol	Lethal Dose 50 (LD50)	14,850 mg/kg	Toxicity Category 5	Production Volume (lbs/year)	>100M - 500M
2764729	Dipyrido[1,2-a:2',1'-c]pyrazinedium, 6,7-dihydro-	Diquat	Lethal Dose 50 (LD50)	30 mg/kg	Toxicity Category 2	Release (lbs/yr)	267,442
928723	Glycine, N-(carboxymethyl)-, disodium salt	Disodium iminodiacetate	Lethal Dose 50 (LD50)	8,070 mg/kg	Toxicity Category 5	Production Volume (lbs/year)	>500M - 1B
298044	Phosphorodithioic acid, O,O-diethyl S-[2-(ethylthio)ethyl] ester	Disulfoton	Reference Dose (RfD)	0.00004 mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	3.81
330541	Urea, N-(3,4-dichlorophenyl)-N,N-dimethyl-	Diuron	No Observed Effect Level (NOEL)	0.63 mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	23.3
27176870	Benzenesulfonic acid, dodecyl-	Dodecylbenzenesulfonic acid	Lethal Dose 50 (LD50)	650 mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
2439103	Guanidine, dodecyl-, monoacetate	Dodine	Reference Dose (RfD)	0.004 mg/kg-day	Toxicity Category 3	Release (lbs/yr)	151,870
115297	6,9-Methano-2,4,3-benzodioxathiepin, 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3-oxide	Endosulfan	No Observed Adverse Effect Level (NOAEL)	0.7 mg/kg-day	Toxicity Category 2	Release (lbs/yr)	1,604,700
759944	Carbamothioic acid, dipropyl-, S-ethyl ester	EPTC	Reference Dose (RfD)	0.025 mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	40

Appendix 2

CASRN	Substance Name	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
66230044	Benzeneacetic acid, 4-chloro-.alpha.-(1-methylethyl)-, cyano(3-phenoxyphenyl)methyl ester, [S-(R*,R*)]-	Esfenvalerate	Lethal Dose 50 (LD50)	325	mg/kg	Toxicity Category 3	Release (lbs/yr)	229,386
140670	Benzene, 1-methoxy-4-(2-propenyl)-	Estragole	TD50	51.8	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
64175	Ethanol	Ethanol	Lowest Observed Adverse Effect Level (LOAEL)	1.43	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	> 1B
16672870	Phosphonic acid, (2-chloroethyl)-	Ethephon	Lowest Observed Adverse Effect Level (LOEL)	0.5	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	5,419,825
563122	Phosphorodithioic acid, S,S'-methylene O,O',O'-tetraethyl ester	Ethion	Reference Dose (RfD)	0.0005	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	505,639
13194484	Phosphorodithioic acid, O-ethyl S,S-dipropyl ester	Ethoprop	Acceptable Daily Intake (ADI)	0.0004	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	1.95
141786	Acetic acid ethyl ester	Ethyl acetate	Maximum Recommended Daily Dose (MRDD)	25	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
140885	2-Propenoic acid, ethyl ester	Ethyl acrylate	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	152,024
75047	Ethanamine	Ethylamine	Lethal Dose 50 (LD50)	400	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
107211	1,2-Ethanediol	Ethylene glycol	Tolerable Daily Intake (TDI)	0.05	mg/kg-day	Toxicity Category 4	Release (lbs/yr)	10,076,483
111762	Ethanol, 2-butoxy-	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	Oxirane	Ethylene oxide	Cancer Classification, IARC	1		Toxicity Category 1	Release (lbs/yr)	374,110
96457	2-Imidazolidinethione	Ethylene thiourea	Reference Dose (RfD)	0.00008	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	299
107153	1,2-Ethanediamine	Ethylenediamine	Reference Dose (RfD)	0.09	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
60004	Glycine, N,N'-1,2-ethanediybis[N-(carboxymethyl)-	Ethylenediaminetetraacetic acid	Lethal Dose 50 (LD50)	30	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>10M - 50M
22224926	Phosphoramidic acid, (1-methylethyl)-, ethyl 3-methyl-4-(methylthio)phenyl ester	Fenamiphos	Reference Dose (RfD)	0.00025	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	728,266
13356086	Distannoxane, hexakis(2-methyl-2-phenylpropyl)-	Fenbutatin oxide	Acceptable Daily Intake (ADI)	0.03	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	265,856
14484641	Iron, tris(dimethylcarbamodithioato-.kappa.S..kappa.S')-. (OC-6-11)-	Ferbam	Acceptable Daily Intake (ADI)	0.003	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	317,819
2164172	Urea, N,N-dimethyl-N'-[3-(trifluoromethyl)phenyl]-	Fluometuron	Reference Dose (RfD)	0.01	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	37.8
144490	Acetic acid, fluoro-	Fluoroacetic acid	Lethal Dose 50 (LD50)	0.47	mg/kg	Toxicity Category 1	Production Volume (lbs/year)	>1M - 10M
72178020	Benzamide, 5-[2-chloro-4-(trifluoromethyl)phenoxy]-N-(methylsulfonyl)-2-nitro-	Fomesafen	Risk Specific Dose (RSD)	0.00005	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	1,102,750
944229	Phosphonodithioic acid, ethyl-, O-ethyl S-phenyl ester	Fonofos	No Observed Effect Level (NOEL)	0.2	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	1.2
50000	Formaldehyde	Formaldehyde	TD50	2.19	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	26,992,234
23422539	Methanimidamide, N,N-dimethyl-N'-[3-[[[(methylamino)carbonyloxy]phenyl]-, monohydrochloride	Formetanate hydrochloride	Lethal Dose 50 (LD50)	18	mg/kg	Toxicity Category 2	Release (lbs/yr)	134,821
64186	Formic acid	Formic acid	Lowest Observed Adverse Effect Level (LOAEL)	360	mg/kg-day	Toxicity Category 4	Release (lbs/yr)	10,144,003
110009	Furan	Furan	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	>10M - 50M
98011	2-Furancarboxaldehyde	Furfural	Cancer Studies, NTP	NTPMSR		Toxicity Category 2	Production Volume (lbs/year)	>10M - 50M
96480	2(3H)-Furanone, dihydro-	gamma-Butyrolactone	Lowest Observed Adverse Effect Level (LOAEL)	160.7	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
7440564	Germanium	Germanium	Lowest Observed Adverse Effect Level (LOAEL)	0.32	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	225.1
111308	Pentanedial	Glutaraldehyde	Lowest Observed Adverse Effect Level (LOAEL)	0.3	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>10M - 50M
56815	1,2,3-Propanetriol	Glycerine	Maximum Recommended Daily Dose (MRDD)	999	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
556525	Oxiranemethanol	Glycidol	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
107222	Ethanedial	Glyoxal	Lethal Dose 50 (LD50)	200	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
74975	Methane, bromochloro-	Halon 1011	Reference Dose (RfD)	0.01	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	210
75887	Ethane, 2-chloro-1,1,1-trifluoro-	HCFC-133a	TD50	87.3	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	56,253
75456	Methane, chlorodifluoro-	HCFC-22	Lowest Observed Adverse Effect Level (LOAEL)	13.5	mg/kg-day	Toxicity Category 4	Release (lbs/yr)	7,075,769
142825	Heptane	Heptane	Lowest Observed Adverse Effect Level (LOAEL)	2,857	mg/kg-day	Toxicity Category 5	Production Volume (lbs/year)	>100M - 500M
87683	1,3-Butadiene, 1,1,2,3,4,4-hexachloro-	Hexachlorobutadiene	Reference Dose (RfD)	0.0002	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	10
67721	Ethane, hexachloro-	Hexachloroethane	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	1,015
4719044	1,3,5-Triazine-1,3,5(2H,4H,6H)-triethanol	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	1H-Azepine, hexahydro-	Hexahydroazepine	Lethal Dose 50 (LD50)	20.7	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
822060	Hexane, 1,6-diisocyanato-	Hexamethylene-1,6-diisocyanate	Lethal Dose 50 (LD50)	350	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>50M - 100M

Appendix 2

CASRN	Substance Name	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
124094	1,6-Hexanediamine	Hexamethylenediamine	Lethal Dose 50 (LD50)	750	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	> 1B
100970	1,3,5,7-Tetraazatricyclo[3.3.1.1 ^{3,7}]decane	Hexamethylenetetramine	Lethal Dose 50 (LD50)	569	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
110543	Hexane	Hexane	Reference Dose (RfD)	0.06	mg/kg-day	Toxicity Category 4	Release (lbs/yr)	39,844,882
2691410	1,3,5,7-Tetrazocine, octahydro-1,3,5,7-tetranitro-	HMX	Lowest Observed Adverse Effect Level (LOAEL)	0.99	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>500K - 1M
302012	Hydrazine	Hydrazine	Risk Specific Dose (RSD)	0.0000033	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	165,485
7647010	Hydrochloric acid	Hydrochloric acid	Lethal Dose 50 (LD50)	900	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	> 1B
6386385	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester	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 (H ₂ S)	Hydrogen sulfide	Reference Dose (RfD)	0.003	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	> 1B
123319	1,4-Benzenediol	Hydroquinone	TD50	82.8	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	574,933
868779	2-Propenoic acid, 2-methyl-, 2-hydroxyethyl ester	Hydroxyethyl methacrylate	Lowest Observed Adverse Effect Level (LOAEL)	2.50	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
13463406	Iron carbonyl (Fe(CO) ₅), (TB-5-11)-	Iron pentacarbonyl	Lethal Dose 50 (LD50)	12	mg/kg	Toxicity Category 2	Release (lbs/yr)	43,517
78831	1-Propanol, 2-methyl-	Isobutanol	Lethal Dose 50 (LD50)	74.1	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>100M - 500M
115117	1-Propene, 2-methyl-	Isobutene	Cancer Studies, NTP	NTPMSR		Toxicity Category 3	Production Volume (lbs/year)	> 1B
110190	Acetic acid, 2-methylpropyl ester	Isobutyl acetate	Lethal Dose 50 (LD50)	4,763	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
78820	Propanenitrile, 2-methyl-	Isobutyronitrile	Lethal Dose 50 (LD50)	25	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
29590429	2-Propenoic acid, isoctyl ester	Isocetyl acrylate	Lethal Dose 50 (LD50)	5,000	mg/kg	Toxicity Category 5	Production Volume (lbs/year)	>100M - 500M
121915	1,3-Benzenedicarboxylic acid	Isophthalic acid	Lethal Dose 50 (LD50)	10,400	mg/kg	Toxicity Category 5	Production Volume (lbs/year)	>100M - 500M
78795	1,3-Butadiene, 2-methyl-	Isoprene	Cancer Studies, NTP	NTPMSR		Toxicity Category 2	Production Volume (lbs/year)	>100M - 500M
67630	2-Propanol	Isopropanol	Lowest Observed Adverse Effect Level (LOAEL)	18	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	> 1B
625558	Formic acid, 1-methylethyl ester	Isopropyl formate	Lethal Dose 50 (LD50)	1.4	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
75310	2-Propanamine	Isopropylamine	Lethal Dose 50 (LD50)	111	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>100M - 500M
6846500	Propanoic acid, 2-methyl-, 2,2-dimethyl-1-(1-methylethyl)-1,3-propanediyl ester	Kodaflex txb	No Observed Effect Level (NOEL)	30	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
77501634	Benzoic acid, 5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-nitro-, 2-ethoxy-1-methyl-2-oxoethyl ester	Lactofen	Reference Dose (RfD)	0.002	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	390,240
78977	Propanenitrile, 2-hydroxy-	Lactonitrile	Lethal Dose 50 (LD50)	31	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>10M - 50M
91465086	Cyclopropanecarboxylic acid, 3-(2-chloro-3,3,3-trifluoro-1-propenyl)-2,2-dimethylcyano(3-phenoxyphenyl)methyl ester, 1.alpha.(S*),3.alpha.(Z)-(+ -)-	lambda-Cyhalothrin	Lethal Dose 50 (LD50)	56	mg/kg	Toxicity Category 3	Release (lbs/yr)	321,987
1335326	Lead, bis(acetato-kappa-O)tetrahydroxytri-	Lead acetate	Cancer Classification, EPA		B	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
330552	Urea, N-(3,4-dichlorophenyl)-N-methoxy-N-methyl-	Linuron	Lowest Observed Effect Level (LOEL)	0.63	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	1.4
554132	Carbonic acid, dilithium salt	Lithium carbonate	Lowest Observed Adverse Effect Level (LOAEL)	0.017	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	211,661
7447418	Lithium chloride (LiCl)	Lithium chloride	Lowest Observed Adverse Effect Level (LOAEL)	0.009	mg/kg-day	Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
121755	Butanedioic acid, ((dimethoxyphosphinothioyl)thio)-, diethyl ester	Malathion	No Observed Effect Level (NOEL)	0.23	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	9.58
108316	2,5-Furandione	Maleic anhydride	Lethal Dose 50 (LD50)	390	mg/kg	Toxicity Category 3	Release (lbs/yr)	769,446
123331	3,6-Pyridazinedione, 1,2-dihydro-	Maleic hydrazide	Lowest Observed Effect Level (LOEL)	500	mg/kg-day	Toxicity Category 4	Release (lbs/yr)	2,147,846
109773	Propanedinitrile	Malononitrile	Reference Dose (RfD)	0.0001	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	854,039
12427382	Manganese, [[1,2-ethanediybis(carbamodithioato)](2-)-]	Maneb	Reference Dose (RfD)	0.005	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	3,046,585
94746	Acetic acid, (4-chloro-2-methylphenoxy)-	MCPA	Reference Dose (RfD)	0.0005	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	18.6
108394	Phenol, 3-methyl-	m-Cresol	Cancer Classification, EPA		C	Toxicity Category 3	Release (lbs/yr)	374,903
541731	Benzene, 1,3-dichloro-	m-Dichlorobenzene	Minimal Risk Level (MRL)	0.03	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	22.4
108781	1,3,5-Triazine-2,4,6-triamine	Melamine	Cancer Studies, NTP	NTPMSR		Toxicity Category 2	Production Volume (lbs/year)	>100M - 500M
24307264	Piperidinium, 1,1-dimethyl-, chloride	Mepiquat chloride	Reference Dose (RfD)	0.03	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	182,976
68111	Acetic acid, mercapto-	Mercaptoacetic acid	Lethal Dose 50 (LD50)	114	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
150505	Phosphorotriethioic acid, tributyl ester	Merphos	Reference Dose (RfD)	0.00003	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	12
79390	2-Propenamide, 2-methyl-	Methacrylamide	Lethal Dose 50 (LD50)	451	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>50M - 100M
79414	2-Propenoic acid, 2-methyl-	Methacrylic acid	Lowest Observed Adverse Effect Level (LOAEL)	5	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>100M - 500M
126987	2-Propenenitrile, 2-methyl-	Methacrylonitrile	Reference Dose (RfD)	0.0001	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	89,330

Appendix 2

CASRN	Substance Name	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
10265926	Phosphoramidothioic acid, O,S-dimethyl ester	Methamidophos	Reference Dose (RfD)	0.00005	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	967,698
67561	Methanol	Methanol	Lowest Observed Adverse Effect Level (LOAEL)	3.1	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	201,697,278
3268493	Propanal, 3-(methylthio)-	Methional	Lethal Dose 50 (LD50)	1.52	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>100M - 500M
16752775	Ethanimidothioic acid, N-[[[(methylamino)carbonyloxy]-], methyl ester	Methomyl	Lowest Observed Adverse Effect Level (LOAEL)	0.1	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	3
79209	Acetic acid, methyl ester	Methyl acetate	Lethal Dose 50 (LD50)	3,705	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	> 1B
96333	2-Propenoic acid, methyl ester	Methyl acrylate	Reference Dose (RfD)	0.03	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	206,487
74839	Methane, bromo-	Methyl bromide (Bromomethane)	Reference Dose (RfD)	0.001	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	43
598550	Carbamic acid, methyl ester	Methyl carbamate	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	>1M - 10M
74931	Methanethiol	Methyl mercaptan	Lethal Dose 50 (LD50)	61	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	> 1B
80626	2-Propenoic acid, 2-methyl-, methyl ester	Methyl methacrylate	Lowest Observed Adverse Effect Level (LOAEL)	0.36	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	3,657,567
1634044	Propane, 2-methoxy-2-methyl-	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	Methanamine	Methylamine	Lethal Dose 50 (LD50)	100	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>50M - 100M
12108133	Manganese, tricarbonyl[(1,2,3,4,5-eta.)-1-methyl-2,4-cyclopentadien-1-yl]-	Methylcyclopentadienyl manganese tricarbonyl	Lethal Dose 50 (LD50)	8	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
93152	Benzene, 1,2-dimethoxy-4-(2-propenyl)-	Methyleugenol	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
4553622	Pentanedinitrile, 2-methyl-	Methylglutaronitrile	Lethal Dose 50 (LD50)	10	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>10M - 50M
75796	Silane, trichloromethyl-	Methyltrichlorosilane	Lethal Dose 50 (LD50)	800	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
9006422	Metiram	Metiram	Acceptable Daily Intake (ADI)	0.03	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	1,388,363
51218452	Acetamide, 2-chloro-N-(2-ethyl-6-methylphenyl)-N-(2-methoxy-1-methylethyl)-	Metolachlor	Cancer Classification, EPA	C		Toxicity Category 3	FW/AW-Max Value (ug/L)	77.6
171118095	Metolachlor ethanesulfonic acid	Metolachlor ethanesulfonic acid (ESA)	Reference Dose (RfD)	Parent data	mg/kg-day	Toxicity Category 3	FW/AW	Parent
152019733	Metolachlor oxanilic acid	Metolachlor oxanilic acid (OA)	Reference Dose (RfD)	Parent data	mg/kg-day	Toxicity Category 3	FW/AW	Parent
21087649	1,2,4-Triazin-5(4H)-one, 4-amino-6-(1,1-dimethylethyl)-3-(methylthio)-	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	Microcystin-LR	Reference Dose (RfD)	0.000003	mg/kg-day	Toxicity Category 1	FW/AW	Supplemental
64285069	Anatoxin-a	Anatoxin-a	Reference Dose (RfD)	0.0005	mg/kg-day	Toxicity Category 2	FW/AW	Supplemental
143545908	Cylindrospermopsin	Cylindrospermopsin	Reference Dose (RfD)	0.00003	mg/kg-day	Toxicity Category 1	FW/AW	Supplemental
2212671	1H-Azepine-1-carbothioic acid, hexahydro-, S-ethyl ester	Molinate	No Observed Effect Level (NOEL)	0.2	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	200
7439987	Molybdenum	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 oxide (MoO3)	Molybdenum trioxide	Cancer Studies, NTP	NTPMSR		Toxicity Category 3	Release (lbs/yr)	2,102,324
105555	Thiourea, N,N'-diethyl-	N,N-Diethylthiourea	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
127195	Acetamide, N,N-dimethyl-	N,N-Dimethylacetamide	Maximum Recommended Daily Dose (MRDD)	0.58	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>10M - 50M
108010	Ethanol, 2-(dimethylamino)-	N,N-Dimethylethanolamine	Maximum Recommended Daily Dose (MRDD)	15	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
300765	Phosphoric acid, 1,2-dibromo-2,2-dichloroethyl dimethyl ester	Naled	No Observed Effect Level (NOEL)	0.2	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	606,781
91203	Naphthalene	Naphthalene	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	FW/AW-Max Value (ug/L)	906
123864	Acetic acid, butyl ester	n-Butyl acetate	Lethal Dose 50 (LD50)	14,000	mg/kg	Toxicity Category 5	Production Volume (lbs/year)	>100M - 500M
97881	2-Propenoic acid, 2-methyl-, butyl ester	N-Butyl methacrylate	Lowest Observed Adverse Effect Level (LOAEL)	3.57	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
126307	1,3-Propanediol, 2,2-dimethyl-	Neopentyl glycol	No Observed Effect Level (NOEL)	100	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
7440020	Nickel	Nickel	Cancer Classification, IARC	1		Toxicity Category 1	FW/AW-Max Value (ug/L)	666
	Nickel compounds	Nickel compounds	Cancer Classification, IARC	1		Toxicity Category 1	Release (lbs/yr)	34,676,669
7440031	Niobium	Niobium	Cancer Classification, EPA	A		Toxicity Category 1	Production Volume (lbs/year)	>1M - 10M
139139	Glycine, N,N-bis(carboxymethyl)-	Nitrioltriacetic acid	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	30,679
98953	Benzene, nitro-	Nitrobenzene	Reference Dose (RfD)	0.0005	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	100
1836755	Benzene, 2,4-dichloro-1-(4-nitrophenoxy)-	Nitrofen	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	25,300
55630	1,2,3-Propanetriol, trinitrate	Nitroglycerin	Lowest Observed Adverse Effect Level (LOAEL)	0.008	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	55,979
75525	Methane, nitro-	Nitromethane	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	>10M - 50M
872504	2-Pyrrolidinone, 1-methyl-	N-Methyl-2-pyrrolidone	Lowest Observed Adverse Effect Level (LOAEL)	120	mg/kg-day	Toxicity Category 4	Release (lbs/yr)	6,311,503
924425	2-Propenamide, N-(hydroxymethyl)-	N-Methylolacrylamide	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	12,306
55185	Ethanamine, N-ethyl-N-nitroso-	N-Nitrosodiethylamine (NDEA)	Risk Specific Dose (RSD)	0.00000007	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	1,000
62759	Methanamine, N-methyl-N-nitroso-	N-nitrosodimethylamine (NDMA)	Reference Dose (RfD)	0.000008	mg/kg-day	Toxicity Category 1	FW/AW	DBP
924163	1-Butanamine, N-butyl-N-nitroso-	N-Nitroso-di-n-butylamine (NDBA)	Risk Specific Dose (RSD)	0.000002	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	5

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CASRN	Substance Name	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
621647	1-Propanamine, N-nitroso-N-propyl-	N-Nitroso-di-n-propylamine (NDPA)	Risk Specific Dose (RSD)	0.00001	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	506
86306	Benzenamine, N-nitroso-N-phenyl-	N-Nitrosodiphenylamine	Cancer Studies, NTP		NTPMSR	Toxicity Category 1	Release (lbs/yr)	14
10595956	Ethanamine, N-methyl-N-nitroso-	N-Nitrosomethylethylamine (NMEA)	Risk Specific Dose (RSD)	0.000004	mg/kg-day	Toxicity Category 1	FW/AW	DBP
684935	Urea, N-methyl-N-nitroso-	N-Nitroso-N-methylurea	TD50	0.093	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	5
930552	Pyrrolidine, 1-nitroso-	N-nitrosopyrrolidine (NPNR)	Risk Specific Dose (RSD)	0.000005	mg/kg-day	Toxicity Category 1	FW/AW	DBP
27314132	3(2H)-Pyridazinone, 4-chloro-5-(methylamino)-2-[3-(trifluoromethyl)phenyl]-	Norflurazon	Reference Dose (RfD)	0.04	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	44.0
103651	Benzene, propyl-	n-Propylbenzene	Lowest Observed Adverse Effect Level (LOAEL)	2.5	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	47
88733	Benzene, 1-chloro-2-nitro-	o-Chloronitrobenzene	Reference Dose (RfD)	0.001	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
95498	Benzene, 1-chloro-2-methyl-	o-Chlorotoluene	Reference Dose (RfD)	0.02	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	52.4
556672	Cyclotetrasiloxane, octamethyl-	Octamethylcyclotetrasiloxane	Lethal Dose 50 (LD50)	1,540	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
20325400	[1,1'-Biphenyl]-4,4'-diamine, 3,3'-dimethoxy-dihydrochloride	o-Dianisidine dihydrochloride	Cancer Studies, NTP		NTPMSR	Toxicity Category 1	Release (lbs/yr)	46
528290	Benzene, 1,2-dinitro-	o-Dinitrobenzene	Reference Dose (RfD)	0.0001	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	105,280
88722	Benzene, 1-methyl-2-nitro-	o-Nitrotoluene	Cancer Studies, NTP		NTPMSR	Toxicity Category 1	Production Volume (lbs/year)	>10M - 50M
95534	Benzenamine, 2-methyl-	o-Toluidine	Cancer Classification, IARC		2A	Toxicity Category 2	Release (lbs/yr)	10,774
636215	Benzenamine, 2-methyl-, hydrochloride	o-Toluidine hydrochloride	Cancer Studies, NTP		NTPMSR	Toxicity Category 1	Release (lbs/yr)	22
19666309	1,3,4-Oxadiazol-2(3H)-one, 3-[2,4-dichloro-5-(1-methylethoxy)phenyl]-5-(1,1-dimethylethyl)-	Oxadiazon	No Observed Effect Level (NOEL)	0.5	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	28,822
75569	Oxirane, methyl-	Oxirane, methyl-	Risk Specific Dose (RSD)	0.000042	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	433,536
301122	Phosphorothioic acid, S-[2-(ethylsulfanyl)ethyl] O,O-dimethyl ester	Oxydemeton-methyl	Lethal Dose 50 (LD50)	10	mg/kg	Toxicity Category 2	Release (lbs/yr)	154,565
42874033	Benzene, 2-chloro-1-(3-ethoxy-4-nitrophenoxy)-4-(trifluoromethyl)-	Oxyfluorfen	No Observed Effect Level (NOEL)	0.3	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	706,799
10028156	Ozone	Ozone	TD50	1.9	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	715,830
72559	Benzene, 1,1'-(dichloroethenylidene)bis[4-chloro-	p,p'-DDE	Risk Specific Dose (RSD)	0.000029	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	0.062
4685147	4,4'-Bipyridinium, 1,1'-dimethyl-	Paraquat	Lowest Observed Adverse Effect Level (LOAEL)	0.93	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	6,899,701
100005	Benzene, 1-chloro-4-nitro-	p-Chloronitrobenzene	TD50	473	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
106434	Benzene, 1-chloro-4-methyl-	p-Chlorotoluene	Reference Dose (RfD)	0.02	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	22.5
120718	Benzenamine, 2-methoxy-5-methyl-	p-Cresidine	Cancer Studies, NTP		NTPMSR	Toxicity Category 1	Release (lbs/yr)	0
100254	Benzene, 1,4-dinitro-	p-Dinitrobenzene	Reference Dose (RfD)	0.0001	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	28,711
32534819	Benzene, 1,1'-oxybis-, pentabromo deriv.	Pentabromodiphenyl ethers	Reference Dose (RfD)	0.002	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
76017	Ethane, pentachloro-	Pentachloroethane	Cancer Studies, NTP		NTPMSR	Toxicity Category 1	Release (lbs/yr)	865
115775	1,3-Propanediol, 2,2-bis(hydroxymethyl)-	Pentaerythritol	No Observed Effect Level (NOEL)	100	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
3296900	1,3-Propanediol, 2,2-bis(bromomethyl)-	Pentaerythritol dibromide	Cancer Studies, NTP		NTPMSR	Toxicity Category 1	Production Volume (lbs/year)	>1M - 10M
110623	Pentanal	Pentanal	Lethal Dose 50 (LD50)	5.66	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>50M - 100M
14797730	Perchlorate	Perchlorate	No Observed Effect Level (NOEL)	0.007	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	420
52645531	Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, (3-phenoxyphenyl)methyl ester	Permethrin	No Observed Effect Level (NOEL)	5	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	1,068,390
335671	Octanoic acid, pentadecafluoro-	PFOA (Perfluorooctanoic acid)	Lowest Observed Adverse Effect Level (LOAEL)	1.0	mg/kg-day	Toxicity Category 2	FW/AW	Supplemental
77098	1(3H)-Isobenzofuranone, 3,3-bis(4-hydroxyphenyl)-	Phenolphthalein	Cancer Studies, NTP		NTPMSR	Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
101848	Benzene, 1,1'-oxybis-	Phenyl ether	Lethal Dose 50 (LD50)	2,450	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
62384	Mercury, (acetato-kappa.O)phenyl-	Phenylmercury acetate	Reference Dose (RfD)	0.00008	mg/kg-day	Toxicity Category 1	Production Volume (lbs/year)	>1M - 10M
57410	2,4-Imidazolinedione, 5,5-diphenyl-	Phenytoin	TD50	59.1	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	15,981
732116	Phosphorodithioic acid, S-[(1,3-dihydro-1,3-dioxo-2H-isindol-2-yl)methyl] O,O-dimethyl ester	Phosmet	Lethal Dose 50 (LD50)	26	mg/kg	Toxicity Category 2	Release (lbs/yr)	1,336,387
7723140	Phosphorus	Phosphorus	Reference Dose (RfD)	0.00002	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	52,750
88993	1,2-Benzenedicarboxylic acid	Phthalic acid	Lowest Observed Adverse Effect Level (LOAEL)	0.56	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
110894	Piperidine	Piperidine	Lethal Dose 50 (LD50)	22.4	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
156105	Benzenamine, 4-nitroso-N-phenyl-	p-Nitrosodiphenylamine	Cancer Studies, NTP		NTPMSR	Toxicity Category 1	Release (lbs/yr)	0
99990	Benzene, 1-methyl-4-nitro-	p-Nitrotoluene	Reference Dose (RfD)	0.01	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M

Appendix 2

CASRN	Substance Name	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
26062793	2-Propen-1-aminium, N,N-dimethyl-N-2-propenyl-, chloride, homopolymer	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	Potassium	Lowest Observed Adverse Effect Level (LOAEL)	0.94	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	23,955
156434	Benzenamine, 4-ethoxy-	p-Phenetidine	Lowest Observed Adverse Effect Level (LOAEL)	0.24	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
41198087	Phosphorothioic acid, O-(4-bromo-2-chlorophenyl) O-ethyl S-propyl ester	Profenofos	Lowest Observed Adverse Effect Level (LOAEL)	0.05	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	881,702
1610180	1,3,5-Triazine-2,4-diamine, 6-methoxy-N,N'-bis(1-methylethyl)-	Prometon	Reference Dose (RfD)	0.015	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	40
107120	Propanenitrile	Propanenitrile	Lethal Dose 50 (LD50)	35.8	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>10M - 50M
2312358	Sulfurous acid, 2-[4-(1,1-dimethylethyl)phenoxy]cyclohexyl 2-propynyl ester	Propargite	Reference Dose (RfD)	0.02	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	20
107197	2-Propyn-1-ol	Propargyl alcohol	Lethal Dose 50 (LD50)	20	mg/kg	Toxicity Category 2	Release (lbs/yr)	64,096
123386	Propanal	Propionaldehyde	Cancer Classification, DSSTOX	LM		Toxicity Category 3	Release (lbs/yr)	699,803
79094	Propanoic acid	Propionic acid	Lethal Dose 50 (LD50)	1,640	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
1639607	Benzeneethanol, .alpha.-[([R]-2-(dimethylamino)-1-methylethyl)-.alpha.-phenyl-, propanoate (ester), hydrochloride, (.alpha.S)-	Propoxyphene hydrochloride	Lowest Observed Adverse Effect Level (LOAEL)	0.0013	mg/kg-day	Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
57556	1,2-Propanediol	Propylene glycol	Lowest Observed Adverse Effect Level (LOAEL)	5	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	> 1B
107982	2-Propanol, 1-methoxy-	Propylene glycol 1-methyl ether	Reference Dose (RfD)	0.7	mg/kg-day	Toxicity Category 5	Production Volume (lbs/year)	>100M - 500M
108656	2-Propanol, 1-methoxy-, acetate	Propylene glycol monomethyl ether acetate	No Observed Effect Level (NOEL)	300	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
57018527	2-Propanol, 1-(1,1-dimethylethoxy)-	Propylene glycol mono-t-butyl ether	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	>1M - 10M
1698608	3(2H)-Pyridazinone, 5-amino-4-chloro-2-phenyl-	Pyrazon	Lethal Dose 50 (LD50)	493	mg/kg	Toxicity Category 3	Release (lbs/yr)	118,553
110861	Pyridine	Pyridine	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Release (lbs/yr)	1,302,842
2176627	Pyridine, pentachloro-	Pyridine, pentachloro-	Lethal Dose 50 (LD50)	435	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
14808607	Quartz (SiO2)	Quartz (SiO2)	Cancer Classification, IARC	1		Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
91225	Quinoline	Quinoline	Risk Specific Dose (RSD)	0.0000033	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	28,629
76578126	Quizalofop	Quizalofop	Reference Dose (RfD)	Surrogate data	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	341,564
121824	1,3,5-Triazine, hexahydro-1,3,5-trinitro-	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	1,4-Benzenediamine, N-(1,3-dimethylbutyl)-N-phenyl-	Santoflex 13	No Observed Effect Level (NOEL)	6	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>50M - 100M
135988	Benzene, (1-methylpropyl)-	sec-Butylbenzene	Lowest Observed Adverse Effect Level (LOAEL)	4.42	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	22
74051802	2-Cyclohexen-1-one, 2-[1-(ethoxymino)butyl]-5-[2-(ethylthio)propyl]-3-hydroxy-	Sethoxydim	No Observed Effect Level (NOEL)	8.9	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	1,721,030
7440213	Silicon	Silicon	Lethal Dose 50 (LD50)	3,160	mg/kg	Toxicity Category 4	FW/AW-Max Value (ug/L)	98,916
7440235	Sodium	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 (Na(N3))	Sodium azide	Lowest Observed Adverse Effect Level (LOAEL)	0.25	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	66,425
532321	Benzoic acid, sodium salt	Sodium benzoate	Lethal Dose 50 (LD50)	1,600	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
7647156	Sodium bromide (NaBr)	Sodium bromide	Lowest Observed Adverse Effect Level (LOAEL)	0.13	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
7775099	Chloric acid, sodium salt	Sodium chlorate	Lowest Observed Adverse Effect Level (LOAEL)	1.4	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	7,277,453
3926623	Acetic acid, chloro-, sodium salt	Sodium chloroacetate	Lethal Dose 50 (LD50)	95	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
128041	Carbamodithioic acid, dimethyl-, sodium salt	Sodium dimethyldithiocarbamate	Lethal Dose 50 (LD50)	300	mg/kg	Toxicity Category 3	Release (lbs/yr)	129,318
25155300	Benzenesulfonic acid, dodecyl-, sodium salt	Sodium dodecylbenzenesulfonate	Lethal Dose 50 (LD50)	438	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>50M - 100M
62748	Acetic acid, fluoro-, sodium salt	Sodium fluoroacetate	Reference Dose (RfD)	0.00002	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	0
7681529	Hypochlorous acid, sodium salt	Sodium hypochlorite	Lowest Observed Adverse Effect Level (LOAEL)	2.2	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
137428	Carbamodithioic acid, methyl-, monosodium salt	Sodium methyldithiocarbamate	Lethal Dose 50 (LD50)	50	mg/kg	Toxicity Category 3	Release (lbs/yr)	60,154,489
1313822	Sodium sulfide (Na2S)	Sodium sulfide	Lethal Dose 50 (LD50)	205	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>100M - 500M
13718268	Vanadate (VO31-), sodium	Sodium vanadate	Lowest Observed Adverse Effect Level (LOAEL)	0.62	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
50704	D-Glucitol	Sorbitol	Maximum Recommended Daily Dose (MRDD)	833	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M

Appendix 2

CASRN	Substance Name	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
131929607	1H-as-Indaceno[3,2-d]oxacycloclododecin-7,15-dione, 2-[(6-deoxy-2,3,4-tri-O-methyl- α -L-mannopyranosyl)oxy]-13-[[[(2R,5S,6R)-5-(dimethylamino)tetrahydro-6-methyl-2H-pyran-2-yl]oxy]-9-ethyl-2,3,3a,5a,5b,6,9,10,11,12,13,14,16a,16b-tetradecahydro-14-methyl-	Spinosyn A	Acceptable Daily Intake (ADI)	0.02	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	117,572
57114	Octadecanoic acid	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	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	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	Sulfuryl fluoride	Lethal Dose 50 (LD50)	100	mg/kg	Toxicity Category 3	Release (lbs/yr)	142,720
35400432	Phosphorodithioic acid, O-ethyl O-[4-(methylthio)phenyl] S-propyl ester	Sulprofos	Lowest Observed Adverse Effect Level (LOAEL)	0.6	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	308,713
1934210	1H-Pyrazole-3-carboxylic acid, 4,5-dihydro-5-oxo-1-(4-sulfophenyl)-4-[[[(4-sulfophenyl)azo]-, trisodium salt	Tartrazine	Lowest Observed Adverse Effect Level (LOAEL)	0.014	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
107534963	1H-1,2,4-Triazole-1-ethanol, α -[2-(4-chlorophenyl)ethyl]- α -(1,1-dimethylethyl)-	Tebuconazole	Acceptable Daily Intake (ADI)	0.03	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	479,616
112410238	Benzoic acid, 3,5-dimethyl-, 1-(1,1-dimethylethyl)-2-(4-ethylbenzoyl)hydrazide	Tebufenozide	Acceptable Daily Intake (ADI)	0.02	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	104,642
34014181	Urea, N-[5-(1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl]-N,N'-dimethyl-	Tebuthiuron	No Observed Effect Level (NOEL)	7	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	17.3
13494809	Tellurium	Tellurium	Lethal Dose 50 (LD50)	20	mg/kg	Toxicity Category 2	FW/AW-Max Value (ug/L)	365.4
13071799	Phosphorodithioic acid, S-[[[(1,1-dimethylethyl)thio]methyl] O,O-diethyl ester	Terbufos	Reference Dose (RfD)	0.000025	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	0.56
56070167	Phosphorodithioic acid, S-[[[(1,1-dimethylethyl)sulfonylmethyl] O,O-diethyl ester	Terbufos sulfone	Reference Dose (RfD)	Parent data	mg/kg-day	Toxicity Category 1	FW/AW	Surrogate
56070156	Terbufos-O-analogue sulfone	Terbufos-O-analogue sulfone	Reference Dose (RfD)	Parent data	mg/kg-day	Toxicity Category 1	FW/AW-Max Value (ug/L)	0.016
100210	1,4-Benzenedicarboxylic acid	Terephthalic acid	Lowest Observed Adverse Effect Level (LOAEL)	142.5	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	> 1B
75650	2-Propanol, 2-methyl-	tert-Butanol	TD50	64.6	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	1,548,617
75912	Hydroperoxide, 1,1-dimethylethyl	tert-Butyl hydroperoxide	Lethal Dose 50 (LD50)	320	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
75649	2-Propanamine, 2-methyl-	tert-Butylamine	Lethal Dose 50 (LD50)	44	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>10M - 50M
98066	Benzene, (1,1-dimethylethyl)-	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	Plumbane, tetraethyl-	Tetraethyl lead	Reference Dose (RfD)	0.0000001	mg/kg-day	Toxicity Category 1	Production Volume (lbs/year)	>1M - 10M
116143	Ethene, tetrafluoro-	Tetrafluoroethene	Cancer Studies, NTP	NTPMSR		Toxicity Category 1	Production Volume (lbs/year)	>50M - 100M
109999	Furan, tetrahydro-	Tetrahydrofuran	Cancer Studies, NTP	NTPMSR		Toxicity Category 2	FW/AW-Max Value (ug/L)	1,430
75570	Methanaminium, N,N,N-trimethyl-, chloride	Tetramethylammonium chloride	Lethal Dose 50 (LD50)	50	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
75592	Methanaminium, N,N,N-trimethyl-, hydroxide	Tetramethylammonium hydroxide	Lethal Dose 50 (LD50)	34	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>10M - 50M
64028	Glycine, N,N'-1,2-ethanediybis(N-(carboxymethyl)-, tetrasodium salt	Tetrasodium EDTA	Lethal Dose 50 (LD50)	2,000	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
25265774	Propanoic acid, 2-methyl-, monoester with 2,2,4-trimethyl-1,3-pentanediol	Texanol	Lethal Dose 50 (LD50)	3,200	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
79277671	2-Thiophenecarboxylic acid, 3-[[[(4-methoxy-6-methyl-1,3,5-triazin-2-yl)amino]carbonyl]amino]sulfonyl]-	Thiencarbazon	Reference Dose (RfD)	Surrogate data	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	105,375
2231574	Carbonylthioic dihydrazide	Thiocarbazine	Lethal Dose 50 (LD50)	6	mg/kg	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
59669260	Ethanimidodithioic acid, N,N'-[[thiobis(methylimino)carbonyloxy]]bis-, dimethyl ester	Thiodicarb	Acceptable Daily Intake (ADI)	0.03	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	823,065
23564058	Carbamic acid, [1,2-phenylenebis(iminocarbonyl)]bis-, dimethyl ester	Thiophanate-methyl	No Observed Effect Level (NOEL)	8	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	454,785

Appendix 2

CASRN	Substance Name	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
108985	Benzenethiol	Thiophenol	Reference Dose (RfD)	0.0001	mg/kg-day	Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
137268	Thioperoxydicarbonic diamide (((H2N)C(S))2S2), tetramethyl-	Thiram	Reference Dose (RfD)	0.005	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	180,203
7440291	Thorium	Thorium-232	Cancer Classification, EPA		A	Toxicity Category 1	FW/AW-Max Value (ug/L)	61.7
26471625	Benzene, 1,3-diisocyanatomethyl-	Toluene diisocyanate	Cancer Studies, NTP		NTPMSR	Toxicity Category 1	Release (lbs/yr)	129,143
66841256	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(1,2,2,2-tetrabromoethyl)-, cyano(3-phenoxyphenyl)methyl ester	Tralomethrin	No Observed Effect Level (NOEL)	0.75	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	23,819
78488	Phosphorotriithioic acid, S,S,S-tributyl ester	Tribufos	Reference Dose (RfD)	0.00003	mg/kg-day	Toxicity Category 1	Release (lbs/yr)	4,929,032
1461229	Stannane, tributylchloro-	Tributyltin chloride	Lethal Dose 50 (LD50)	0.03	mg/kg	Toxicity Category 1	Production Volume (lbs/year)	>1M - 10M
102716	Ethanol, 2,2',2''-nitrioltris-	Triethanolamine	TD50	100	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>100M - 500M
121448	Ethanimine, N,N-diethyl-	Triethylamine	Lowest Observed Adverse Effect Level (LOAEL)	1	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	1,167,219
112276	Ethanol, 2,2'-[1,2-ethanedylbis(oxy)]bis-	Triethylene glycol	Lowest Observed Adverse Effect Level (LOAEL)	3.6	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>100M - 500M
1582098	Benzenamine, 2,6-dinitro-N,N-dipropyl-4-(trifluoromethyl)-	Trifluralin	No Observed Effect Level (NOEL)	0.75	mg/kg-day	Toxicity Category 2	FW/AW-Max Value (ug/L)	1.74
552307	5-Isobenzofurancarboxylic acid, 1,3-dihydro-1,3-dioxo-	Trimellitic anhydride	Lethal Dose 50 (LD50)	1,900	mg/kg	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
512561	Phosphoric acid, trimethyl ester	Trimethyl phosphate	Cancer Studies, NTP		NTPMSR	Toxicity Category 1	Production Volume (lbs/year)	10K - 500K
75503	Methanimine, N,N-dimethyl-	Trimethylamine	Lethal Dose 50 (LD50)	397	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>50M - 100M
77996	1,3-Propanediol, 2-ethyl-2-(hydroxymethyl)-	Trimethylolpropane	Acceptable Daily Intake (ADI)	0.05	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>50M - 100M
118967	Benzene, 2-methyl-1,3,5-trinitro-	Trinitrotoluene	Reference Dose (RfD)	0.0005	mg/kg-day	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
101020	Phosphorous acid, triphenyl ester	Triphenyl phosphite	Lethal Dose 50 (LD50)	444	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
76879	Stannane, hydroxytriphenyl-	Triphenyltin hydroxide (TPTH)	Acceptable Daily Intake (ADI)	0.0005	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	662,418
126727	1-Propanol, 2,3-dibromo-, phosphate (3:1)	Tris(2,3-dibromopropyl) phosphate	Cancer Studies, NTP		NTPMSR	Toxicity Category 1	Release (lbs/yr)	500
140089	Ethanol, 2-chloro-, phosphite (3:1)	Tris(2-chloroethyl) phosphite	Lethal Dose 50 (LD50)	100	mg/kg	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
115968	Ethanol, 2-chloro-, phosphate (3:1)	Tris(chloroethyl)phosphate	Cancer Studies, NTP		NTPMSR	Toxicity Category 1	FW/AW-Median Value (ug/L)	0.20
1120214	Undecane	Undecane	No Observed Effect Level (NOEL)	100	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	>100M - 500M
57136	Urea	Urea	Lowest Observed Adverse Effect Level (LOAEL)	200	mg/kg-day	Toxicity Category 4	Production Volume (lbs/year)	> 1B
51796	Carbamic acid, ethyl ester	Urethane	TD50	16.9	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	96,050
7440622	Vanadium	Vanadium	Reference Dose (RfD)	0.007	mg/kg-day	Toxicity Category 3	FW/AW-Max Value (ug/L)	70.4
1314621	Vanadium oxide (V2O5)	Vanadium pentoxide	Cancer Studies, NTP		NTPMSR	Toxicity Category 1	Production Volume (lbs/year)	>1M - 10M
1929777	Carbamothioic acid, dipropyl-, S-propyl ester	Vernolate	Reference Dose (RfD)	0.001	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	182,187
50471448	2,4-Oxazolidinedione, 3-(3,5-dichlorophenyl)-5-ethenyl-5-methyl-	Vinclozolin	Reference Dose (RfD)	0.025	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	122,226
108054	Acetic acid ethenyl ester	Vinyl acetate	TD50	341	mg/kg-day	Toxicity Category 3	Release (lbs/yr)	3,068,589
75025	Ethene, fluoro-	Vinyl fluoride	Cancer Classification, IARC		2A	Toxicity Category 2	Production Volume (lbs/year)	>1M - 10M
25013154	Benzene, ethenylmethyl-	Vinyltoluene	Reference Dose (RfD)	0.006	mg/kg-day	Toxicity Category 3	Production Volume (lbs/year)	>10M - 50M
137304	Zinc, bis(dimethylcarbamodithioato-kappa.S.,kappa.S)-, (T-4)-	Ziram	TD50	10.7	mg/kg-day	Toxicity Category 2	Release (lbs/yr)	1,996,914