FINAL REPORT: TASK 1

IDENTIFICATION OF *CHEMICALS OF INTEREST* RELATED TO THE REUSE OF PRODUCED WATERS FOR AGRICULTURAL IRRIGATION OF EDIBLE CROPS

Prepared for:

The California Central Valley Region Regional Water Quality Control Board

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GSI Job No. 4874
Issued: 23 March 2020

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Suggested Citation:

GSI Environmental Inc., 2020. Identification of Chemicals of Interest Related to the Reuse of Produced Waters for Agricultural Irrigation of Edible Crops. Central Valley Regional Water Quality Control Board, Fresno, California. March 9, 2020.

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ATSDR – Agency for Toxic Substances and Disease Registry

BMD – Benchmark Dose

CalEPA – California Environmental Protection Agency

CS2 – Carbon disulfide

CASRN – Chemical Abstract Registration Number

CEBS – Chemical Effects in Biological Systems

CICAD – Concise International Chemical Assessment Document

CVRWQCB – Central Valley Regional Water Quality Control Board

d – day

DART – Developmental and Reproductive Toxicology Database

ECHA – European Chemicals Agency

EPA – US Environmental Protection Agency

FDA – Food and Drug Administration

GRAS – Generally Recognized as Safe

GSI – GSI Environmental

HBSL – Human Based Screening Levels

HEAST – Health Effects Assessment Summary Table

HHBP – Human Health Benchmarks for Pesticides

HSDB – Hazardous Substances Data Bank

IARC – International Agency for Research on Cancer

IPCS-INCHEM – International Programme on Chemical Safety Chemical Safety Information from Intergovernmental Organizations

IRIS – Integrated Risk Information System

ITER – International Toxicity Estimates for Risk

kg – kilogram

L – Liter

LOAEL – Lowest Observed Adverse Effect Level

MADL – Maximum Allowable Daily Dose

MCL – Maximum Contaminant Level

mg – Milligram

MOU – Memorandum of Understanding

MRL – Minimal Risk Level

NAWQA – National Water-Quality Assessment

NIEHS – National Institutes of Environmental Health

NIH – National Institutes of Health

NOAEL – No Observed Adverse Effect Level

NOEL – No Observed Effect Level

NORM – Naturally Occurring Radioactive Materials

NSRL – No Significant Risk Level

OECD – Organisation for Economic Co-operation and Development

OEHHA – Office of Environmental Health Hazard Assessment

OPR – Organizational Peer Reviewed

pCi – picoCurie

PET – Polyethylene terephthalate

ppm – parts per million

PPRTV – Provisional Peer-Reviewed Toxicity Values

RA – Read-across

RCRA – Resource Conservation and Recovery Act

REACH – Registration, Evaluation, Authorization and Restriction of Chemicals

REL – Reference Exposure Level

RfD – Reference dose

STV – Surrogate Toxicity Value

TOXNET – Toxicology Data Network

UF – Uncertainty Factor

USGS – United States Geological Survey

VOC – Volatile Organic Compound

WHO – World Health Organization

EXECUTIVE SUMMARY

This report describes work completed under Task 1 of the "Memorandum of Understanding Between the Central Valley Regional Water Quality Control Board and Permit Holders Governing the Solicitation, Management and Review of Academic, Technical and/or Scientific Studies Related to the Irrigation of Crops with Oil Field Produced Water." Task 1 is the first of a three- task project to research and evaluate the safety of using treated, produced water for the irrigation of food crops. The primary objective of Task 1 is to conduct a hazard assessment of chemicals that may be present in the water that comes out of an oil well, along with oil, when crude oil is produced (i.e., produced water). A second objective is to develop a prioritized list of these chemicals for further study in the context of the beneficial use of produced water for the irrigation of food crops. Task 2 entails a literature search for information on the properties and occurrence of the chemicals identified in Task 1 that will support the further evaluation and understanding of the safety aspects of using produced water for irrigation. Task 3, was a continuation of a program of testing crops irrigated with blended produced water that been ongoing in the Cawelo Water District prior to the initiation of this study. As result, Task 3 was started prior to the beginning of Task 1 and continued throughout the development of the Task 1 report. It entailed testing crops to determine if there ae chemical differences in crops irrigated with produced water, when compared against those that are irrigated with conventional water sources and, if so, is this difference attributable to the use of produced water as an irrigation water source. Data collected during Task 3 was used to inform prioritization of the evaluation of the chemicals in Task 1.

The chemicals considered for the prioritization performed in Task 1 include naturally occurring substances known to be present in produced water and chemical additives used in oil and gas production that may subsequently be present in produced water. The chemicals occurring naturally in produced water were identified from reliable published sources. The chemical additives considered in this evaluation are the chemicals reported to the Central Valley Regional Water Quality Control Board (CVRWQCB) by the oil and gas producers and chemical manufacturers. Under the authority of the California Water Code, the CVRWQCB issued directives through September 2018 that required oil and gas producers and chemicals manufacturers to disclose the chemical make-up of additives that are used during petroleum exploration, production, and treatment at facilities that use produced water used for irrigation of food crops. The chemicals identified for further evaluation under this task were identified because they may be present in produced water used for irrigation and not necessarily because they are expected to be found in crops irrigated with produced water.

By combining the list of naturally occurring chemicals and oil field additives mentioned above, we identified 399 chemicals to be prioritized for further evaluation. While fate and transport was part of the evaluation process, chronic oral toxicity of the chemicals was the primary factor used in the evaluation of the chemicals. The emphasis on toxicity was intended to ensure that the most toxic chemicals be retained for further evaluation in Task 2. Chemicals were eliminated from further evaluation if the chemicals had very low

toxicity and if it was clear that exposure at levels that might cause adverse health effects was not plausible. Oral toxicity was the only toxicity route considered because we were interested in the safety of consumption of the irrigated crops. The potential for exposure by inhalation and dermal contact was considered to be insignificant in comparison to ingestion.

Because the toxicity of the 399 chemicals selected for further consideration in this study had not been studied to the same degree, we relied on a variety of sources of information and approaches to assessing the toxicity of the chemicals evaluated in this task. Of the 399 chemicals, GSI identified published toxicity values for 107 of the chemicals. Toxicity values for 23 of the chemicals were identified using a read-across approach in which toxicity values for chemicals with known toxicity were applied to structurally similar chemicals. For the remaining chemicals, GSI was able to identify 71 chemicals of low concern for toxic effects at concentrations normally encountered by humans and at concentrations expected in irrigated crops. These chemicals of low concern for toxic effect included constituents of food, food additives, chemicals considered essentially non-toxic, chemicals with therapeutic oral use and low toxicity, inert compounds, and compounds that break down into one of the previously identified essentially non-toxic chemicals. There are 59 chemicals for which GSI was unable to identify sufficient information to evaluate chronic oral toxicity; these require further evaluation in Task 2. Among the remaining chemicals, 69 chemicals did not show evidence of chronic oral toxicity; and 15 chemicals did not have sufficient information to support conclusions as to their toxicity. For 51 of the chemicals, toxicity studies were available, but no agency had developed toxicity factors for the chemicals. GSI used this available toxicity information, for the specific purpose of this study, and developed project-specific surrogate toxicity values. Using the published toxicity studies and applying uncertainly factors consistent with those used by the Office of Environmental Health Hazard Assessment (OEHHA), GSI developed 51 project-specific surrogate toxicity values for these chemicals; and we used these toxicity factors for purposes of the chemical prioritization process described in this report.

Chemicals with toxicity data were screened as part of the prioritization process for the list of chemicals. Chemicals were screened based on a toxicity criterion and their potential to naturally biodegrade in water. The final list of chemicals that were identified for further review in Task 2 include 143 chemicals. Of those 143 chemicals, 53 had agency derived toxicity values, 12 were identified based on project-specific surrogate toxicity values, 59 did not have any toxicity data, 15 had incomplete information to assess their toxicity based on chronic oral exposure, and there were 4 other identified radionuclides.

The next phase of this project (Task 2) is a literature review focused on the use of produced water for irrigation. The specific topics addressed include the occurrence of the chemicals identified in Task 1 in produced water, and factors that will affect the environmental fate and transport of the identified chemicals. The information collected on environmental fate and transport will include plant uptake, biodegradation in water and soil, fugacity of chemicals in water, and sorption potential of chemicals that could affect

the uptake of the chemicals by plants. It will also investigate processes that could alter the toxicological properties of the identified chemicals or generate degradation products that require further evaluation. The results of the evaluation performed in Task 1 will be used to focus the collection of information in Task 2, to prepare an evaluation of the state of knowledge of the identified chemicals in the context of the reuse of produced water for agricultural irrigation, and to identify key information gaps.

1.0 INTRODUCTION

GSI Environmental (GSI) has been commissioned as a third-party consultant to perform technical work in support of an evaluation of the use effects and health risks associated with the use of treated produced water for purposes of irrigating food crops. The work is being performed in accordance with a Memorandum of Understanding (MOU) between the CVRWQCB and a group of permit holders that generate produced water as a result of their oil and gas extraction activities and a group of permit holders that accepts treated, produced water for beneficial use as agricultural irrigation water[1]. The MOU stipulates that the suppliers and users fund the technical work to support the scientific review of using produced water in irrigated agriculture and that the CVRWQCB direct the technical work performed by the third-party consultant. The technical work completed by the third-party consultant was disseminated to the Food Safety Expert Panel and the CVRWQCB for comments and recommendation via draft reports and presentations during the public Food Safety Meetings. The Scope of Work developed in response to the MOU is available on the CVRWQCB website[2], and it includes three tasks:

1. Selection of “Chemicals of Interest,” from a list of known chemical additives and naturally occurring chemicals in produced water, for further evaluation
2. Literature review focusing on the “Chemicals of Interest” in the context of produced water reuse in agriculture irrigation and other potential sources of these chemicals in the agricultural water supply
3. Sampling and chemical analysis of crops irrigated with produced water and crops grown nearby using conventional sources for irrigation

This report describes the selection criteria, methods, data sources and results that have been used to-date to identify the “Chemicals of Interest” (Task 1). It builds on work by other researchers who conducted a hazard assessment of oil field additive chemicals, which may impact the reuse of produced water for agricultural irrigation (Shonkoff et al., 2016). The Scope of Work document proposed that the following 13 factors could be considered in the selection of the Chemicals of Interest:

- Oral toxicity information/data (with priority given to chronic mammalian toxicity data)

[1] https://www.waterboards.ca.gov/centralvalley/water_issues/oil_fields/food_safety/2017_0627_offs_mou.pdf
[2]https://www.waterboards.ca.gov/centralvalley/water_issues/oil_fields/food_safety/meetings/2018_0725_offs_mtg_sows.pdf

- Dermal toxicity information/data
- Carcinogenicity information/data
- Teratogenicity information/data
- Environmental persistence/degradation information/data, including soil half-life
- Degradation byproducts of the chemicals and their associated toxicities, carcinogenicity, teratogenicity, endocrine disrupting potential, etc.
- Plant uptake information/data
- Amounts and frequency of use in oil fields
- Chemicals that are persistent, bioaccumulative, and toxic, as defined by the US Environmental Protection Agency (EPA) and other government or scientific organizations
- Chemicals detected in any water quality analyses of irrigation water with maximum measured irrigation water concentrations above available risk-based water screening levels (for example, EPA drinking water screening levels or California Public Health Goals)
- Ambient, background concentrations in air and water that can result from agricultural practices and human activities unrelated to produced water reuse
- Whether the chemical is naturally occurring in the environment
- Other sources of the chemical in the environment and the specificity of the chemical to application of produced water for irrigation

An initial review of these 13 factors resulted in GSI focusing on oral toxicity (including consideration of carcinogenicity and teratogenicity) as the primary factor in the selection of the Chemicals of Interest. Biodegradation in water was also a factor in the selection process, although it was not as significant as toxicity in the ranking process. While the other factors identified above are important in determining whether a chemical in irrigation water will end up in the edible part of a plant at a significant concentration, they are not sufficiently well understood or are not definitive considerations in the elimination of chemicals from further consideration. For example, we know that plants can take chemicals up from the soil into edible plant parts; but we do not have precise quantitative plant uptake factors that would support eliminating any chemical from further evaluation because of a low rate of uptake. Similarly, some of the chemicals used in oil production may be used in small quantities, but we do not have sufficient information to show that the volume of use could not result in the accumulation in the edible part of plants a detectable or unsafe level. Water sampling data from samples of produced water and blended irrigation water were considered during the review of factors that might support identification of the Chemicals of Interest. This data, however, was not used as a primary evaluation tool when identifying the Chemicals of Interest. Uncertainties associated with the water sampling with such factors as the timing of when oil production chemicals were used in relationship to when samples were collected or the timing of when samples were

collected in relationship to when blended irrigation water was applied to fields was not known. Because of these, and other information gaps, we could not eliminate chemicals from further consideration simply because they were not detected in produced water or in blended irrigation water. Similarly, because of gaps in our understanding of the fate and transport of chemicals noted above, we could not eliminate chemicals from further concern based on their detection below a *de miminis* concentration. Accordingly, the selection of the Chemicals of Interest was meant to be conservative and respect the theoretical potential for these chemicals to be present in water and to present a chronic toxicity hazard.

Because the crop sampling conducted under Task 3 was a continuation of ongoing crop sampling that had been conducted prior to the MOU between the CVRWQCB and the produced water suppliers and users, Task 3 was being performed concurrently with Tasks 1 and 2. Results of this earlier sampling have been posted on the CVRWQCB website as a series of 2017 crop reports. Data collected as part of Task 3, and previously in 2017, was used as a reference point for chemical concentrations that are likely to be detected in food crops irrigated with blended produced water. These sampling results were used to inform a toxicity cut-off criterion for prioritizing the chemicals for further review in Task 2, discussed in Section 3.1.

Under Task 1 in the SOW, the stated deliverable is a list of “Chemicals of Interest”, including naturally occurring chemicals and chemical additives that were not shown to be of low concern to human health by virtue of their presence in irrigation water by the screening process performed under Task 1. The list of 143 chemicals identified as warranting further evaluation in Task 2 (i.e., the “Chemicals of Interest”) is a primary product of this Task. The list of chemicals and the process by which they were identified is described in this report.

2.0 IDENTIFYING THE LIST OF CHEMICALS TO BE EVALUATED

The extraction of oil and gas from the ground also typically brings a substantial amount of water to the surface along with the oil and gas. The byproduct water is commonly referred to as “produced” water, and volume of water produced in oil and gas extraction is typically far greater than the volume of oil and gas. The ratio of oil to produced water from an oil well is generally more than three and can be more than 20 in some locations (Water Environment Fact sheet). After separating the oil and gas from the water, the oil and gas are typically processed further prior to use; and the larger volume of water needs to be managed.

Differences in the chemical composition of the separated water can affect the ways in which the water is managed, which may involve treatment and use or disposal (Guerra et al., 2011). Typical management practices of produced water consist of water disposal wells, treatment for enhanced oil recovery operations, and/or treatment and discharge to surface impoundments (e.g., ponds). Due to the low salinity and dissolved solids content of the produced water coming from some wells in the Central Valley, at least some of the produced water from these wells has been used for the irrigation of crops meant for

human consumption. Chemicals that may be present in produced water from oil wells in the San Joaquin Valley include chemicals that are naturally occurring in the produced water and chemicals used as additives in various stages of the construction and management of oil wells and the oil/water treatment process. The list of chemicals that may be present in produced water from oil wells in the San Joaquin Valley as a result of naturally occurring sources or local practices in the use of oil field additives is described below.

2.1 Naturally Occurring Chemicals

A number of studies have characterized the naturally occurring chemicals in produced water. These studies have shown there is wide variation in the composition of produced water, which can depend on such factors as the underlying geology, age of the formation, and extraction techniques employed. GSI reviewed a number of peer-reviewed journal articles, government documents, and other published materials and compiled a list of chemicals that have been previously found in produced water and that are seemingly unrelated to the chemical additives. From our review of the literature, GSI identified 45 organic compounds and 45 inorganic compounds, including three radionuclides, likely to be found in produced water, outside of those directly added. See Appendix A for the list of chemicals found in produced water that are likely to be naturally occurring.

2.2 Additives

From December 2017 through September 2018, CVRWQCB staff issued Orders pursuant to California Water Code sections 13267 and 13267.5 to oil companies and chemical manufacturers and distributors. These Orders required, under penalty of perjury, each recipient to submit the chemical make-up of additives used during petroleum exploration, production, and treatment at facilities that use produced water for irrigation of crops for human consumption. From these responses, CVRWQCB staff generated the Oil Field Additive List. The list is periodically updated as the producers provide the Water Board with revised and updated lists of chemicals used in the production of oil and gas. The reported list of additives does not include the amount of each chemical that is used or the frequency of their use. Such data could have been useful in evaluating the potential hazards posed by a given chemical. For example, knowing that specific chemicals are used in small amounts and/or infrequently could have been used as a factor to decide whether or not to include a chemical as a Chemical of Interest for evaluation in Task 2. Similarly, knowing that a specific chemical is used frequently in large volumes could have been important in identifying a chemical as a high priority chemical. Understanding whether chemicals are used in high or low volumes would also have been valuable in evaluating the relative importance of chemical-specific data gaps (i.e., data gaps for chemicals used in small amounts would have been of less importance than data gaps for chemicals used in large amounts).

As of June 2019, the list of additive chemicals used by the oil and gas producers included 347 entries, including two radionuclides. It is possible that some chemicals detected in produced water may be the result of chemical reactions between the mixture of naturally

occurring chemicals and chemical additives or among the chemical additives alone. See Appendix B for the reported list of petroleum extraction-related chemical additives, as evaluated in this report. The combination of chemicals listed in Appendix A and Appendix B represent the chemicals evaluated in Task 1. Between the two lists there are a total of 437 chemicals. An initial review of the combined lists identified 38 entries where chemicals were part of both naturally occurring and additives chemicals, or duplicate entries were present in the list of additives. The resulting list of 399 chemicals were evaluated in Task 1.

3.0 PROCESS FOR EVALUATING THE LIST OF CHEMICALS

In the work presented here, GSI conducted the evaluation of produced water-related chemicals with the goal of eliminating some chemicals from further evaluation and identifying a subset to be evaluated further in Task 2. The steps of the evaluation process are presented below:

1. Identify agency derived published chronic toxicity values for the chemicals on the list, where available;
2. From the list of chemicals remaining after (1), a sub-list was generated in this step that comprises produced water chemicals that are constituents of food, food additives; are considered essentially non-toxic; have therapeutic oral use with low toxicity, inert compounds; and compounds that break down into one of the previously identified chemicals. These were classified as being of low concern for toxic effect
3. From the remaining chemicals—after (1) and (2)—research the available peer reviewed literature, government/industry reports, and relevant databases to identify data that characterize the toxic potential of the remaining chemicals related to chronic oral exposures;
4. From the research activities under (3), identify the sub-list of chemicals for which there are no relevant data characterizing toxic potential related to chronic oral exposures;
5. From the remaining chemicals—after (1), (2), (3), and (4)—create three sub-lists that represent: chemicals with incomplete/inconclusive chronic toxicity data, chemicals that are not chronically toxic at levels likely observed, and chemicals with quantifiable chronic toxicity;
6. For chemicals without agency derived published toxicity factors (e.g., Reference Doses) but for which toxicity test results were available, GSI developed project-specific surrogate toxicity values for the purpose of selecting chemicals for further evaluation in this study.
7. Chemicals with published toxicity values and project-specific surrogate values were further screened based on their level of toxicity and biodegradation in water.
8. Compile the list of chemicals for further review in Task 2. The list includes chemicals that did not have relevant toxicity data, chemicals with unclear/unquantified chronic toxicity, chemicals with toxicity data that met toxicity

level criteria and were inorganic or poorly biodegradable. The steps of this process along with the toxicity and biodegradability criteria used for the screening are discussed in more detail below.

3.1 Toxicity Screening Criteria Based on Consumption

GSI identified chronic oral toxicity level of 0.5 mg/kg as a threshold screening level for the purpose of prioritizing chemicals with higher toxicity for further evaluation in Task 2. This screening level was based on consideration of the amount of food crop a person is likely to consume and the range of concentrations of chemicals detected in food crop samples under Task 3. The basis of this screening criterion and the chemicals screened from further evaluation using it are described below.

The derivation of the chronic oral toxicity value of 0.5 mg/kg/day was based on two calculations. First, the calculation that a dose of 0.5 mg/kg/day is equal to a daily dose of 35 mg for a 70-kilogram person (i.e., 0.5 mg/kg/day x 70 kg = 35 mg/day). The second calculation was that a daily dose of 35 mg/day of a chemical from food crops for a person assumed to ingest 0.318 kg/day of fruits and vegetables would result if the chemical concentration in the food crop were 110 mg/kg (i.e., 35 mg/day ÷ 0.318 kg/day = 110 mg/kg). The produce consumption level of 0.318 kg/day is the average fruit and vegetable consumption level for adults in the U.S. (Rehm et al, 2018).

Except for methanol, all other chemicals were detected in crops irrigated with produced water (and sampled as part the Task 3) at concentrations well under 110 mg/kg. For most chemicals, the level of chemicals detected were at least ten times lower than 110 mg/kg. Using this criterion, chemicals with chronic oral toxicity factors greater than 0.5 mg/kg/day were screened from further consideration as not being sufficiently toxic to warrant being identified as Chemicals of Interest to be carried into Task 2.

Methanol is unique because it is a breakdown product of pectin in fruits and vegetables, which is facilitated by pectin methylesterase (Anthon and Barrett, 2010; Lund et al., 1981; OEHHA, 2012). It has been reported to be present in orange juice in the range of in the range of 11-80 ppm [mg/kg] (Lund et al 1981), for example. While the levels reported by Lund et al (1981) in orange juice are much lower than at least some of the levels reported from Task 3, the results are not directly comparable. Over 90 percent of methanol in juice and fruit smoothies is reported to be associated with pulp (Possner et al 2014); and the concentrations of methanol reported in orange juice by Lund et al (1981) were for extracted juice. The produce samples analyzed under Task 3 of this study were homogenized whole fruit samples; and, thus, are not directly comparable to results from testing extracted juice. Because methanol is a byproduct of the ripening process, another important variable affecting the methanol concentration in produce is the time between harvest and sample preparation in the laboratory. Because we don't have information on that time interval for the published studies, we can't evaluate the significance of that differences in that time interval in the different methanol levels reported in the published studies and the results from Task 3. While we do not have precise estimates of levels of methanol we would expect to find in produce, the results of published studies do

demonstrate that substantial levels of methanol are expected to be present in produce samples.

Another factor to consider when deriving a toxicity screening level based on average adult consumption patterns is whether the screening level addresses children and more vulnerable adults. As discussed above, the objective of the screening level was to support prioritizing chemicals for further evaluation and not necessarily to provide a threshold concentration for levels considered "safe". Rather, we were using the screening level to identify chemicals with higher vs lower level of interest for further evaluation. Nonetheless, the uncertainty associated with using a priority-setting tool warrants evaluation; and variability in both toxic response and exposure levels need to be considered.

Variability in toxic response due to differences between individuals, including children, is one kind of uncertainty associated with using this kind of screening level criterion. The uncertainty surrounding inter-individual variability of toxic response, more specifically sensitivity to exposure, is typically addressed when deriving toxicity values. We recognize that standard uncertainty factors designed to address the response of sensitive subpopulations is not universally adequate. For some chemicals, however, toxicity values have been developed to address the range of toxic sensitivities in the human population. We have not conducted a comprehensive review of the range of sensitivities addressed by the toxicity values that were screened using the screening-level criterion. Accordingly, there is some uncertainty in knowing if the screening-level criterion fully addresses the sensitivity of all subpopulations. The sensitivity of children and other subpopulations is at least partially addressed by the uncertainty factors originally used to derive the toxicity values that were screened in the selection of the Chemicals of Interest in Task 1.

Differences in individual consumption levels of fruits and vegetables are another uncertainty associated with the toxicity screening value used in Task 1. One specific question is whether the screening level adequately addressed the higher consumption level of fruits and vegetables by children, when consumption is estimated on the basis of kg of produce consumed per kg of body weight. According to the USEPA's (2009) Child-Specific Exposure Factors Handbook, a 13.8 kg three-year old child, for example, consumes an average of 0.19 kg of fruits and vegetables per day. Using these child-specific exposure factors and the 0.5 mg/kg toxicity factor, a chemical concentration in produce of 36.3 mg/kg would translate to an ingested dose of 0.5 mg/kg-day (0.5 mg/kg/day x 13.8 kg = 6.9 mg/day; 6.9 mg/day ÷ 0.19 kg/day = 36.3 mg/kg). Beside methanol (which was detected at a few hundred mg/kg in some crops, including mandarins, almonds, and tomatoes), zinc (which was detected at 39 mg/kg in almonds) was the only other chemical detected in food crop samples above 36 mg/kg. As noted above, methanol is a product of the ripening process; and zinc is typically found in almonds grown in California at levels in the range found in this study[1] (Yada, et al., 2013).

[1] As shown in Table 3 in the Task 3 report, zinc was detected in almond samples at levels ranging from 14 to 39 mg/kg in almonds irrigated with blended produced water and 14 to 36 mg/kg in

If we assume that the 36 mg/kg level in produce would address children and adults with higher than average produce consumption, it seems reasonable to conclude that the 0.5 mg/kg toxicity levels is a reasonable criterion to use for prioritizing the Chemicals of Interest.

3.1.1 Using Consumption Criteria to Identify Chemicals with Low Chronic Oral Toxicity

For some chemicals with available animal toxicity studies, GSI was able to classify a group as *Chemicals with Low Chronic Oral Toxicity*. To be classified to this group, respective animal studies needed to satisfy the following two conditions.

The first condition was that a no observed effect level (NOEL) needed to be identified. The NOEL is the highest exposure level used in a study where no effect is observed. The NOEL is similar to the no observed adverse effect level (NOAEL), but in identifying a NOEL an adverse effect is not observed at any exposure level used in the study. In contrast for the NOAEL, an adverse effect is observed above some exposure level.

The second condition that needed to be satisfied was that the NOEL had to be 500 mg/kg/d or larger. The value of 500 mg/kg/day was derived by applying a factor of 1000 to the factor of 0.5 mg/kg/day described above. The factor of 1000 is based on standard practices of applying a ten-fold factor to account for uncertainty associated with the uncertainty associated with extrapolating test results from animals to humans, a ten-fold factor to account for the possible presence of sensitive subpopulations in the human population, and another ten-fold factor to account for the extrapolation of sub-chronic animal studies to chronic human exposures.

3.2 Biodegradation Screening Criterion

While toxicity was the primary factor used in the selection of chemicals for further evaluation, biodegradation was also a factor in the selection of chemicals for further evaluation. More specifically, chemicals identified by the Organisation for Economic Cooperation and Development (OECD) as “poorly degradable” were identified as Chemicals of Interest and carried forward for further evaluation in Task 2. Biodegradability in water was used as the primary fate and transport screening criteria to identify the prioritized list of chemicals with toxicity data. Biodegradability classifications of ‘readily,’ ‘inherently,’ and, ‘poorly’ biodegradable, and inorganic are reported below. A memorandum from the Scientific Advisor for the CVRWQCB [Dr. William Stringfellow] provided background information on the use and interpretation of standardized tests for biodegradation in water, attached as Appendix C. In summary, these standardized tests are conservative in that they are unlikely to falsely report compounds as biodegradable when they are not. However, the tests may report compounds as not biodegradable in water when in fact they are. In general, there are three basic biodegradability classifications: readily biodegradable, inherently biodegradable, and poorly

control almonds. Yada et al., 2013, reported that zinc is present in almonds grown in California at levels of ~20 to 40 mg/kg.

biodegradable. Compounds that are classified as “readily biodegradable” by OECD guidelines can be considered to degrade rapidly in any environment; they normally report degradation of ≥ 60% in 28 days. Compounds classified as “inherently biodegradable” will degrade in the environment but may not rapidly degrade under all conditions and report degradation of > 20% but < 60% biodegradation in 28 days by naturally occurring organisms. Poorly biodegradable compounds will degrade less than 20% in 28 days under the same testing conditions and timeframe.

The biodegradation criterion was only applied to chemicals with toxicity data. If a chemical was missing biodegradation data, or if a toxicity assessment was not made, the chemical was retained for further review in Task 2.

3.3 Overview of the Evaluation

Following this procedure, GSI was able to evaluate and categorize the list of identified chemicals associated with oil and gas production that could be present in produced water; Figure 1 gives an overview of this process. Of the 399 chemicals on the list, GSI identified agency derived toxicity factors for 107 of the chemicals. For 23 of the chemicals, GSI was able to identify toxicity factors by extrapolating from the agency derived toxicity factors, as they are chemically or biologically similar chemicals. This resulted in a total of 130 chemicals with agency derived toxicity factors (Table 2)[1]. From the remaining chemicals, GSI was able to identify 71 chemicals of low concern for toxic effects at concentrations normally encountered by humans and at concentrations expected in irrigated crops (Table 4). These chemicals are constituents of food, food additives, considered non-toxic, have therapeutic oral use with low toxicity, inert compounds, or compounds that break down into one of the previously identified non-toxic chemicals. There are 59 chemicals for which GSI was unable to identify sufficient literature or data to evaluate their relevant chronic oral toxicity; these require further evaluation (Table 5). Among the remaining chemicals where relevant toxicologic data and literature were available, 69 chemicals did not show evidence of chronic toxicity from oral exposure (Table 6). There were 15 chemicals that did not have sufficient information to derive conclusions as to their toxicity (Table 7). Reasons for their inconclusive toxicity are discussed further below. For the remaining chemicals, GSI developed project-specific toxicity values that could be used as part of the process of identifying the chemicals of interest. GSI developed 51 project-specific surrogate toxicity values; they are reported in section *6.5. Chemicals with Quantified Chronic Oral Toxicity Values* (Table 3). A group of five radionuclides were identified; these comprise both naturally occurring and additive materials. One of these, uranium, was included in the group with agency derived toxicity factors due to its non-cancer toxicity; there were 4 others. After evaluating and screening these chemicals, based on the available information, 143 chemicals were identified as “Chemicals of Interest” for further review in Task 2. The remaining chemicals were not

[1] Table references are reported in this section and appear out of order. They have been identified in 3.3 as reference to the general evaluation, however, are numbered to reflect their presentation in the main content of this report. Table 1 begins the enumeration of these tables in Section 5.1.

prioritized for review in Task 2 as there is limited concern with regard to hazards they may create.

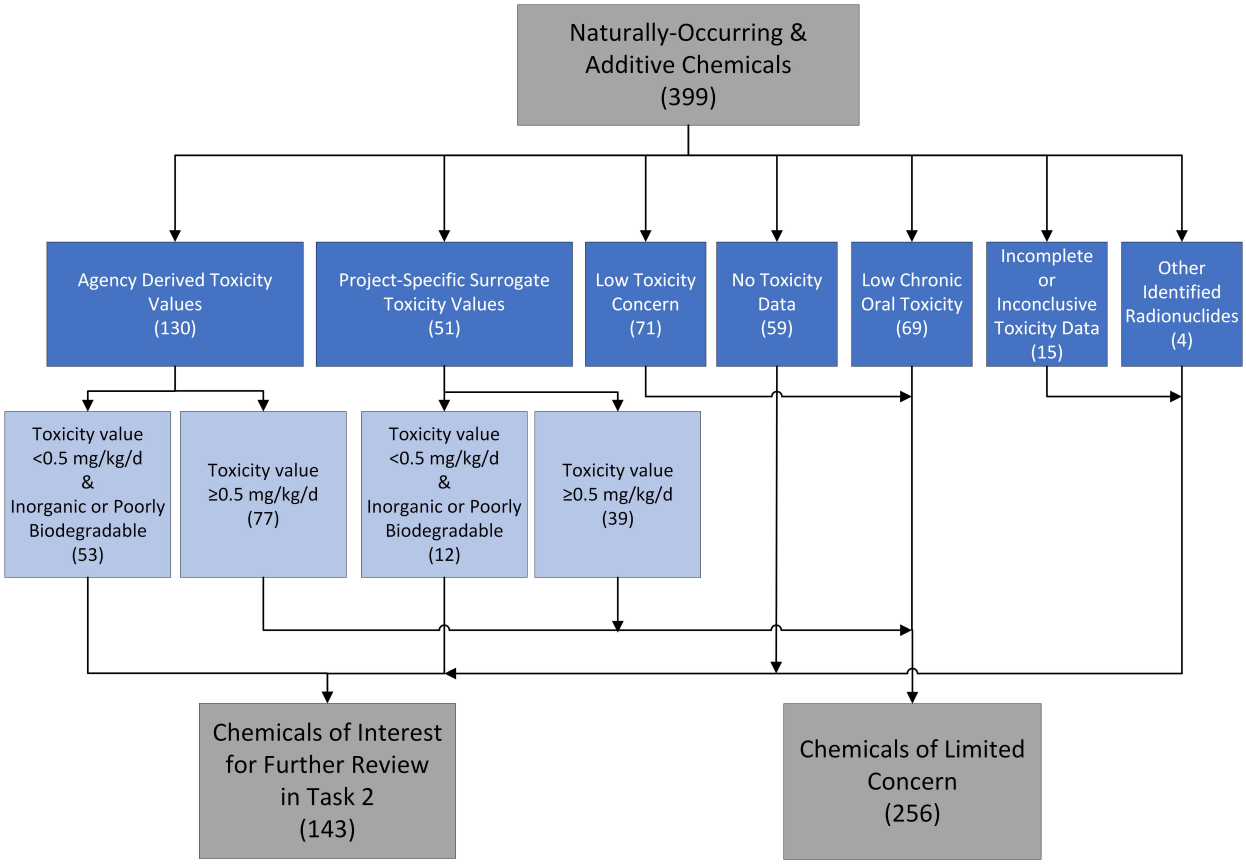

Figure 1: Flowchart presenting overview of risk-based hazard assessment of produced water related chemicals in the context of agricultural irrigation of food crops

4.0 PUBLISHED DATA USED TO EVALUATE TOXICITY

As previously noted, chronic oral toxicity was the primary factor used to prioritize chemicals for further evaluation. Oral toxicity is the most relevant route of toxicity for the evaluation of health risks from chemical exposures related to edible crops. Chronic toxicity, rather than acute toxicity, was the most relevant exposure duration because the crops need to be safe for a lifetime of consumption, and chronic toxicity limits are much lower that acute exposure limits. The first step in the search for relevant toxicity information was the review of the published government agency data described below. The units of the various toxicity values we found were standardized to represent a dose quantified in milligrams per kilogram body mass per day (mg/kg/d). Toxicity values related to non-cancer outcomes are typically reported in mg/kg/d; however, toxicity values related to cancer outcomes are typically reported in units associated with a measure of risk. These units of risk are called slope factors, unit risk values, or cancer potency values; and they need to be converted to risk-specific doses to be presented in the same

units of mg/kg/d as the non-cancer toxicity values presented to be used in the screening process described in this report.

In the case of carcinogens, published toxicity values are typically reported as cancer potency; and are usually presented as a slope factor or unit risk factor. Slope factors and unit risk factors represent the increase in cancer risk associated with a lifetime exposure of some incremental unit of exposure. For this assessment, slope factors associated with oral exposure were used to estimate risk-specific doses. This risk-specific dose is a constant lifetime average exposure level [mg/kg/d] associated with a predefined increase in cancer risk. For this assessment, the predefined lifetime excess cancer risk of 1 in 100,000 was used to calculate the standardized toxicity values. We used this value as a reference level to facilitate comparisons with non-cancer toxicity values, which are also expressed in units of mg/kg/d. Equation 1 reports the calculation for the cancer slope factor risk-specific dose. The lifetime incremental cancer risk of 1 in 100,000 is the level of risk above which warning is required under The Safe Drinking Water and Toxic Enforcement Act of 1986 (also known as Proposition 65 in California). It is also toward the lower end of the acceptable cancer risk range of 1 to 100 in a million set out in the National Contingency Plan (40 CFR 300.430), which is often cited as the basis for regulatory decision making. To put the 1 in 100,000 lifetime risk level in context, the lifetime risk for males in the United States of developing cancer is approximately 40%; for women it is approximately 38% (ACS, 2018). A 1 in 100,000 increase risk of cancer, when compared to the average risk of cancer, would represent an increased risk of about a 0.0025% above the average cancer risk in the United States.

$$risk\ specific\ dose = \frac{{}^{1}/_{100000}}{cancer\ slope\ factor\left[\frac{1}{\frac{mg}{kg}/d}\right]} = dose\ in\ \frac{mg}{kg}/d$$

Equation 1

The sources of toxicity factors used for our prioritization are identified below. A brief description of the program under which the toxicity factors were developed and how they are intended to be used in regulatory and public health programs is provided. For some chemicals, multiple agency-derived toxicity factors were available. In such cases, we selected the lowest published value for our prioritization process.

a. EPA Integrated Risk Information System (IRIS) Reference Dose (RfD)
b. EPA IRIS Oral Slope Factor for Cancer
c. EPA Provisional Peer-Reviewed Toxicity Values (PPRTV) Oral RfD
d. EPA Human Health Benchmarks for Pesticides (HHBP)
e. PPRTV Oral Slope Factor
f. Agency for Toxic Substances and Disease Registry (ATSDR) Minimal Risk Level (MRL) Oral Chronic Exposure
g. California Office of Environmental Health Hazard Assessment (OEHHA) Oral Slope Factor
h. OEHHA Child-Specific RfD

i. OEHHA Cancer No Significant Risk Level (NSRL) Oral Exposure
j. OEHHA Reproductive/Developmental Maximum Allowable Daily Dose (MADL) Oral Exposure
k. United States Geological Survey (USGS) Noncancer Human Based Screening Levels (HBSL)
l. USGS Cancer HBSL
m. Human Health Toxicity Values in Superfund Risk Assessments Health Effects Assessment Summary Table (HEAST) Oral Slope Factor
n. HEAST Chronic Oral RfD
o. HEAST Oral Exposure NOAEL
p. Other Toxicity Values Derived by Authoritative Organizations to Protect Health

4.1 United States Environmental Protection Agency Integrated Risk Information System

The United States Environmental Protection Agency (EPA) Integrated Risk Information System (IRIS) is a program within the EPA that characterizes health hazards associated with chemicals in the environment. IRIS published toxicologic assessment values that can be used in identifying risks associated with levels of exposure. Two of the toxicity values published in the IRIS database, oral chronic RfD and oral cancer slope factor, were used as potential criteria in the evaluation of the list of identified chemicals.

The oral RfD is an estimate of the chronic upper daily oral dose that is unlikely to cause an appreciable increase in risk to health during a lifetime. It can be derived from a NOAEL, lowest observed adverse effect level (LOAEL), or benchmark dose (BMD). To these observed [NOAEL and LOAEL] or derived [BMD] effect levels, it is convention in developing RfDs that uncertainty factors are applied to derive a health protective toxicity value; this is discussed in more detail later. The RfD is used to characterize risks associated with exposures related to non-cancer outcomes.

The US EPA, through IRIS, also reports oral slope factors for cancer outcomes (discussed above).

4.2 Superfund Program's Provisional Peer Review Toxicity Values

Within the Superfund Program, through the EPA, toxicological assessments of certain chemicals were made to support health hazard identification and risk assessments associated with the Superfund Program. Provisional Peer Reviewed Toxicity Values (PPRTV) are derived from review of the scientific literature; Agency methodologies, practices, and guidance are then employed for the development of toxicity values (US EPA, PPRTV). PPRTVs are available for provisional oral RfDs, provisional inhalation reference concentrations, provisional oral slope factors, and provisional inhalation unit risks. In evaluating the identified list of oil and gas extraction chemicals, provisional oral RfDs and provisional oral slope factors were used from the PPRTV database.

4.3 Agency for Toxic Substances and Disease Registry Minimal Risk Levels

The Agency for Toxic Substances and Disease Registry (ATSDR) develops Minimal Risk Levels (MRL) for hazardous substances under its responsibility to characterize chemicals likely to be found at Superfund sites. These evaluations are done in coordination with the EPA using similar methods to those used by the EPA in developing RfDs (ATSDR, 2018). That is, they may incorporate both human and animal data. Like the EPA IRIS RfD, they build in the assumption that humans are more sensitive to these chemicals than animals. They are derived for multiple exposure time regimes: acute (1-14 days), intermediate (> 14-364)[1], and chronic (≥ 365 days). It should be noted that MRLs are only defined for non-cancer outcomes and are based on the most sensitive outcome of human relevance. MRLs are not based on serious outcomes, such as irreparable kidney damage or birth defects; because of uncertainty factors that are built into the assigned toxicity value, exposures above the MRL are not expected to cause adverse health effects.

4.4 Office of Environmental Health Hazard Assessment

The Office of Environmental Health Hazard Assessment (OEHHA) is a department of the California Environmental Protection Agency (CalEPA) whose mission is to protect and enhance public health and the environment by objective scientific evaluation of risks posed by hazardous substances. Not only does OEHHA provide many of the same kinds of support in the derivation of toxicity values as the federal EPA's IRIS, but it also supports The Safe Drinking Water and Toxic Enforcement Act of 1986, otherwise known as Proposition 65. In the context of Proposition 65, OEHHA derives toxicity related dose levels for cancer, reproductive and developmental outcomes. In the evaluation of the identified chemicals related to oil and gas extraction, GSI identified the following toxicity values published by OEHHA: oral child specific RfD, oral slope factors, maximum allowable dose level (MADL) and no significant risk level (NSRL).

4.5 United States Geological Survey Human Based Screening Levels

The United States Geological Survey (USGS) Human Based Screening Levels (HBSL) are derived water standards used to supplement US EPA Maximum Contaminant Levels (MCLs) and Human Health Benchmarks for Pesticides (HHBPs). HBSLs are used to determine whether contaminants found in surface-water or groundwater sources of drinking water are a potential human-health concern. HBSLs were developed by the U.S. Geological Survey National Water-Quality Assessment (NAWQA) Project for contaminants without US EPA MCLs or HHBPs. Since HBSLs are published as water concentration values, we converted the water concentrations to the equivalent daily dose (mg/kg-day) to facilitate comparison to other toxicity values. This was done using the same assumptions used to develop the HBSL (70 kg adult drinking 2L of water per day). Ultimately, none of toxicity values based on the HBSLs were selected as reference values for the prioritization of the chemicals evaluated here.

[1] This time regime is commonly referred to as sub-chronic

4.6 Health Effects Assessment Summary Tables for Superfund

Health Effects Assessment Summary Tables (HEASTs) were published databases of human health toxicity values developed for the EPA Superfund and Resource Conservation and Recovery Act (RCRA) hazardous waste programs. Toxicity values published in these databases are provisional; as of 2002 they have been superseded by the PPRTV database. GSI included this database our search for agency-derived toxicity factors, but we did not select any values from this collection of toxicity factors.

4.7 Other Sources of Toxicological data

GSI used a web search approach to identify other published toxicity factors from government agencies or other authoritative sources and to identify toxicity data to be used for the other toxicity criteria used in the selection of chemicals for further evaluation in Task 2. In addition to Google Web Search and Google Scholar, we used health and toxicologic specific databases available on the internet; these included PubMed, National Institutes of Environmental Health (NIEHS), Chemical Effects in Biological Systems (CEBS), National Institutes of Health (NIH), Toxicology Data Network (TOXNET), NIH PubChem, World Health Organization (WHO) Concise International Chemical Assessment Document (CICAD), International Programme on Chemical Safety Information from Intergovernmental Organizations (IPCS-INCHEM), and the database of registration dossiers through the European Chemical Agency's (ECHA) Registration, Evaluation, Authorization and Restriction of Chemicals (REACH) program.

TOXNET is a metasearch database comprised of a number of health-related databases. GSI used it to identify relevant literature by focusing on results from the following databases that it contained: Hazardous Substances Data Bank (HSDB) contains peer-reviewed toxicology data for over 5,000 hazardous chemicals; TOXLINE contains 4 million references to literature on biochemical, pharmacological, physiological, and toxicological effects of drugs and other chemicals; Developmental and Reproductive Toxicology Database (DART) contains references to developmental and reproductive toxicology literature; the Household Products Database, which contains data identifying potential health effects of chemicals in more than 10,000 common household products; Haz-Map, which links jobs and hazardous tasks with occupational diseases and their symptoms and also identifies specific chemicals and hazards associated with them; and International Toxicity Estimates for Risk (ITER), which contains risk information for over 600 chemicals from authoritative groups worldwide.

Through the REACH program in the European Union, companies are required to register their substances in combination with other companies who are registering the same substance. From the registration dossier, GSI was able to identify chemical and physical properties, environmental fate and pathway information, and toxicological information. Most importantly, within the toxicological section, data from difficult-to-find and unpublished reports were made available that identified the presence or absence of relevant health effects associated with repeated dose oral exposures. These toxicity report data were used to develop project-specific surrogate toxicity values.

5.0 DEVELOPING PROJECT-SPECIFIC SURROGATE TOXICITY VALUES FOR NON-ASSESSED CHEMICALS

Toxicity values have not been derived and published by regulatory agencies or other authoritative bodies for a large number of the chemicals related to oil and gas extraction, even though toxicity information is available for some of the chemicals. There can be a variety of reasons why organizations do not develop toxicity factors for chemicals even when toxicity information is available. Such reasons may include a lack of resources, low concern for toxicity, or low concern for exposure to a chemical. In some cases, the available toxicity data may not be considered sufficient to support the derivation of a toxicity factor with a sufficient degree of confidence to be to be used for regulatory decision making. The reason an organization does not develop a toxicity factor for a chemical is not usually provided.

For purposes of this study, GSI did identify chemicals for which toxicity information was available even though a regulatory agency or other authoritative organization had not developed an exposure limit or toxicity factor. GSI reviewed the available peer-reviewed literature and industry studies to identify which of these chemicals had human or animal toxicologic data related to chronic oral exposures. GSI then used that data, to derive project-specific surrogate toxicity values following procedures used by OEHHA (e.g., application of uncertainty factors) when they develop regulatory Reference Exposure Levels (OEHHA, 2008). We recognize that technical judgement is necessary when developing exposure limits and that the values we have developed may not be the same values that OEHHA would have developed or that would have been adopted following the peer review process that OEHHA toxicity factors undergo. The toxicity values developed here are project-specific values selected for the purposes of prioritizing and selecting chemicals for further evaluation. While we have followed OEHHA guidance for developing toxicity factors, the toxicity values we have developed for the specific purpose of this evaluation are not intended to be equivalent to toxicity factors developed by OEHHA or other regulatory agencies. They are developed solely for the purpose of prioritizing chemicals for further evaluation in this project.

5.1 Methods to Develop Comparable Toxicity Values for Non-Assessed Chemicals

The toxicity values that GSI developed for this assessment were of the same form as an RfD, i.e., a dose level reported in mg/kg/d that is unlikely to adversely affect health under chronic exposure. As noted above, the methods that GSI employed in the development of these values were guided by the process employed by California's OEHHA (Salmon et al, 2002) and other government agencies when establishing health protective exposure levels, including the US EPA (US EPA, 2002). In short, the process can be thought to have four main steps: (1) development and evaluation of a database identifying studies that identify adverse outcomes related to exposures to a specific chemical; (2) identification of the critical effect, defined as "the first adverse effect, or its known precursor, that occurs to the most sensitive species as the dose rate of an agent increases"; (3) identifying the NOAEL or LOAEL associated with the critical effect; and (4)

developing the exposure level by adjusting the NOAEL or LOAEL based on uncertainty factors specific to the study in which the NOEAL or LOAEL were identified.

For nearly all chemicals that GSI developed project-specific values, there was insufficient toxicologic literature to develop databases of the scope that is typically used in these kinds of evaluations, i.e., inclusion of tens to hundreds of studies looking at outcomes in multiple species to various biologic systems. These large databases allow the EPA and other agencies to thoroughly evaluate a chemical's toxicity based on the following criteria:

- Have adequate studies been conducted to establish the target organs/endpoints?
- Have the effects been characterized for both sexes and all life stages?
- Are data pertaining to potentially susceptible subpopulations available?
- Are the responses consistent across species? Are the results of the studies biologically plausible?
- Are the route and matrix of exposure relevant to the specific reference value being derived?
- Is the duration of exposure appropriate for the specific reference value being derived?
- Is the animal species and strain appropriate for extrapolation to humans?
- To what degree may the biological endpoints be extrapolated (qualitatively and quantitatively) to humans?
- Are toxicokinetic data available? Are they available for both sexes, for relevant life stages, or for other susceptible subpopulations?
- Is the shape of the dose-response curve consistent with the known toxicokinetics of the test compound?
- Are the metabolism and toxicokinetics in the animal species similar to those of humans?
- Has the dose-response curve been replicated by, or is it consistent with, data from other laboratories and other test species?
- Have the data for all relevant endpoints been adequately modeled by the BMD or other appropriate quantitative analysis to determine the most sensitive endpoint(s)?
- How well is the toxicity characterized? Do the results of the identified studies indicate the possibility of effects on particular systems that have not yet been explored sufficiently, or do they indicate that additional studies may reveal effects not yet characterized?

For many of the chemicals, only a few relevant studies were available. GSI evaluated the toxicological studies of the non-assessed chemicals as best practicable, congruent with the overarching principles of evaluation criteria above. However, due to the limited number of available studies, truncated evaluations of the chemicals were conducted. For

inclusion in the evaluation, the studies related to toxicological properties of a chemical needed to satisfy the following:

- Is the outcome physiologically relevant to humans? In other words, do humans have the same physiological structure that the chemical can act on?
- Can the toxicokinetics of the chemical associated with the outcome in animals be plausibly extrapolated to humans? This criterion would only exclude studies if it was positively known that specific metabolic pathways of action did not apply to humans.
- Is the outcome associated with oral exposure in the sub-chronic (90-365 day) to chronic (> 1 year) exposure time period?

In identifying the critical effect, the outcome with the lowest published NOAEL or LOAEL that satisfied the three minimum criteria (above) was chosen to develop a toxicity value. As the final step in the evaluation, based on parameters specific to the identified study, a toxicity value comparable to the EPA RfD is developed by adjusting the NOAEL or LOAEL by a combination of uncertainty factors. In a few cases, GSI conducted a 'read-across assessment' when toxicity data were not available for a specific chemical. Read-across assessments are common non-testing technique used to fill data gaps and have been growing in use over the last several years for a variety of reasons, including reducing the need for animal testing (van Leeuwen et al., 2009).

For the read-across assessment, toxicity data from similar chemicals with similar functional groups were used as a substitute for the naturally occurring or additive chemical on the list. For example, toxicity data from benzenesulfonic acid C10-16-alkyl derivatives was used in the assessment of the similar alkylarylsulfonate amine salt, which does not have any specific toxicity data available. Alkylarylsulfonate amine salt is benzenesulfonic acid compounded with isopropylamine. Isopropylamine is a known irritant that can cause chemical burns with oral exposure at high concentrations, with no other known systemic effects. In addition, isopropylamine is readily biodegradable in water (ECHA, Isopropylamine), and hence, unlikely to contribute significantly to any overt toxicity of concern here, which is in addition to the benzenesulfonic acid. Read-across assessments of this kind are explicitly identified for chemicals evaluated in this report.

After following the process outlined above to identify a NOAEL or LOAEL for a critical effect, guidance was taken from the approach used in California by OEHHA to develop Reference Exposure Levels (REL). An REL is derived by taking the NOAEL or LOAEL and dividing it by a number of uncertainty factors. In developing the project-specific surrogate toxicity value comparable to a REL, up to five uncertainty factors were used to account for uncertainties in extrapolating the animal NOAEL or LOAEL to humans. These uncertainty factors were based on the studies' characteristics and include factors for: LOAEL to NOAEL extrapolation, sub-chronic to chronic extrapolation, interspecies uncertainty, intraspecies uncertainty, and database deficiency factors. Equation 2 represents the calculation of the REL. The denominator is a product of a number of potential uncertainty factors, UF_i.

$$REL = \frac{NOAEL\ or\ LOAEL}{\prod UF_i}$$ **Equation 2**

he general guidelines from the EPA in developing a RfD are to apply factors of 10 for each of the following: adjusting from animal to human, adjusting for sub-chronic to chronic, adjusting for susceptible populations, and adjusting a LOAEL to NOAEL (US EPA, 2002). The California approach is slightly more nuanced and can account for our understanding about toxicokinetics and toxicodynamics in the inter- and intraspecies extrapolations, the degree of sub-chronic extrapolation, and adjustment for data gaps. Table 1 reports the uncertainty factors used in this work based on the California guidance.

All of the chemicals for which we develop project-specific toxicity values were non-carcinogenic chemicals. Accordingly, we did not need to address carcinogenic potency of any chemicals without agency-derived toxicity factors.

6.0 RESULTS OF THE REVIEW OF CHEMICALS

The following sections report the results of the toxicologically focused prioritization assessment of chemicals that may be present in produced water. Six tables discussed in this section present the results of the review process described above and include: (1) the list of chemicals with agency derived peer-reviewed published toxicity values (Table 2); (2) chemicals for which we developed project-specific surrogate toxicity values (Table 3); (3) chemicals that are of low concern for chronic oral toxicity (Table 4); (4) chemicals without applicable toxicity data (Table 5); (5) chemicals that are not chronically oral toxicants at levels we might expect to see in food crops (Table 6); and (6) chemicals with incomplete toxicity information (Table 7) . A final table presents the results of screening the list of chemicals in (1) and (6) based on toxicity level and biodegradability in water (Table 9).

6.1 Chemicals with Agency Derived, Peer-Reviewed Toxicity Values

Table 2 identifies 130 chemicals within the list of 399 chemicals potentially present in produced water that have agency derived, peer-reviewed toxicity values based on chronic oral exposure. The chemicals are ordered from lowest to highest assigned screening toxicity values. For each chemical listed in Table 2, other relevant information is also presented including, chemical identification through chemical name and Chemical Abstract Service Registry Number (CASRN), the Organisation for Economic Co-operation and Development (OECD) biodegradation in water classification, and an indicator representing whether the chemical is naturally occurring and/or is an oil an additive. There are two categories of screening toxicity values reported in Table 2 based in the source of the screening value. The first source is organizational peer reviewed (OPR) published toxicity values; these are toxicity values that are published by government agencies or other authoritative organizations and used for risk assessments or the protection of public health. This also includes risk-specific doses calculated using agency derived cancer slope factors. The second source are values based on read-across

assessments in which the basis of the chemical-specific read-across value is an agency-derived toxicity factor. The “Source of Value” column in Table 2 notes if a value is based on toxicity values from regulatory agencies or other authoritative organizations (“OPR”) or if the value was derived by read-across methods (“RA – OPR”).

Chemicals in this list were eliminated from further consideration if they had a toxicity screening value greater than 0.5 mg/kg/d and they were not identified by the OECD as being “poorly biodegradable” or inorganic.

6.2 Chemicals with Project-Specific Surrogate Toxicity Values

Table 3 reports the list of 51 chemicals for which GSI developed project-specific surrogate toxicity values. The information in Table 3 is similar to that in Table 2, with the addition of a short description of the data/study that informed the development of the project-specific surrogate toxicity value. As in Table 2, chemicals in Table 3 are listed from the lowest to the highest assigned toxicity screening value.

The screening evaluation of chemicals based on the project-specific surrogate toxicity values are being reported separately from those with published toxicity values, as there were more limited data available for the derivation of the screening toxicity factors presented in Table 3. Uncertainties related to database deficiencies in these assessments may unduly bias the developed values. This bias could serve to make chemicals appear more toxic than they are for the simple reason that additional uncertainty factors were applied due to the more limited toxicity data.

Like the chemicals addressed in Table 2 and as indicated in Figure 1, chemicals were eliminated from further consideration if they had a toxicity value greater than 0.5 mg/kg/d and were not identified by the OECD as “poorly biodegradable”.

6.3 Chemicals of Low Concern for Chronic Oral toxicity

After identifying chemicals with published values, GSI identified 71 of the chemicals (see Table 4) that are of low concern for chronic oral toxicity, based on:

- Known constituents of the human diet, in that they are normally and naturally found in unadulterated food for humans
- Common food additives or supplements; this includes chemicals that have therapeutic use through ingestion that are known to be essentially non-toxic
- Other chemicals considered to be essentially non-toxic, i.e., those where human exposures have not shown adverse effects
- Inert chemicals
- Upon combination with water, the chemical will react and become one of the previously mentioned groups

Many of the chemicals in Table 3 are readily recognized as not being of toxicological concern, but additional discuss in provided below for 13 of the chemicals that may not be

readily recognized as being of low concern for toxicity if present in irrigation water. These 13 chemicals include:

1. Dimethyl siloxane and silicones, which are used in the biomedical field and in cosmetics as emollients, have been heavily researched and found to be virtually non-toxic to mammals through ingestion (Moretto et al., 2005). It is also called simethicone and used as an over-the-counter medication to break up bubbles and relieve the symptoms of bloat/gas.

2. The same assessment can be applied to polydimethylsiloxane emulsion as for dimethyl siloxane and silicones (Moretto et al., 2005). All of the siloxane compounds may be the same. CASRN identification was not provided for 2 of 3 entries in the list of additive chemicals.

3. Hydroxymethyl cellulose, which is used as a thickening agent, is not absorbed to an appreciable degree and appears unchanged in feces after ingestion (Bingham et al., 2001).

4. Ethoxylated sorbitan monooleate, otherwise known as polysorbate 80 is used in both the food and cosmetics industry where it is regarded as safe by ingestion (Rowe et al., 2006).

5. Magma fiber, which is a mineral fiber that is soluble in acidic environments, typically contains calcium oxide (CaO), magnesium oxide, and aluminum (III) oxide. Under acidic aqueous environments, this may enrich waters with calcium, magnesium, and aluminum ions. Of the three, there is some concern over increased aluminum concentrations. Toxicity with chronic aluminum exposure is addressed later in the list of Chemicals of Interest.

6. Polyethylene terephthalate (PET) oral toxicity is expected to be low. It is used as a packaging material and health concerns are related to irritation (DAK Americas, 2008). Some concern exists over antimony migration from PET into water due to residual antimony left over from its production (Keresztes et al., 2009). Potential antimony exposures are specifically addressed later in the list of chemicals of interest.

7. Hydrochloric acid is naturally produced in the stomach as a digestive agent (pH 1.5 to 3.0). Its toxicity is related to its corrosivity, which is directly related to its pH level. We do not expect hydrochloric acid to be present in produced water at levels that would measurably affect pH, much less be corrosive to tissue. Other than an imperceptible effect on pH, hydrochloric acid will increase the concentration of chloride ions. Chloride ions are found in food and table salt and would not be of any toxicological consequence in produced water from ingestion.

   The reported pH of blended produced water ranges between 5.9 to 8.1 with a mean of 7 and a standard deviation of 0.5. This suggests that any hydrochloric acid used

in oil production is substantially diluted and neutralized by the time it makes its way into blended irrigation water.

8. Cellophane is produced by treating cellulose with an alkali and carbon disulfide to create viscose. In its production, toxicity arises due to the carbon disulfide (CS_2) that is used during manufacturing of viscose (Kuo et al., 1997), which is the parent material of cellophane. CS_2, however, is carefully recovered during manufacturing, allowing the cellophane to be used to wrap food stuff. It has been used since the early 1900's to wrap food stuff with no known concerns to health; it is readily biodegradable (Lamot and Voets, 1978). Given its long history of use with no known health concerns, and the innocuous nature of its biodegradation by-products, there is no reason to carry cellophane forward as a Chemical of Interest for this project.

9. Saponite is a group of clay minerals with some research looking at their toxicities. Saponite is a subtype of smectite. In one study, rats were fed montmorillonite (a different subtype of smectite) with their chow during pregnancy; and no effects were observed in the dam or offspring (Wiles et al., 2004). It is expected that there is low toxicity associated with these clays (Zoltan et al., 2005). Smectite clays are used in the production of pelletized animal food (Odom et al., 1984).

10. Because of the chemical similarity of smectite and saponite clays and the historical use of smectite clays in pelletized animal food, we expect that both clays have low toxicity.

11. Sodium hypochlorite is the active ingredient in common household bleach. It is widely used in drinking water to control bacteria, viruses, and parasites. Sodium hypochlorite reacts in water to form hypochlorous acid, and it forms hypobromous acid in the presence of bromine. These acids can react with organic compounds in the water creating by-products known as trihalomethanes. Trihalomethanes are common disinfection by-products but are highly volatile. In a review of the available blended irrigation water quality data from the study area, chloroform, bromoform, bromodichloromethane, and dibromochloromethane were all reported as non-detects. These results suggest that trihalomethanes are not a concern in blended irrigation water. The fact that trihalomethanes were not present at detectable levels may be attributable to sodium hypochlorite being significantly diluted and/or is only used in small amounts. The absence of detectable levels of trihalomethanes may also be attributable to the fact that trihalomethanes are volatile and would be expected to volatilize from water during storage and transport in open ponds and irrigation canals.

12. Magnesium is a dietary requirement and is commonly ingested as a dietary supplement. The tolerable upper limit for supplemental magnesium in a young child is 65 mg and for an adult is 350 mg (IOM, 1997). For a 10 kg child, a more sensitive receptor, the upper tolerable limit is 6.5 mg/kg/day. It is not expected that levels of magnesium in produced water would be very high; it was reported in

Guerra et al. (2011) that magnesium in produced water was in the range of 1.2 mg/L, which for a 10 kg child, drinking 1 L per day would equate to a dose of 0.12 mg/kg/d. While adverse effects from too much magnesium consumption have been reported following the ingestion of too much magnesium in dietary supplements, laxatives, or antacids, there are no reports of magnesium as a food safety issue. Because exposure at levels expected to cause even mild effects are not reasonably expected, there is no reason to carry magnesium forward as a Chemical of Interest.

13. Ammonium chloride is an acidifying agent used to treat alkalosis and metabolized as ammonia, which doesn't appear to demonstrate chronic toxicity through ingestion (TOXNET, 2015a).

6.4 Chemicals Without Data to Identify Toxicity

Table 5 reports 59 chemicals where there was insufficient data to evaluate their chronic oral toxicity. For the chemicals on this this list, we were not able to identify agency-derived toxicity values or toxicity studies. We were also not able to identify toxicity data for structurally or biologically similar chemicals to support evaluation using read-across methods. Several of the chemicals on the list identified with ambiguous names and without an CASRN. Because toxicity factors and toxicity tests generally involve identifiable substances, if not specific molecules, the ambiguous identification of some chemicals prevented us from identifying toxicity information for the chemicals. Several substances on the list appear to be chemicals in commerce but which may not have been tested for oral toxicity because the opportunity for exposure by ingestion was not likely (e.g., lignite and tall oil). Some of the chemicals in Table 5 are polymers. While polymers are generally considered to have low toxicity themselves, chemicals that could pose toxicity concerns may leach from the polymers. The chemicals listed in Table 5 could not be eliminated from needing further evaluation and are being identified as requiring further evaluation under Task 2.

6.5 Chemicals with Low Chronic Oral Toxicity

The 69 chemicals listed in Table 6 were identified as not exhibiting chronic oral toxicity at exposure levels reasonably expected to be associated with the ingestion of crops irrigated with produced water or through the oral route of exposure. Because of the low chronic oral toxicity exhibited by these chemicals, we identified them as not warranting further evaluation. The chemicals in Table 6 are similar to the chemicals listed in Table 3 in that chemicals in both tables were eliminated from further evaluation because of low toxicity. Unlike the chemicals in Table 3, which includes chemicals approved as food additives, constituents of over-the-counter medicines, dietary supplements, or were essentially inert, the chemicals in Table 6 have not been approved for such uses. Nonetheless, they do exhibit such low chronic oral toxicity that they can be eliminated from further evaluation as Chemicals of Interest in produced water used for food crop irrigation.

Some of the chemicals in Table 6 are only toxic through routes of exposure other than oral (e.g., crystalline silica through inhalation), and some are recognized as being

toxicologically inert (e.g., polyethylene). We also eliminated from further consideration chemicals where animal test data reported no observed effects for carcinogenic, reproductive/developmental, and systemic effects and the NOEL was greater than or equal to 500 mg/kg/d. The basis of the 500 mg/kg/day cutoff level is based on the evaluation of the likely level of consumption of fruits and vegetables discussed earlier in Section 3.1.

6.6 Chemicals with Incomplete or Inconclusive Chronic Oral Toxicity

For the 15 chemicals listed in Table 7, data found during the literature search for oral toxicity data was available but was either insufficient or contradictory, which prevented eliminating the chemicals from further evaluation. Specific reasons for classification of each of the chemicals in this group are provided in the table. In four cases, there was a lack of congruence between the chemical name provided and the CASRN, precluding identification of the unique chemical and evaluation of the toxicity of a specific chemical or substance. Another oil field additive was reported as “aromatic amine”, which is a chemically ambiguous identification. As discussed, more fully below, “aromatic amines” can include a variety of specific chemicals with relatively high toxicity.

Aromatic amines are a broad group of chemicals listed as oil field additives by the producers. The lack of specificity in identifying the specific aromatic amines used in the additives made it difficult to evaluate toxicity of the identified additive. Aromatic amines can cause moderate to severe poisoning, with symptoms ranging from headache, dizziness, and ataxia to anemia, cyanosis, and reticulocytosis and cancer (Patnaik, 1992). In general, the most sensitive outcomes related to chronic exposure to aromatic amines appear to be cancer related. For example, the non-cancer RfD published by EPA in the IRIS database for Benzidine is 0.003 mg/kg/d. In contrast, for the same chemical, a dose associated with a 1 in 100,000 increase in cancer is 0.0004 mg/kg/d—a dose that is nearly 10 times smaller. IARC has evaluated a number of aromatic amines as to their carcinogenicity in Monograph 99 (IARC, 2010a). Below, in Table 7, is the list of aromatic amines evaluated in the monograph and the conclusions drawn from their scientists’ evaluations as to their carcinogenicity.

6.7 Radionuclides

Naturally occurring radioactive materials are known to exist in produced water (Otto, 1989). They are incorporated in the petroleum deposit materials due to the dissolution of surrounding minerals over a long period of time. Zielinski and Otton (1999) identified radium (Ra) and uranium (U) as two naturally occurring elements that are found in produced water. Radium is typically found in produced water as only two of 33 known isotopes, Ra-226 and Ra-228. Radium produces both alpha and gamma radiation. Uranium has toxicity separate from its radioactivity, and this facet of its toxicity is identified in the peer-reviewed published toxicity values and is included in Table 2. In addition, two radionuclides were reported as being present in additives used by the oil and gas industry during production; these were krypton 85 (Kr-85) and xenon 133 (Xe-133). The additive radionuclides emit beta radiation, and a small amount of gamma radiation in the case of

Kr-85. A more comprehensive review of these radioactive elements, their decay products and half-life in the context of water quality measurements taken of the produced water will follow in the literature review, Task 2.

6.8 Chemicals of Interest

Table 9 reports the final priority screening of naturally occurring and additive chemicals with toxicity data. Chemicals were screened based on toxicity and biodegradation in water. For toxicity, chemicals that had sufficiently low oral chronic toxicity (i.e., chemicals with a toxicity or toxicity comparison value greater than 0.5 mg/kg/d) were screened from further evaluation in addition to those to that were 'inherently' and 'readily' biodegradable. Application of this selection rule resulted in a list that contains 65 of the 180 chemicals listed in Tables 2 and 3. Of the 65 chemicals, 53 are based on agency derived toxicity values and 12 are based on project-specific surrogate toxicity values.

The complete list of Chemicals of Interest to be reviewed further in Task 2 is comprised of chemicals for which we have toxicity data of varying degrees. The list of chemicals includes: 53 chemicals for which there are agency derived, peer reviewed toxicity values; 12 chemicals where project-specific surrogate values were developed for their assessment; 59 chemicals with no relevant toxicity data, 15 chemicals with incomplete or inconclusive information needed to make an assessment, and an additional 4 identified radionuclides. This list of chemicals is summarized in Tables 4, 6, 9, and the 4 other radionuclides discussed in Section 6.7. This total list representing the 'Chemicals of Interest' is reported in Appendix D.

7.0 DISCUSSION

The work described in this report was a risk-based evaluation of produced water-related chemicals that potentially pose human health risks associated with the reuse of produced water for agricultural irrigation. This work began with the development of a list of 399 chemicals that may be present in the produced water. The list includes naturally occurring compounds that have been detected in produced water from a variety of oil fields and reported chemical additives associated with oil production in the San Joaquin Valley. We recognize that the chemistry of different production zones and the produced water from different oil fields will vary. For this reason, all of the identified naturally occurring chemicals may not be present in the produced water that is the subject of the MOU. The list of oil field additives includes chemicals reported to the CVRWQCB that are used during oil production in the San Joaquin Valley. Use of this more inclusive approach to identifying candidate chemicals for the screening evaluation is intended to minimize the chances of overlooking important chemicals. Starting with a longer list of chemicals also enhances the value of the results of this exercise for any future evaluations of the beneficial use of produced water in other oil fields. We also recognize that new chemicals not evaluated in this study may be used in the future.

As discussed above, 256 of the 399 initially identified chemicals were eliminated from further concern because it is unlikely that they pose a human health risk to people consuming crops irrigated with produced water. The 143 chemicals carried forward for

further evaluation in Task 2 are not necessarily expected to pose a health risk, but we did not have enough information from the initial screening performed in Task 1 to eliminate them from further concern. While the primary focus in Task 1 was the toxicity of the chemicals, the primary focus in Task 2 will be a review of the literature to provide a better understanding about how these chemicals will behave in an agricultural environment. Table 10 reports the outline and summary of sections in the Task 2 literature review. We recognize that the movement of chemicals in irrigation water through the soil to the roots and the subsequent uptake by plants involves complicated and incompletely understood chemical and biological processes. Accordingly, we do not expect to be able to eliminate a substantial fraction of the chemicals carried forward to Task 2 based on rigorous fate and transport criteria. While the primary focus of Task 2 is to understand the ultimate fate of these chemicals in an agricultural environment, we will also search for additional information on the toxicity of some of the chemicals that could not be eliminated from further concern by the Task 1 screening evaluation (e.g., the polymers). The Task 2 report will include a discussion of the movement of chemicals through soil and plant uptake and will identify some of the key uncertainties associated with the soil migration and plant uptake of chemicals in produced water. The Task 3 report will include results from laboratory analyses of crops irrigated with produced water will include a comparison of the results from testing crops irrigated with produced water and crops irrigated with irrigation water that does not include produced water.

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Table 1: Uncertainty factors used to develop RELs

Uncertainty Factor	Value Used
LOAEL Factor	1 if NOAEL, any effect 10 if LOAEL, any effect
Interspecies Factor	1 human observation √10 non-human primate 10 when no data on toxicokinetics or toxicodynamic differences between humans and non-primate test species
Intraspecies Factor	1 if human study including sensitive subpopulations (e.g., infants and children) √10 if studies including human studies with normal adult subjects only, but no reason to suspect additional susceptibility of children 10 if suspect additional susceptibility of children (e.g., exacerbation of asthma, neurotoxicity)
Subchronic Factor	1 if study duration >12% of estimated lifetime √10 if study duration 8-12% of estimated lifetime 10 if study duration <8% of estimated lifetime
Database Deficiency Factor	1 if no substantial data gaps √10 if substantial data gaps including, but not limited to, developmental toxicity

Table 2: List of chemicals with agency derived, peer-reviewed toxicity values ordered from most to least toxic

CASRN	Chemical Name	Notes	Toxicity Screening Value (mg/kg/d)	Source of Value[1]	OECD Biodegradation Category	Oil Field Additive?	Naturally Occurring?
79-06-1	Acrylamide	1 in 100000 cancer risk dose (CalEPA, OEHHA)	0.000002	OPR	Readily Biodeg.	Y	N
53-70-3	Dibenzo(a,h)anthracene	1 in 100000 cancer risk dose (CalEPA, OEHHA)	0.000002	OPR	Poorly Biodeg.	N	Y
50-32-8	Benzo(a)pyrene	1 in 100000 cancer risk dose (CalEPA, OEHHA)	0.000003	OPR	Poorly Biodeg.	N	Y
119-65-3	Isoquinoline	1 in 100000 cancer risk dose (US EPA, IRIS); quinoline used as a read-across compound	0.000003	RA - OPR	Poorly Biodeg.	Y	N
111-44-4	Bis (2-chloroethyl) ether	1 in 100000 cancer risk dose (CalEPA, OEHHA)	0.000004	OPR	Poorly Biodeg.	N	Y
7440-38-2	Arsenic	1 in 100000 cancer risk dose (US EPA, IRIS)	0.000007	OPR	Inorganic	N	Y
56-55-3	Benzo(a)anthracene	1 in 100000 cancer risk dose (CalEPA, OEHHA)	0.000008	OPR	Poorly Biodeg.	N	Y
205-99-2	Benzo(b)fluoranthene	1 in 100000 cancer risk dose (CalEPA, OEHHA)	0.000008	OPR	Poorly Biodeg.	N	Y
193-39-5	Indenopyrene	1 in 100000 cancer risk dose (CalEPA, OEHHA)	0.000008	OPR	Poorly Biodeg.	N	Y
100-44-7	Benzyl chloride	1 in 100000 cancer risk dose (US EPA, IRIS)	0.00006	OPR	Readily Biodeg.	Y	N
218-01-9	Chrysene	1 in 100000 cancer risk dose (CalEPA, OEHHA)	0.00008	OPR	Poorly Biodeg.	N	Y
91-20-3	Naphthalene	1 in 100000 cancer risk dose (CalEPA, OEHHA)	0.00008	OPR	Inherent Biodeg.	Y	Y
123-91-1	1,4 Dioxane	1 in 100000 cancer risk dose (US EPA, IRIS)	0.0001	OPR	Non-biodeg.	Y	N
71-43-2	Benzene	1 in 100000 cancer risk dose (CalEPA, OEHHA)	0.0001	OPR	Readily Biodeg.	Y	Y
7440-43-9	Cadmium	MRL (CDC, ATSDR)	0.0001	OPR	Inorganic	Y	Y
7439-97-6	Mercury	REL (CalEPA, OEHHA)	0.0002	OPR	Inorganic	Y	Y
7440-48-4	Cobalt	RfD (US EPA, PPRTV)	0.0003	OPR	Inorganic	N	Y
7439-92-1	Lead	Based on FDA's provisional total tolerable intake level (PTTIL) for lead by small children (20 kg) of 6 micrograms per day (FDA, 2006)	0.0003	OPR	Inorganic	Y	Y
7440-36-0	Antimony	RfD (US EPA, IRIS)	0.0004	OPR	Inorganic	N	Y
1309-64-4	Antimony trioxide	See Antimony, RfD (US EPA, IRIS).	0.0004	RA - OPR	Inorganic	Y	N
107-02-8	Acrolein	RfD (US EPA, IRIS)	0.0005	OPR	Readily Biodeg.	Y	N
50-00-0	Formaldehyde	1 in 100000 cancer risk dose (CalEPA, OEHHA)	0.0005	OPR	Readily Biodeg.	Y	N
100-41-4	Ethylbenzene	1 in 100000 cancer risk dose (CalEPA, OEHHA)	0.0009	OPR	Readily Biodeg.	Y	Y

[1] OPR: Organizational Peer Reviewed Toxicity Value [usually agency derived]; RA – OPR: Read-across assessment using an Organizational Peer Reviewed Toxicity Value

CASRN	Chemical Name	Notes	Toxicity Screening Value (mg/kg/d)	Source of Value[1]	OECD Biodegradation Category	Oil Field Additive?	Naturally Occurring?
5064-31-3	Trisodium nitrilotriacetate	1 in 100000 cancer risk dose (CalEPA, OEHHA)	0.001	OPR	Readily Biodeg.	Y	N
7440-41-7	Beryllium	RfD (US EPA, 2018)	0.002	OPR	Inorganic	Y	Y
111-42-2	Diethanolamine	RfD (US EPA, PPRTV)	0.002	OPR	Readily Biodeg.	Y	N
7439-93-2	Lithium	RfD (EPA, PPRTV)	0.002	OPR	Inorganic	N	Y
554-13-2	Lithium carbonate	See Lithium, RfD (EPA, PPRTV)	0.002	RA - OPR	Inorganic	Y	N
13453-71-9	Lithium chlorate	See Lithium, RfD (EPA, PPRTV)	0.002	RA - OPR	Inorganic	Y	N
7447-41-8	Lithium chloride	See Lithium, RfD (EPA, PPRTV)	0.002	RA - OPR	Inorganic	Y	N
1310-65-2	Lithium hydroxide	See Lithium, RfD (EPA, PPRTV)	0.002	RA - OPR	Inorganic	Y	N
13840-33-0	Lithium hypochlorite	See Lithium, RfD (EPA, PPRTV)	0.002	RA - OPR	Inorganic	Y	N
107-19-7	Propargyl alcohol	RfD (US EPA, IRIS)	0.002	OPR	Readily Biodeg.	Y	N
7440-47-3	Chromium	RfD (US EPA, IRIS)	0.003	OPR	Inorganic	Y	Y
7440-61-1	Uranium	RfD (US EPA, IRIS)	0.003	OPR	Inorganic	N	Y
91-57-6	2-Methylnaphthalene	RfD (US EPA, IRIS)	0.004	OPR	Readily Biodeg.	N	Y
140-88-5	Ethyl acrylate	RfD (US EPA, PPRTV)	0.005	OPR	Readily Biodeg.	Y	N
7439-98-7	Molybdenum	RfD (US EPA, IRIS)	0.005	OPR	Inorganic	N	Y
7782-49-2	Selenium	RfD (US EPA, IRIS)	0.005	OPR	Inorganic	N	Y
7440-22-4	Silver	RfD (US EPA, IRIS)	0.005	OPR	Inorganic	N	Y
90-12-0	1-Methylnaphthalene	RfD (US EPA, PPRTV)	0.007	OPR	Readily Biodeg.	N	Y
526-73-8	1,2,3-Trimethylbenzene	RfD (US EPA, IRIS)	0.01	OPR	Readily Biodeg.	Y	N
95-63-6	1,2,4-Trimethylbenzene	RfD (US EPA, IRIS)	0.01	OPR	Readily Biodeg.	Y	N
108-67-8	1,3,5-Trimethylbenzene	RfD (US EPA, IRIS)	0.01	OPR	Readily Biodeg.	Y	N
7440-50-8	Copper	MRL (ATSDR)	0.01	OPR	Inorganic	Y	Y
7758-99-8	Copper sulfate pentahydrate	MRL (CDC, ATSDR); read across, copper sulfate used as read-across, based on acute gastrointestinal effects	0.01	RA - OPR	Inorganic	Y	N
7553-56-2	Iodine	MRL (CDC, ATSDR)	0.01	OPR	Inorganic	Y	N
7440-02-0	Nickel	REL (CalEPA, OEHHA)	0.01	OPR	Inorganic	Y	Y
7786-81-4	Nickel sulfate	REL (CalEPA, OEHHA)	0.01	OPR	Inorganic	Y	N
7440-62-2	Vanadium	MRL (CDC, ATSDR)	0.01	OPR	Inorganic	N	Y

CASRN	Chemical Name	Notes	Toxicity Screening Value (mg/kg/d)	Source of Value[1]	OECD Biodegradation Category	Oil Field Additive?	Naturally Occurring?
105-67-9	2,4-Dimethylphenol	RfD (US EPA, IRIS)	0.02	OPR	Readily Biodeg.	N	Y
108-90-7	Chlorobenzene	RfD (US EPA, IRIS)	0.02	OPR	Poorly Biodeg.	N	Y
129-00-0	Pyrene	RfD (US EPA, IRIS)	0.03	OPR	Poorly Biodeg.	N	Y
64742-95-6	Solvent naphtha, petroleum, light arom.	RfD (US EPA, PPRTV)	0.03	OPR	Poorly Biodeg.	Y	N
29868-05-1	Alkanolamine phosphate	See Monoethanolamine	0.04	RA - OPR	Poorly Biodeg.	Y	N
206-44-0	Fluoranthene	RfD (US EPA, IRIS)	0.04	OPR	Poorly Biodeg.	N	Y
86-73-7	Fluorene	RfD (US EPA, IRIS)	0.04	OPR	Readily Biodeg.	N	Y
123-31-9	Hydroquinone	RfD (US EPA, PPRTV)	0.04	OPR	Inherent Biodeg.	Y	N
141-43-5	Monoethanolamine	NSF International evaluated the noncancer oral toxicity data for ethanolamine and calculated a reference dose (RfD) of 0.04 mg/kg-day. The RfD was based on a NOAEL of 120 mg/kg-day for maternal toxicity observed in pregnant rats that received ethanolamine via gavage (Hellwig and Liberacki, 1997).	0.04	OPR	Readily Biodeg.	Y	N
1341-49-7	Ammonium bifluoride	MRL (CDC, ATSDR) as fluoride	0.05	OPR	Readily Biodeg.	Y	N
16984-48-8	Fluoride	MRL (CDC, ATSDR)	0.05	OPR	Inorganic	N	Y
7664-39-3	Hydrofluoric acid	MRL (CDC, ATSDR) as fluoride	0.05	OPR	Inorganic	Y	N
95-48-7	o-Cresol	RfD (US EPA, IRIS)	0.05	OPR	Readily Biodeg.	N	Y
83-32-9	Acenaphthene	RfD (US EPA, IRIS)	0.06	OPR	No data	N	Y
208-96-8	Acenaphthylene	RfD (US EPA, PPRTV)	0.06	OPR	Inherent Biodeg.	N	Y
111-76-2	2-Butoxyethanol	MRL (CDC, ATSDR)	0.07	OPR	Readily Biodeg.	Y	N
108-88-3	Toluene	RfD (US EPA, IRIS)	0.08	OPR	Readily Biodeg.	Y	Y

CASRN	Chemical Name	Notes	Toxicity Screening Value (mg/kg/d)	Source of Value[1]	OECD Biodegradation Category	Oil Field Additive?	Naturally Occurring?
104-76-7	2-Ethylhexan-1-ol	NSF International evaluated the noncancer oral toxicity data for 2-ethylhexanol (2-EH) and calculated a reference dose (RfD) of 0.1 mg/kg-day. The RfD was based on a NOAEL of 36 mg/kg-day observed in a chronic gavage study in Fischer rats (Astill et al., 1996), in which there was a reduction in mean body weight of 10% or greater, and altered organ weights compared to concurrent controls. NSF International applied a composite uncertainty factor of 300 (10 each for inter- and intraspecies extrapolation and 3 for database deficiencies).	0.1	OPR	Inherent Biodeg.	Y	N
98-82-8	Cumene	RfD (US EPA, IRIS)	0.1	OPR	Readily Biodeg.	Y	N
5989-27-5	d-Limonene	d-Limonene is a major component in the oil of citrus fruit peels. IPCS has evaluated the noncancer oral toxicity data for d-Limonene, and derived a tolerable daily intake (TDI) of 0.1 mg/kg-day based on a NOAEL of 10 mg/kg-day for increased relative liver weight observed in rats in a subchronic oral gavage study (Webb et al., 1989) and a composite uncertainty factor of 100 (10 each for intraspecies and interspecies differences).	0.1	OPR	Readily Biodeg.	Y	N
84-74-2	di-n-Butylphthalate	RfD (US EPA, IRIS)	0.1	OPR	Readily Biodeg.	N	Y
111-30-8	Glutaraldehyde	MRL (CDC, ATSDR)	0.1	OPR	Readily Biodeg.	Y	N
7439-96-5	Manganese	RfD (US EPA, IRIS)	0.1	OPR	Inorganic	N	Y
14797-65-0	Nitrite	RfD (US EPA, IRIS)	0.1	OPR	Inorganic	N	Y
8028-48-6	Orange terpenes	See d-Limonene as read-across assessment. This is an unspecified mixture of compounds derived from citrus. Many of the compounds are reported as citrus terpenes or d-Limonene.	0.1	RA - OPR	Readily Biodeg.	Y	N
59-50-7	p-Chloro-m-cresol	RfD (US EPA, PPRTV)	0.1	OPR	Readily Biodeg.	N	Y
106-44-5	p-Cresol	MRL (CDC, ATSDR)	0.1	OPR	Readily Biodeg.	N	Y
7446-09-5	Sulfur dioxide	MADL (CalEPA, OEHHA)	0.1	OPR	Inorganic	Y	N
79-10-7	Acrylic Acid	RfD (US EPA, PPRTV)	0.2	OPR	Readily Biodeg.	Y	N
7727-43-7	Barite	See Barium, MRL (CDC, ATSDR)	0.2	OPR	Inorganic	Y	N
7440-39-3	Barium	MRL (CDC, ATSDR)	0.2	OPR	Inorganic	Y	Y
7440-42-8	Boron	Rfd (US EPA, IRIS)	0.2	OPR	Inorganic	N	Y

CASRN	Chemical Name	Notes	Toxicity Screening Value (mg/kg/d)	Source of Value[1]	OECD Biodegradation Category	Oil Field Additive?	Naturally Occurring?
108-91-8	Cyclohexylamine	RfD (US EPA, IRIS)	0.2	OPR	Readily Biodeg.	Y	N
107-22-2	Glyoxal	IPCS has evaluated the noncancer oral toxicity data for glyoxal, and derived a tolerable daily intake (TDI) of 0.2 mg/kg-day based on a NOAEL of 100 mg/kg-day for a dose-related decrease of water and food consumption and body weight observed in a 28-day rat drinking water study (Societe Francaise Hoechst, 1987). IPCS applied a total uncertainty factor of 500 (10 each for inter- and intraspecies differences and 5 for less-than-lifetime exposure).	0.2	OPR	Readily Biodeg.	Y	N
12179-04-3	Sodium tetraborate pentahydrate	MRL (CDC, ATSDR) as boron	0.2	OPR	Inorganic	Y	N
1330-20-7	Xylene	RfD (US EPA, IRIS)	0.2	OPR	Readily Biodeg.	Y	Y
120-12-7	Anthracene	RfD (US EPA, 2018)	0.3	OPR	Poorly Biodeg.	N	Y
128-37-0	Butylhydroxytoluene	RfD (US EPA, PPRTV)	0.3	OPR	Inherent Biodeg.	N	Y
110-54-3	Hexane	RfD (US EPA, PPRTV) for n-Hexane	0.3	OPR	Readily Biodeg.	N	Y
8008-20-6	Kerosene	MRL (CDC, ATSDR)	0.3	OPR	Inherent Biodeg.	Y	N
108-95-2	Phenol	RfD (US EPA, IRIS)	0.3	OPR	Readily Biodeg.	N	Y
7440-31-5	Tin	MRL (CDC, ATSDR)	0.3	OPR	Inorganic	N	Y
7440-66-6	Zinc	RfD (US EPA, IRIS)	0.3	OPR	Inorganic	Y	Y
7646-85-7	Zinc chloride	as Zinc, RfD (US EPA, IRIS)	0.3	OPR	Inorganic	Y	N
68424-85-1	Alkyl dimethylbenzyl ammonium chloride	RfD (US EPA, 2006)	0.4	OPR	Readily Biodeg.	Y	N
139-08-2	Benzyl dimethyl dodecyl ammonium chloride	Read-across assessment; see Alkyl dimethylbenzyl ammonium chloride	0.4	RA - OPR	Readily Biodeg.	Y	N
122-18-9	Benzyl dimethyl hexadecyl ammonium chloride	Read-across assessment; see Alkyl dimethylbenzyl ammonium chloride	0.4	RA - OPR	Readily Biodeg.	Y	N
122-19-0	Benzyl dimethyl octadecyl ammonium chloride	Read-across assessment; see Alkyl dimethylbenzyl ammonium chloride	0.4	RA - OPR	Readily Biodeg.	Y	N
68081-81-2	Alkyl benzenesulfonate	Read-across assessment; see Benzenesulfonic acid, C10-16-alkyl derivs	0.5	RA - OPR	Readily Biodeg.	Y	N

CASRN	Chemical Name	Notes	Toxicity Screening Value (mg/kg/d)	Source of Value[1]	OECD Biodegradation Category	Oil Field Additive?	Naturally Occurring?
68910-32-7	Alkylaryl sulfonates	This is Benzenesulfonic acid, mono-C10-16-alkyl derivs., compds. with ethanolamine. Ethanolamine has less toxicity than the benzosulfonic acid. Read-across assessment, Benzenesulfonic acid, C10-16-alkyl derivs	0.5	RA - OPR	Poorly Biodeg.	Y	N
90218-35-2	Alkylarylsulfonate amine salt	This is also known as benzenesulfonic acid, C10-16-alkyl derives., compds. with 2-propanamine. Read-across assessment, Benzenesulfonic acid, C10-16-alkyl derivs. The chronic oral toxicity of 2-propanamine is unclear. This represents the best-known toxicity of this compound.	0.5	RA - OPR	Poorly Biodeg.	Y	N
68910-31-6	Ammonium alkylaryl sulfonates	This is Benzenesulfonic acid, mono-C10-16-alkyl derivs., ammonium salt. Read across from Benzenesulfonic acid, C10-16-alkyl derivs., potassium salts	0.5	RA - OPR	Poorly Biodeg.	Y	N
68584-22-5	Benzenesulfonic acid, C10-16-alkyl derivs	Rfd (US EPA, Human Benchmark for Pesticides)	0.5	OPR	Poorly Biodeg.	Y	N
68584-27-0	Benzenesulfonic acid, C10-16-alkyl derivs., potassium salts	Rfd (US EPA, Human Benchmark for Pesticides)	0.5	RA - OPR	Poorly Biodeg.	Y	N
68855-24-3	C14-30 Alkyl Derivatives [Benzenesulfonic acid, mono-C10-16-alkyl derivs., ammonium salts]	This is Benzenesulfonic acid, mono-C10-16-alkyl derivs., ammonium salt. Read across from Benzenesulfonic acid, C10-16-alkyl derivs., potassium salts	0.5	RA - OPR	Poorly Biodeg.	Y	N
7722-84-1	Hydrogen peroxide	NSF International has evaluated the noncancer oral toxicity data for hydrogen peroxide and derived a reference dose (RfD) of 0.5 mg/kg-day based on a BMDL05 of 49 mg/kg-day estimated from data on duodenal hyperplasia observed in catalase-deficient mice following subchronic drinking water exposure (Weiner et al., 2000). NSF International applied an uncertainty factor of 100 (10 for intraspecies variability and 3 each for interspecies variability and database deficiencies).	0.5	OPR	Inorganic	Y	N
78-93-3	2-Butanone	RfD (US EPA, IRIS)	0.6	OPR	Readily Biodeg.	N	Y
7440-24-6	Strontium	RfD (US EPA, IRIS)	0.6	OPR	Inorganic	N	Y
141-78-6	Ethyl acetate	RfD (US EPA, PPRTV)	0.7	OPR	Readily Biodeg.	Y	N
17375-41-6	Ferrous sulfate, monohydrate	RfD (EPA, PPRTV) for iron in iron compounds	0.7	OPR	Inorganic	Y	N
7439-89-6	Iron	RfD (US EPA, PPRTV)	0.7	OPR	Inorganic	N	Y
107-21-1	Ethylene glycol	MRL (CDC, ATSDR)	0.8	OPR	Readily Biodeg.	Y	N

CASRN	Chemical Name	Notes	Toxicity Screening Value (mg/kg/d)	Source of Value[1]	OECD Biodegradation Category	Oil Field Additive?	Naturally Occurring?
67-64-1	Acetone	RfD (US EPA, IRIS)	0.9	OPR	Readily Biodeg.	Y	N
1344-28-1	Aluminium oxide	RfD (US EPA, PPRTV)	1	OPR	Inorganic	Y	N
7429-90-5	Aluminum	RfD (US EPA, PPRTV)	1	OPR	Inorganic	N	Y
7446-70-0	Aluminum chloride	Read-across assessment; see Aluminum.	1	RA - OPR	Inorganic	Y	N
1327-41-9	Aluminum chlorohydrate	Read-across assessment; see Aluminum.	1	RA - OPR	Inorganic	N	N
7726-95-6	Bromine (Br)	In 1966, a FAO/WHO meeting on pesticide residue recommended an acceptable daily intake (ADI) for humans of 0–1 mg/kg body weight bromide, based on a minimum pharmacologically effective dosage in humans of approximately 600 mg of bromide ion. A more recent meeting of the group in 1988 reaffirmed the ADI of 0–1 mg/kg body weight (WHO, 2009).	1	OPR	Inorganic	N	Y
124-04-9	Adipic acid	RfD (US EPA, PPRTV) for Hexanedioic Acid	2	OPR	Readily Biodeg.	Y	N
67-63-0	Isopropanol	RfD (US EPA, PPRTV)	2	OPR	Inorganic	Y	N
67-56-1	Methanol	RfD (US EPA, IRIS)	2	OPR	Readily Biodeg.	Y	N
14797-55-8	Nitrate	RfD (US EPA, IRIS)	2	OPR	Inorganic	N	Y
8012-95-1	Mineral Oil	RfD (US EPA, PPRTV)	3	OPR	Readily Biodeg.	Y	N
1863-63-4	Ammonium benzoate	Read-across assessment; see Benzoic acid	4	RA - OPR	Readily Biodeg.	Y	N
65-85-0	Benzoic acid	RfD (US EPA, IRIS)	4	OPR	Readily Biodeg.	Y	Y
532-32-1	Sodium benzoate	Read-across assessment; see Benzoic acid	4	RA - OPR	Readily Biodeg.	Y	N
57-55-6	Propylene glycol	RfD (US EPA, PPRTV)	20	OPR	Readily Biodeg.	Y	N
7664-38-2	Phosphoric acid	RfD (US EPA, PPRTV)	49	OPR	Inorganic	Y	N
7785-84-4	Sodium trimetaphosphate	RfD (US EPA, PPRTV)	49	OPR	Inorganic	Y	N

CASRN	Chemical Name	Notes	Toxicity Screening Value (mg/kg/d)	Source of Value[1]	OECD Biodegradation Category	Oil Field Additive?	Naturally Occurring?
143-07-7	Dodecanoic acid	NSF International has evaluated the noncancer oral toxicity data for dodecanedioic acid and calculated a reference dose (RfD) of 70 mg/kg-day based on a NOAEL of 74 mg/kg-day from a human clinical study (Passi et al., 1983). No critical effect was identified in humans or laboratory animals over the tested dose ranges (Du Pont, 1992 - unpublished, as reported in OECD/SIDS, 1996). NSF International used a composite uncertainty factor of 1, since sufficient data to fulfill all areas of uncertainty were identified.	70	OPR	Readily Biodeg.	Y	N

Table 3: Chemicals with derived project-specific surrogate toxicity values ordered from lowest to highest values and OECD biodegradation classification

CASRN	Chemical Name	Notes	Toxicity Screening Value (mg/kg/d)	NOAEL/LOAEL (mg/kg/d)	Uncertainty Factor	Source of Toxicity Value[1]	OECD Biodegradation Category	Oil Field Additive ?	Naturally Occurring ?
60-24-2	2-mercaptoethanol	In a sub-chronic rat study, changes in body weight gain and food consumption in addition to (in males) ptyalism, minimal to marked vacuolated hepatocytes accompanied by lower cholesterol and triglyceride levels, paleness and accentuated lobular pattern of the liver were observed. NOAEL = 15 mg/kg/d (ECHA, 2-mercaptoethanol).	0.005	15	3000	STV	Poorly Biodeg.	Y	N
55566-30-8	Phosphonium, tetrakis (hydroxymethyl)- sulfate (2:1) salt	Hepatocyte cytoplasmic vacuolation was noted in the portal area of the liver in both species with apoptosis in hepatocytes of the dog only. Raised levels of liver enzymes ALT and AST were also noted in rat studies. NOAEL = 0.75 mg/kg/d (ECHA, Tetrakis(hydroxymethyl)phosphonium sulphate (2:1)).	0.008	0.75	100	STV	Inherent Biodeg.	Y	N
108-74-7	Hexahydro- 1,3,5, trimethyl S triazine	In a sub-chronic rat study, at 100 mg/kg/d, toxicity consisted of clinical signs (salivation, rales and/or piloerection),slightly decreased total protein and albumin, a thickened limiting ridge of the stomach at macroscopic examination and microscopic findings for the stomach (lymphogranulocytic inflammation of the glandular stomach and hyperplasia of the epithelium of the limiting ridge and eyes (females only: degeneration of the retina) NOAEL = 30 mg/kg/d (ECHA, Hexahydro-1,3,5-trimethyl-1,3,5-triazine).	0.01	30	3000	STV	Readily Biodeg.	Y	N
124-68-5	2-Amino-2-methylpropanol	A chronic rat study found adverse hepatic systemic effects. NOAEL from the 2-generation study performed using the associated chemical 4,4-dimethyl oxazolidine. This substance hydrolyses almost immediately in the stomach following oral dosing; releasing formaldehyde and AMP. NOAEL = 11 mg/kg/d (ECHA,2-Amino-2-methylpropanol).	0.04	11	300	STV	Readily Biodeg.	Y	N
64742-53-6	Distillates, hydrotreated light naphthenic	A sub-chronic rat study found hematologic effects. LOAEL = 125 mg/kg/d (ECHA, Distillates (petroleum), hydrotreated light naphthenic).	0.04	125	3000	STV	No data, as mixture	Y	N

[1] STV: Project-specific Surrogate Toxicity Value; RA – STV: Read-Across assessment using an project-specific Surrogate Toxicity Value

CASRN	Chemical Name	Notes	Toxicity Screening Value (mg/kg/d)	NOAEL/LOAEL (mg/kg/d)	Uncertainty Factor	Source of Toxicity Value[1]	OECD Biodegradation Category	Oil Field Additive ?	Naturally Occurring ?
68648-87-3	Benzene, c10-c16 alkyl derivatives	In a rat study looking at reproductive effects, a NOAEL of 5mg/kg/day was identified for exposure during gestation. Outcomes were depressed weight gains in adults, smaller litters, and fewer live pups; decreased pup survival and lower pup weights were also found at some higher dosing levels (Robinson and Schroeder, 1992).	0.05	5	100	STV	Readily Biodeg.	Y	N
25265-78-5	Benzene, tetrapropylene-	This is a linear alkyl benzene. See Benzene, c10-c16 alkyl derivatives	0.05	NA	NA	RA - STV	Readily Biodeg.	Y	N
26172-55-4	Methylchloroisothiazolinone	A sub-chronic rat study found decreased cumulative body weight gain and decreased feed consumption effects. Read-across study with the unchlorinated 2-methyl-2H-isothiazol-3-one used for the assessment. Both chlorinated and non-chlorinated are similarly used as biocides with similar biological activity strengths. NOAEL = 19 mg/kg/d (ECHA, 2-methyl-2H-isothiazol-3-one).	0.06	19	300	RA - STV	Inherent Biodeg.	Y	N
126-97-6	Ethanolamine thioglycolate	A chronic rat study found reproductive effects. NOAEL = 20 mg/kg/d (ECHA, 2-hydroxyethyl)ammonium mercaptoacetate).	0.07	20	300	STV	Poorly Biodeg.	Y	N
140-01-2	Pentasodium diethylenetriamine pentaacetate	A sub-chronic rat study found body weight and histopathological changes of the urinary tract with corroborating results of the urinalyses effects. NOAEL = 75 mg/kg/d (ECHA, Pentasodium (carboxylatomethyl)iminobis(ethylenenitrilo)tetraacetate).	0.08	75	1000	STV	Readily Biodeg.	Y	N
13598-36-2	Phosphonic acid	A sub-chronic rat study found labored respiration, rales, gasping, piloerection, chromodacryorrhoea of the snout, lethargy, hunched posture, salivation, hypothermia and lean appearance effects. NOAEL = 250 mg/kg/d (ECHA, Phosphonic acid).	0.08	250	3000	STV	Readily Biodeg.	Y	N
27176-87-0	Branched DDBSA	A sub-chronic rat study found squamous cell hyperplasia of stomach effects. NOAEL = 100 mg/kg/d (ECHA, Dodecylbenzenesulphonic acid).	0.1	100	1000	STV	Readily Biodeg.	Y	N
64742-55-8	Paraffinic petroleum distillate, hydrotreated light	A sub-chronic rat study found hematologic effects. LOAEL = 125 mg/kg/d (ECHA, Distillates (petroleum), hydrotreated light paraffinic).	0.1	125	1000	STV	Inherent Biodeg.	Y	N

CASRN	Chemical Name	Notes	Toxicity Screening Value (mg/kg/d)	NOAEL/LOAEL (mg/kg/d)	Uncertainty Factor	Source of Toxicity Value[1]	OECD Biodegradation Category	Oil Field Additive ?	Naturally Occurring ?
2634-33-5	1,2 Benzisothiazol-3(2H)-one	A sub-chronic rat study found elevated alkaline phosphatase levels and decreased body weight. NOAEL = 69 mg/kg/d (ECHA, 1,2-benzisothiazol-3(2H)-one).	0.2	69	300	STV	Readily Biodeg.	Y	N
115-19-5	2-methyl-3-Butyn-2-ol	A sub-chronic rat study found systemic toxicity manifested on kidney, as well as reproductive organs epididymis, testis, and ovary effects. NOAEL = 45 mg/kg/d (ECHA, 2-methylbut-3-yn-2-ol).	0.2	45	300	STV	Poorly Biodeg.	Y	N
68308-87-2	Cottonseed, flour	Cottonseed flour contains gossypol, which is a liver, erythrocyte, and male reproductive toxicant; these are related to acute exposure and generally reversible once exposure has ended. Work had been done to test gossypol as a male contraceptive, however this work was stopped because in some cases fertility didn't return once gossypol was no longer being taken (Coutinho, 2002). In the case of male fertility, the contraceptive action of gossypol appears to be reversible at a daily dose of 5 mg/kg/day (Gu et al., 2000). GSI has applied a factor of 10 to account for susceptible populations	0.2	5	30	STV	No data on gossypol	Y	N
26027-38-3	Ethoxylated 4- nonphenol	A reproductive rat study that exposed dams to nonoxynol-9 during gestation found developmental effects. NOAEL = 50 mg/kg/d (Meyer et al., 1988). This is a read-across study substituting NP-9 for NP-4	0.2	50	300	STV	Poorly Biodeg.	Y	N
No CASRN	Nonylphenol ethoxylates	This is a polyoxyethylene alkylphenols, see Ethoxylated 4-nonphenol	0.2	NA	NA	RA - STV	Poorly Biodeg.	Y	N
127087-87-0	Nonylphenol polyethylene glycol ether	This is a polyoxyethylene alkylphenols, see Ethoxylated 4-nonphenol	0.2	NA	NA	RA - STV	Poorly Biodeg.	Y	N
68412-54-4	Oxyalkylated alkylphenol	This is a polyoxyethylene alkylphenols, see Ethoxylated 4-nonphenol	0.2	NA	NA	RA - STV	Poorly Biodeg.	Y	N

CASRN	Chemical Name	Notes	Toxicity Screening Value (mg/kg/d)	NOAEL/LOAEL (mg/kg/d)	Uncertainty Factor	Source of Toxicity Value[1]	OECD Biodegradation Category	Oil Field Additive ?	Naturally Occurring ?
2836-32-0	Sodium glycolate	Sodium glycolate is the sodium salt of glycolic acid, also known as hydroxyacetic acid. In a rat study where glycolic acid was orally administered for 90 day at 0, 150,300, and 600 mg/kg/day, systemic effects were observed; the NOAEL = 150 mg/kg/day. Glycolic acid is naturally occurring in some vegetables, i.e., pineapple, tomatoes, and papaya (TOXNET, 2014). It is metabolized to oxalic acid like ethylene glycol, which is where its systemic toxicity likely arises.	0.2	150	620	*RA* - STV	Readily Biodeg.	Y	N
No CASRN	Severely hydrotreated paraffinic	See Solvent dewaxed heavy paraffinic	0.2	NA	NA	RA - STV	Inherent Biodeg.	Y	N
No CASRN	Solvent dewaxed heavy paraffinic	For insufficiently refined lubricant-based oils, using "Distillates (petroleum), hydrotreated heavy paraffinic" CAS 64742-54-7 as a read-across chemical: Subchronic rat study LOAEL 125mg/kg/day hematological effects observed. (ECHA, Distillates (petroleum), hydrotreated heavy paraffinic)	0.2	125	620	RA – STV	Inherent Biodeg.	Y	N
111-46-6	Diethylene glycol	Snelling et al. (2017) used long term animal studies to derive a human equivalent reference dose of 0.3 mg/kg/d.	0.3	NA	NA	STV	Readily Biodeg.	N	Y
2809-21-4	Hydroxyethylidenediphosphonic acid	A chronic rat study found prolonged anemia in both sexes at the top dose, with a slight retardation of bone marrow development. Severe pallor of the skin of the top dose group animals and slight pallor in the mid dose rats was seen. A pale color was also noted for organs well supplied with blood (spleen and kidneys). These observations are consistent with perturbation of iron homeostasis. The NOAEL takes into consideration the most susceptible juvenile life period. NOAEL = 34 mg/kg/d (ECHA, Etidronic acid).	0.3	34	100	STV	Poorly Biodeg.	Y	N
79-21-0	Peracetic acid	A chronic rat study found statistically significant reduction in terminal body weight, corrected body weight and body weight gain from days 5 to 20 at the high dose level were found in dams. NOAEL = 12.5 mg/kg/d (ECHA, Peracetic acid).	0.3	30	100	STV	Readily Biodeg.	Y	N

CASRN	Chemical Name	Notes	Toxicity Screening Value (mg/kg/d)	NOAEL/LOAEL (mg/kg/d)	Uncertainty Factor	Source of Toxicity Value[1]	OECD Biodegradation Category	Oil Field Additive ?	Naturally Occurring ?
68439-70-3	Alkyl amine	In a chronic rat study given a diet containing 0, 0.01, 0.1 or 0.2 % test substance ad libitum for 104 weeks. No substance related effect was observed except decreased mean body weight in the highest dose group. NOAEL = 50 mg/kg/d (ECHA, Amines, C12-16-alkyldimethyl).	0.4	42.3	100	STV	Poorly Biodeg.	Y	N
75-12-7	Formamide	A chronic mouse study found split NOAEL values of 80 mg/kg bw/day for males, based on the reduced body weight (-25%), erythron changes, and histopathological changes (degeneration of the germinal epithelium) in the testes and in the epididymis, and 40 mg/kg bw/day for females, based on reduced body weights (-20%) at 160 mg/kg bw/day and hematological changes at 80 mg/kg bw/day. NOAEL = 40 mg/kg/d (ECHA, Formamide).	0.4	40	100	STV	Readily Biodeg.	Y	N
9003-01-4	Polyacrylic acid	A chronic rat study found decreased food and water intakes, and decreased body and organ weights effects. NOAEL = 83 mg/kg/d (ECHA, 2-Propenoic acid, homopolymer).	0.4	40	100	STV	Readily Biodeg.	Y	N
61790-41-8	Quaternary ammonium compound	A sub-chronic rat study found clinical signs of toxicity including reduced body weight gain, reduced food efficiency and occurrence of haemosiderine in kidneys of high dose animals. NOAEL = 40 mg/kg/d (ECHA, Quaternary ammonium compounds, trimethylsoya alkyl, chlorides).	0.4	40	100	STV	Poorly Biodeg.	Y	N
9003-04-7	Sodium polyacrylate	Sodium salt of polyacrylic acid (see Polyacrylic acid)	0.4	NA	NA	RA - STV	Readily Biodeg.	Y	N

CASRN	Chemical Name	Notes	Toxicity Screening Value (mg/kg/d)	NOAEL/LOAEL (mg/kg/d)	Uncertainty Factor	Source of Toxicity Value[1]	OECD Biodegradation Category	Oil Field Additive ?	Naturally Occurring ?
98-00-0	Furfuryl alcohol	Oral carcinogenicity studies with furfural in rats and mice (NTP, 1999) showed some evidence of carcinogenic activity for male rats, based on the occurrence of uncommon cholangiocarcinomas in two animals and bile duct dysplasia with fibrosis in two other animals at the high dose of 60 mg/kg bw/day. In mice there was an increased incidence of hepatocellular adenoma at the highest dose (175 mg/kg bw/day). These carcinomas were associated with hepatotoxicity (chronic inflammation and pigmentation) which was also seen at 100 mg/kg bw/day. It was assumed that the observed liver tumors were induced via some mechanism involving liver toxicity, and that at levels at which no liver toxicity is induced, tumors will not arise (NTP, 1999).	0.5	53	100	STV	Readily Biodeg.	Y	N
79-14-1	Glycolic acid	A sub-chronic rat study found renal oxalate crystal nephropathy effects. NOAEL = 150 mg/kg/d (ECHA, Glycollic acid).	0.5	150	300	STV	Readily Biodeg.	Y	N
8002-09-3	Pine oil	Maternal and developmental effects observed in a rat study of dams exposed to pine oil during gestation. NOAEL = 50 mg/kg/day. (HAZMAP, Pine Oil)	0.5	50	100	STV	Inherent Biodeg.	Y	N
7783-20-2	Ammonium sulfate	A chronic rat study found increased kidney and liver weight; decreased absolute spleen weight effects. NOAEL = 256 mg/kg/d (ECHA, Ammonium sulphate).	0.9	256	300	STV	Inorganic	Y	N
10192-30-0	Ammonium bisulfate	A chronic rat study found occult blood in the faeces and changes in gastric morphology effects using sodium metabisulfite as a read across chemical. NOAEL ammonium bisulfate dose equivalent = 113 mg/kg/d (ECHA, Ammonium hydrogensulphite).	1	113	100	STV	Inorganic	Y	N
108-93-0	Cyclohexanol	A read-across study using cyclohexanone for a sub-chronic rat study found hematological changes that are probably a result of slight changes in lipid metabolism or of reduced water consumption., NOAEL = 143 mg/kg/d (ECHA, Cyclohexanol).	1	143	100	STV	Readily Biodeg.	Y	N

CASRN	Chemical Name	Notes	Toxicity Screening Value (mg/kg/d)	NOAEL/LOAEL (mg/kg/d)	Uncertainty Factor	Source of Toxicity Value[1]	OECD Biodegradation Category	Oil Field Additive ?	Naturally Occurring ?
123-42-2	Diacetone Alcohol	In a sub-acute reproductive study looking at effects related to exposure of diacetone alcohol in pregnant rabbits from day 6-28 of gestation, found effects of fetal malformation with NOAEL = 100 mg/kg/d. Experimental toxicokinetics suggests that diacetone alcohol and its metabolites do not bioaccumulate. For this reason, no uncertainty factor for length of exposure is applied as exposures in this study represent near full gestational period for the rabbits. (ECHA, 4-hydroxy-4-methylpentan-2-one).	1	100	100	STV	Readily Biodeg.	Y	N
34590-94-8	Dipropylene glycol monomethyl ether	A sub-chronic rat study the only effects observed during this study were salivation and increased liver weights at the highest dose level. The liver weight increase observed at the highest dose level was only slight and no histopathologic changes, except for hypertrophy, accompanied this effect. There were no changes in clinical chemistry (ALP, ASP) indicating a liver damage. The same effect was observed with other structurally related molecules, e.g. propylene glycol methyl ether has been shown to cause liver weight increases via a phenobarbital-like enzyme induction mode of action and it is highly likely that dipropylene glycol methyl ether liver weight increases occur via the same mode of action. As this is an adaptive effect typical for many glycol ethers, it is not considered as adverse. The excessive salivation is the adverse effect observed here. NOAEL = 1000 mg/kg/d (ECHA, (2-methoxymethylethoxy)propanol).	1	1000	1000	STV	Inherent Biodeg.	Y	N
7783-18-8	Inorganic sulfur compound [Ammonium thiosulfate]	A sub-chronic rat study found occult blood in the feces and changes in gastric morphology effects. NOAEL = 168 mg/kg/d (ECHA, Ammonium thiosulphate).	1	108	100	STV	Inorganic	Y	N
110-85-0	Piperazine	Toxicity has been noted at therapeutic or near therapeutic doses. Doses as low as 30 mg/kg/day in patients with renal failure and 50 to 75 mg/kg/day in patients with normal renal function have resulted in toxicity. Transient neurologic dysfunction was observed in a 2-year-old girl receiving an estimated dose of piperazine 300 mg/kg/day for 2 days. Neurologic dysfunction resolved within 72 hours of admission. (ECHA, Piperazine).	1	30	30	STV	Readily Biodeg.	Y	N

CASRN	Chemical Name	Notes	Toxicity Screening Value (mg/kg/d)	NOAEL/LOAEL (mg/kg/d)	Uncertainty Factor	Source of Toxicity Value[1]	OECD Biodegradation Category	Oil Field Additive ?	Naturally Occurring ?
7631-90-5	Sodium bisulfite	A chronic rat study found occult blood in the feces and changes in gastric morphology effects using sodium metabisulfite as a read across chemical. NOAEL SO2 dose equivalent = 72 mg/kg/d (ECHA, Sodium hydrogensulfite).	1	118	100	STV	Inorganic	Y	N
7775-09-9	Sodium Chlorate	A sub-chronic rat study evidence of anemia. NOAEL = 100 mg/kg/d (ECHA, Sodium chlorate).	1	100	100	STV	Inorganic	Y	N
2893-78-9	Sodium dichloroisocyanurate	A sub-chronic rat study found labored breathing, emaciation, accumulation of yellow material in the anogenital region, decreased activity and death effects. NOAEL = 115 mg/kg/d (ECHA, Troclosene sodium).	1	115	100	STV	Poorly Biodeg.	Y	N
9005-67-8	Ethoxylated sorbitan monostearate	Also known as polysorbate 60, this is a food and pharmaceutical additive used as an emulsifier and thickener. A chronic rat study showed lifelong diarrhea and enlargement to the cecum with 2-year exposure. Most animals on the highest emulsifier dosage had livers which were enlarged and more friable than normal. NOAEL = 1000 mg/kg/d [ECHA, Sorbitan monostearate, ethoxylated]	3	1000	300	STV	Inherent Biodeg.	Y	N
26316-40-5	Oxyalated Ethylenediamine	In a sub-chronic rat study, the only treatment-related effects indicative of systemic toxicity were lower red blood cell counts, hemoglobin concentrations and hematocrits in males and females administered 1000 mg/kg/day. NOAEL = 300 mg/kg/d (ECHA, Ethylenediamine, ethoxylated and propoxylated).	3	300	100	STV	Inherent Biodeg.	Y	N
68439-57-6	Sodium C14-16 olefin sulfonate	A chronic rat study found depressed weight gain. NOAEL = 70 mg/kg/d (ECHA, Sulfonic acids, C14-16 (even numbered)-alkane hydroxy and C14-16 (even numbered)-alkene, sodium salts).	3	259	100	STV	Readily Biodeg.	Y	N
64742-94-5	Heavy aromatic naphtha	In a reproductive rat study, the NOAEL was identified based on reduced body weight in dams and in pups. NOAEL = 750 mg/kg/d (ECHA, Solvent naphtha (petroleum), heavy arom.).	8	750	100	STV	Readily Biodeg.	Y	N
64742-48-2	Hydrotreated heavy naphtha	Read-across assessment; see Heavy aromatic naphtha.	8	NA	NA	RA - STV	Readily Biodeg.	Y	N

CASRN	Chemical Name	Notes	Toxicity Screening Value (mg/kg/d)	NOAEL/LOAEL (mg/kg/d)	Uncertainty Factor	Source of Toxicity Value[1]	OECD Biodegradation Category	Oil Field Additive ?	Naturally Occurring ?
64742-47-8	Hydrotreated Light Petroleum Distillate	A sub-chronic rat study found reduced body weight in dams and pups. NOAEL = 750 mg/kg/d (ECHA, Distillates (petroleum), hydrotreated light).	8	750	100	STV	Readily Biodeg.	Y	N
25322-68-3	Polyethylene oxide	A sub-chronic rat study found changes in liver and kidney weight effects. NOAEL = 8000 mg/kg/d (ECHA, Poly(oxy-1,2-ethanediyl), α-hydro-ω-hydroxy- Ethane-1,2-diol, ethoxylated).	80	8000	100	STV	Readily Biodeg.	Y	N

Table 4: Chemicals that are of low concern for chronic oral toxicity

CASRN	Chemical Name	Assessment Classification	Additional Notes
64-19-7	Acetic acid	Food additive	
90320-37-9	Almond Shell	Considered virtually non-toxic	
12125-02-9	Ammonium Chloride	Therapeutic oral use	See main text (TOXNET, 2015a)
1302-78-9	Bentonite	Therapeutic oral use	Bulk laxative
No CASRN	Bicarbonate	Food additive	
7440-70-2	Calcium	Component of food	
471-34-1	Calcium carbonate	Therapeutic oral use	Antacid
1305-78-8	Calcium Oxide	Hydrolyzes	
7778-18-9	Calcium sulfate	Food additive	
7440-44-0	Carbon	Therapeutic oral use	Ingested as activated charcoal; does not dissolve in water
124-38-9	Carbon dioxide	Food additive	
No CASRN	Carbonate	Food additive	
No CASRN	Cedar fiber	Considered virtually non-toxic	Wood fiber
9005-81-6	Cellophane	Food additive	See main text on cellophane
9004-34-6	Cellulose, microcrystalline	Food additive	
16887-00-6	Chloride (Cl^-)	Component of food	
77-92-9	Citric acid	Food additive	
25155-15-1	Cymenes	Food additive	p-Cymene is a known volatile compound in oranges (Teranishi et al., 1963).

CASRN	Chemical Name	Assessment Classification	Additional Notes
63148-62-9	Dimethyl siloxanes and silicones	Considered virtually non-toxic	See main text (Moretto et al., 2005)
7758-16-9	Disodium pyrophosphate	Food additive	
64-17-5	Ethanol	Food additive	
84012-43-1	Extract of walnut	Considered virtually non-toxic	Walnut shell powder; does not dissolve in water
61790-12-3	Fatty acids, tall-oil	Food additive	Tall Oil Acid is approved for use as an indirect food additive. When fed to rats as 15% of the total caloric intake, Tall Oil Acid was nontoxic; however, it had a growth-retarding effect. No treatment-related effects were observed in rats fed diets containing 5% and 10% Tall Oil Acid over two generations. (Tall oil, 1989)
61790-45-2	Fatty acids, tall-oil, sodium salts	Food additive	See Fatty acids, tall-oil
56-81-5	Glycerol	Food additive	
7782-42-5	Graphite	Considered virtually non-toxic	Does not dissolve in water
7647-01-0	Hydrochloric Acid	Considered virtually non-toxic	See main text
9004-62-0	Hydroxyethyl cellulose	Considered virtually non-toxic	See main text (Bingham et al., 2001)
20461-54-5	Iodide	Food additive	
7439-90-9	Krypton	Inert	
1317-65-3	Limestone	Therapeutic oral use	Contains calcium carbonate
No CASRN	Magma fiber	Inert	
7439-95-4	Magnesium	Component of food	See main text (IOM, 1997)
1302-93-8	Mullite	Inert	Does not dissolve in water
7727-37-9	Nitrogen	Inert	

CASRN	Chemical Name	Assessment Classification	Additional Notes
No CASRN	Nutshell	Considered virtually non-toxic	Does not dissolve in water
112-80-1	Oleic acid	Component of food	Common non-saturated fat in the human diet
13397-24-5	Phosphogypsum [Gypsum]	Food additive	Gypsum is made of Calcium Sulfate which is a food additive
7723-14-0	Phosphorous	Component of food	Toxicity concern, white phosphorus (very unlikely to be found)
No CASRN	Polydimethylsiloxane emulsion	Considered virtually non-toxic	See main text (Moretto et al., 2005)
74-84-0	Polyethylene [Ethane]	Inert	See main text (Browning and Snyder, 1987)
25038-59-9	Polyethylene terephthalate	Considered virtually non-toxic	Low oral toxicity, see main text (DAK Americas, 2008; Keresztes et al., 2009)
7440-09-7	Potassium	Component of food	
127-08-2	Potassium acetate	Food additive	
7447-40-7	Potassium chloride	Food additive	
12136-45-7	Potassium Oxide	Hydrolyzes	
16068-46-5	Potassium phosphate	Food additive	
1319-41-1	Saponite	Food additive	Animal food additive. See main text (Odom et al., 1984; Wiles et al., 2004; Zoltan et al., 2005)
1318-93-0	Smectite	Food additive	Animal food additive. See main text (Odem et al., 1984; Wiles et al., 2004; Zoltan et al., 2005)
7440-23-5	Sodium	Component of food	
127-09-3	Sodium acetate	Food additive	
144-55-8	Sodium bicarbonate	Food additive	
497-19-8	Sodium carbonate	Food additive	

CASRN	Chemical Name	Assessment Classification	Additional Notes
9063-38-1	Sodium carboxymethyl starch	Therapeutic oral use	Also known as sodium starch glycolate is commonly used in pharmaceuticals as a disintegrant (Shah and Augsburger, 2002)
9004-32-4	Sodium carboxymethylcellulose	Food additive	
7647-14-5	Sodium chloride	Food additive	
6381-77-7	Sodium erythorbate	Food additive	
7681-52-9	Sodium Hypochlorite	Food additive	Can be used to disinfect drinking water, see main text
7681-82-5	Sodium iodide	Food additive	
1313-59-3	Sodium Oxide	Hydrolyzes	
7757-82-6	Sodium sulfate	Food additive	
7772-98-7	Sodium thiosulfate	Food additive	
9005-65-6	Sorbitan monooleate, ethoxylated	Considered virtually non-toxic	See main text (Rowe et al., 2006)
57-11-4	Stearic Acid	Food additive	(Mortensen et al., 2017)
No CASRN	Sulfate (SO_4^{2-})	Food additive	
7704-34-9	Sulfur	Considered virtually non-toxic	(US EPA, 1991)
13463-67-7	Titanium dioxide	Food additive	
7732-18-5	Water	Considered virtually non-toxic	
No CASRN	Wood dust	Considered virtually non-toxic	Does not dissolve in water
11138-66-2	Xanthan gum	Food additive	
7440-63-3	Xenon	Inert	

Table 5: Chemicals with insufficient data to identify chronic toxicity

CASRN	Chemical Name	Alternate Chemical Name /Other Notes	Oil Field Additive ?	Naturally Occurring ?
27646-80-6	2-Methylamino-2-methyl-1-propanol		Y	N
67990-40-3	2-Propen-1-aminium, N,N-dimethyl-N-2-propenyl-, chloride, polymer with 2-hydroxypropyl 2-propenoate and 2-propenoic acid		Y	N
145417-45-4	2-Propenoic acid, 2-methyl-, polymer with methyl 2-methyl-2-propenoate, octadecyl 2-methyl 2 propenoate and 2propenoic acid, sodium salt		Y	N
9033-79-8	2-propenoic acid, polymer with sodium 2-propenoate	Sodium Acrylate Copolymer (absorbant polymer)	Y	N
130800-24-7	2-Propenoic acid, telomer with 2-methyl-2-(1-oxo-2-propenyl)-1-propanesulfonic acid, sodium salt		Y	N
300-92-5	Aluminum distearate		Y	N
No CASRN	Amide surfactant acid salt		Y	N
No CASRN	Amides, Non Ionics		Y	N
61791-24-0	Amine derivative	Polyethylene glycol soyamine	Y	N
67924-33-8	Amine salt	Ethanol, 2,2',2''-nitrilotris-, homopolymer, hydrochloride	Y	N

CASRN	Chemical Name	Alternate Chemical Name /Other Notes	Oil Field Additive ?	Naturally Occurring ?
NP-U2856	Amine salt		Y	N
64346-44-7	Amine sulfate	Bis(isopropylammonium) sulphate	Y	N
68239-30-5	Bis (HDMA) EPI Copolymer hydrochloride		Y	N
69418-26-4	Cationic acrylamide copolymer	Polyquaternium-33	Y	N
44992-01-0	Cationic acrylamide monomer	2-(Dimethylamino)ethyl acrylate methochloride; Ethanaminium, N,N,N-trimethyl-2-[(1-oxo-2-propenyl)oxy]-, chloride	Y	N
54076-97-0	Cationic polymer	Ethanaminium, N,N,N-trimethyl-2-((1-oxo-2-propenyl)oxy)-, chloride, homopolymer	Y	N
681331-04-4	Causticized Lignite		Y	N
64743-05-1	Coke (petroleum), calcined		Y	N
25987-30-8	Copolymer of acrylamide and sodium acrylate	2-Propenoic acid, polymer with 2-propenamide, sodium salt	Y	N
129828-31-5	Crosslinked polyol ester	2-Propenoic acid, polymer with 4-(1,1-dimethylethyl)phenol, formaldehyde, 2,5-furandione, 2-methyloxirane, 4-nonylphenol and oxirane	Y	N

CASRN	Chemical Name	Alternate Chemical Name /Other Notes	Oil Field Additive ?	Naturally Occurring ?
2673-22-5	Diester of sulfosuccinic acid sodium salt		Y	N
No CASRN	Drilling paper		Y	N
61791-26-2	Ethoxylated amine	PEG-10 Hydrogenated tallow amine	Y	N
9081-83-8	Ethoxylated octylphenol		Y	N
5877-42-9	Ethyl octynol	4-Ethyl-3-hydroxy-1-octyne	Y	N
63428-92-2	Formaldehyde, polymer with 2-methyloxirane, 4-nonylphenol and oxirane	p-Nonylphenol, formaldehyde copolymer, ethoxylated and propoxylated	Y	N
30704-64-4	Formaldehyde, polymer with 4-(1,1-dimethylethyl)phenol, 2-methyloxirane and oxirane	p-tert-Butylphenol-formaldehyde resin, copolymer with ethylene oxide and propylene oxide	Y	N
30846-35-6	Formaldehyde, polymer with 4-nonylphenol and oxirane		Y	N
No CASRN	Heavy catalytic reformed naptha		Y	N
61790-59-8	Hydrogenated tallow amine acetone		Y	N
68648-89-5	Kraton G1702H	Benzene, ethenyl-, polymer with 2-methyl-1,3-butadiene, hydrogenated		
129521-66-0	Lignite		Y	N

CASRN	Chemical Name	Alternate Chemical Name /Other Notes	Oil Field Additive ?	Naturally Occurring ?
PE-M2464	Methyl oxirane polymer		Y	N
No CASRN	Organic acid ethoxylated alcohols		Y	N
68171-44-8	Oxyalkylated alkylphenolic resin	Formaldehyde, polymer with 4-(1,1-dimethylethyl)phenol, 4-nonylphenol and oxirane	Y	N
68910-19-0	Oxyalkylated polyamine	Diethylenetriamine, propoxylated, ethoxylated	Y	N
67939-72-4	Oxyalkylated polyamine	Triethylenetetramine polymer with oxirane and methyl oxirane	Y	N
68123-18-2	Phenol, 4,4'-(1-methylethylidene) bis-, polymer with 2-(chloromethyl)oxirane, 2-methyloxirane and oxirane		Y	N
68425-75-2	Phosphate ester salt	Ethanol, 2-amino-, polymer with alpha-tridecyl-omega-hydroxypoly(oxy-1,2-ethanediyl) phosphate	Y	N
9005-70-3	POE (20) Sorbitan Trioleate	Polysorbate 85. No chronic oral studies are available, dermal studies show minor erythema (Mezei., 1975).	Y	N
68938-70-5	Poly (triethanolamine.mce)		Y	N

CASRN	Chemical Name	Alternate Chemical Name /Other Notes	Oil Field Additive ?	Naturally Occurring ?
68955-69-1	Polyamine salts	Hexanedinitrile, hydrogenated, high-boiling fraction, polymer with epichlorohydrin, acetate (salt)	Y	N
26062-79-3	Polydimethyl diallyl ammonium chloride	Polyquaternium-6; Quaternium-40	Y	N
68036-92-0	Polyglycol diepoxide	Oxirane, methyl-, polymer with oxirane, ether with 1,2,3-propanetriol (3:1), ether with (chloromethyl)oxirane polymer with 4,4'-(1-methylethylidene)bis(phenol)	Y	N
68036-95-3	Polyglycol diepoxide	Oxirane, methyl-, polymer with oxirane, ether with (chloromethyl)oxirane polymer with 4,4'-(1-methylethylidene)bis(phenol)	Y	N
No CASRN	Polyhydroxyalkanoates (PHA)		N	Y

CASRN	Chemical Name	Alternate Chemical Name /Other Notes	Oil Field Additive ?	Naturally Occurring ?
64741-71-5	Polymers (petroleum) viscous	TSCA Definition 2018: A complex combination of hydrocarbons obtained from distillation of products from the polymerization of propylene or butylene. It has a carbon number range from C12 upward and a boiling range from approximately 220.degree.C (428.degree.F) upward. The hydrocarbons are predominantly monoolefinic.	Y	N
36484-54-5	Polyoxyalkylene glycol		Y	N
61790-86-1	Polyoxyalkylenes	Fatty acids, tall-oil, monoesters with sorbitan, ethoxylated	Y	N
9014-93-1	Polyoxyethylene dinonylphenol	Nonyl nonoxynol-10	Y	N
12068-19-8	Polyoxyethylene nonyl phenyl ether phosphate	PEG-6 Nonyl phenyl ether phosphate, sodium salt	Y	N
70142-34-6	Polyoxyl 15 hydroxystearate		Y	N
42751-79-1	Polyquaternary amine	Dimethylamine, polymer with epichlorohydrin and ethylenediamine	Y	N
68609-18-7	Quaternized condensed alkanolamines	Ethanol, 2,2',2''-nitrilotris-, homopolymer, reaction products with chloromethane	Y	N

CASRN	Chemical Name	Alternate Chemical Name /Other Notes	Oil Field Additive ?	Naturally Occurring ?
No CASRN	Steranes or cyclopentanoperhydrophenanthrene		N	Y
68140-11-4	Tall oil, DETA/ midazoline acetates		Y	N
72480-70-7	Tar bases, quinoline derivatives, quaternized benzyl chloride		Y	N
68527-49-1	Thiourea, polymer with formaldehyde and 1-phenylethanone		Y	N
64114-46-1	Triethanolamine homopolymer		Y	N

Table 6: Chemicals with low chronic oral toxicity

CASRN	Chemical Name	Notes
629-73-2	1-Hexadecene	NOAEL > 1000mg/kg/day for females and males because the findings were not evidence of true systemic toxicity, as the compound was aspirated during delivery (ECHA, Hexadecene)
75-07-0	Acetaldehyde	A sub-chronic rat study found hyperkeratosis of the forestomach. This is not an effect that is toxicologically relevant to humans. No other effects were observed up to a dosage of 625 mg/kg/d. (ECHA, Acetaldehyde).
No CASRN	Alcohols, C-10-14 ethoxylated	Alcohol ethoxylates are a class of non-ionic surfactants with hundreds of different potential forms depending on length of the carbon chains and saturation arrangement. There is no published data suggesting chronic systemic human toxicity and in animal models, no health effects have been observed with repeated dose studies. In multiple 90-day repeated dose rat studies conducted by adding ethoxylated alcohols to food: adding C14-15 alcohol ethoxylates to food, no relevant local or systemic effects were observed with doses of 500 mg/kg/day (Procter and Gamble Ltd., 1978); adding C12-15 alcohol ethoxylates to food, no relevant local or systemic effect with dose of 102 mg/kg/day (Unilever, 1978a); adding C12-C14 alcohol ethoxylates to food, no relevant local or systemic effects with dose of 110 mg/kg/day; and adding C14-15 alcohol ethoxylates to food, no relevant local or systemic effects--including reproductive--were observed with daily dose of 785 mg/kg/day (Proctor and Gamble, 1974).
68551-12-2	Alcohols, C12-16, ethoxylated	See Alcohol, C-10-14 ethoxylated
68951-67-7	Alcohols, C14-C15, ethoxylated	See Alcohol, C-10-14 ethoxylated
No CASRN	Alcohols, C9-11, ethoxylated	See Alcohol, C-10-14 ethoxylated

CASRN	Chemical Name	Notes
90622-58-5	Alkanes, C11-15-iso	Using a read across study using other alkanes, no effects found in both rats and dogs (Johannsen and Levinskas, 1987); No effects observed in a study with C12-C14 isoalkane exposures up to 5000 mg/kg/day, as reported in the registration dossier for ECHA REACH program (ECHA, Alkanes, C12-14-iso).
90622-46-1	Alkanes, C14-16	See Dodecane, registration dossier reports toxicologic data for mixed hydrocarbons with length of 10 or more carbons.
926-39-6	Amine sulfate [Ethanolamine-O-sulfate]	Ethanolamine-O-sulfate has a known acute diuretic and enzymatic inhibitory effect; these effects are acute and transitory (MeSH, Ethanolamine-O-sulfate). In a study where rats were given 250 mg/kg and 500 mg/kg of ethanolamine-O-sulfate though repeated intraperitoneal injections, this produced decreases in body weight and increases in brain GABA levels (Howard et al., 1980). Ethanolamine-O-sulfate is a GABA transferase inhibitor, which will increase GABA levels in the brain. Most studies were found to give it intraventricularly, as it poorly crosses the blood brain barrier (Anlezark et al., 1976; Gudelsky et al.,1983). As such, chronic oral exposure is likely to be of minimal risk.

CASRN	Chemical Name	Notes
7664-41-7	Ammonia	Ammonia is a gas with solubility in water; it creates a basic solution. For example, a 1 molar aqueous solution of ammonia has a pH of approximately 11.6, which is about 10 times less basic than household bleach, which can have pH as high as 12.6. Ammonia's toxicity in oral exposure is related to its caustic properties. In the context of using produced water for irrigation with ammonia, anhydrous ammonia is used as a fertilizer, and therefore unlikely to affect the quality of crops. It is not assessed under IRIS for oral exposure and not classifiable as a human carcinogen (US EPA, 2016a).
191-24-2	Benzo(ghi)perylene	Under IRIS, it is not assessed for oral exposure or classifiable as to human carcinogenicity (US EPA. 1990). Available studies were deemed by the EPA to be inadequate to make an assessment of carcinogenicity due to oral exposure, where they used lung implant, skin-painting and subcutaneous injection bioassays. ,Results from those studies do not suggest overt carcinogenicity (US EPA, 1990). It is also classified by IARC as Group 3 (Not classifiable as to its carcinogenicity to humans).
106-97-8	Butane	Butane is a gas with low toxicity with little risk of oral exposure. A 10-minute inhalation exposure at 10,000 ppm of butane gas results in drowsiness, but no other evidence of systemic effects (ACGIH, 2012).
68551-19-9	C12-C14 Isoalkanes	See Alkanes, C11-15-iso
68551-20-2	C12-C14 Isoalkanes	See Alkanes, C11-15-iso
61791-31-9	Cocamide DEA	Known risks associated with cocamide diethanolamine exposure are through dermal/inhalation exposures (IARC, 2013)

CASRN	Chemical Name	Notes
14464-46-1	Crystalline silica (cristobalite)	The route of exposure of concern for crystalline silica is inhalation. The available data are insufficient to demonstrate an association for an adverse outcome with oral exposure (ATSDR, 2017).
14808-60-7	Crystalline silica (quartz)	The route of exposure of concern for crystalline silica is inhalation. The available data are insufficient to demonstrate an association for an adverse outcome with oral exposure (ATSDR, 2017).
14808-60-7	Crystalline silica (quartz)	The route of exposure of concern for crystalline silica is inhalation. The available data are insufficient to demonstrate an association for an adverse outcome with oral exposure (ATSDR, 2017).
15468-32-3	Crystalline silica (tridymite)	The route of exposure of concern for crystalline silica is inhalation. The available data are insufficient to demonstrate an association for an adverse outcome with oral exposure (ATSDR, 2017).
15468-32-3	Crystalline silica (tridymite)	The route of exposure of concern for crystalline silica is inhalation. The available data are insufficient to demonstrate an association for an adverse outcome with oral exposure (ATSDR, 2017).
124-18-5	Decane	In a sub-chronic rat study (90 days), given a mixture of light hydrotreated aliphatic hydrocarbons C9-C14 (MRD-89-582) no effects were observed up to a dosage of 5000 mg/kg/day (ECHA, Decane).
577-11-7	Dioctyl sulfosuccinate sodium salt	In a 90-day rat study, no effects were observed up to 1000 mg/kg/d. (ECHA, Docusate sodium).

CASRN	Chemical Name	Notes
10042-91-8	Diphosphoric acid, sodium salt	Polyphosphates have low oral toxicity (Madsen et al., 2001). No mutagenicity or carcinogenicity was observed with the Ames Test and in a chromosomal aberration assay in vitro using a Chinese hamster fibroblast cell line (Ishidate et al. 1984). Sodium triphosphate was shown to have no reproductive effects with doses up to 238 mg/kg/day (IPCS 1982).
125005-87-0	Diutan	Repeated dose exposures found no effects at up to 1000 mg/kg/day in a 28-day repeat dose oral toxicity study using OECD Test Guideline 407 (US EPA, 2016b).
112-40-3	Dodecane	No effects observed in a study with exposures up to 5000 mg/kg/day of mixed alkanes with lengths of 10 or more carbon atoms, reported in the registration dossier for ECHA REACH program (ECHA, Dodecane)
78330-21-9	Ethoxylated alcohol C11-14	See Alcohol, C-10-14 ethoxylated
68439-45-2	Ethoxylated alcohol C6-12	See Alcohol, C-10-14 ethoxylated
No CASRN	Ethoxylated C11 Alcohol	See Alcohol, C-10-14 ethoxylated
61791-12-6	Ethoxylated castor oil	Studies in a range of mammals (mouse, rat, and dog [beagle]) report no adverse effects observed in exposures ranging from 1250-5000 mg/kg/d looking at local, systemic, and reproductive effects (ECHA, Castor oil, ethoxylated)
67762-38-3	Fatty acid ester	No effects observed in a study with exposures up to 1000 mg/kg/day, reported in the registration dossier for ECHA REACH program (ECHA, 'Fatty acids, C16-18 and C18-unsatd., Me esters')

CASRN	Chemical Name	Notes
61788-91-8	Fatty alkyl amines	Risks associated with fatty acid amines is the presence of nitrosamine contamination. Nitrosamines are known carcinogens with one of the most potent being nitrosodiethanolamine, a liver carcinogen in rats (IARC, 1978).
97722-02-6	Glycerides, tall oil mono-, di, and tri	A sub-chronic rat study found no toxicologically relevant effects in clinical signs, functional observations, body weights, food consumption, clinical pathology, macroscopy, organ weights, and histopathology effects up to 1000 mg/kg/d (ECHA, Glycerides, tall-oil mono-, di-, and tri-).
142-62-1	Hexanoic acid	The only effects observed were marked hyperplasia of the squamous epithelium of the forestomach in all high dose animals, and to a minimal degree, in 3 intermediate dose group animals. The forestomach is not a structure found in humans, making the finds of no toxicological relevance (Potakar, 1983). Moody and Reddy (1977) exposed rats to 2, 4 and 8% hexanoic acid (corresponding to 1000, 2000, 4000 mg/kg/day) in diet for 3 weeks before alterations in body weight gain, liver size, hepatic enzyme activity and hepatic peroxisome proliferation were examined. No effects were observed by hexanoic acid, the authors concluded that the NOAEL was ≥ 4000 mg/kg bw/day.

CASRN	Chemical Name	Notes
7783-06-4	Hydrogen sulfide	Hydrogen sulfide is a common nuisance contaminant in drinking water. The taste and odor threshold in water is estimated to be between 0.05 and 0.1 mg/L (WHO, 2017a). No reliable human or animal studies have been published that have investigated chronic oral exposures (ATSDR, 2006). It is unexpected that it would be difficult for a person to consume a toxic dose of hydrogen sulfide in drinking water (WHO, 2017b); this likely holds for hydrogen sulfide in crops. During final distribution of irrigation waters, there is ample opportunity for the water to oxygenate. Sulfide oxidizes readily in oxygenated waters to either sulfur or sulfate, both with limited toxicity.
No CASRN	Ionic Surfactants	A review of animal toxicity studies looking at chronic oral exposures to a large variety of anionic and cationic surfactants did not indicate increased risk for adverse carcinogenic, chronic systemic, or reproductive outcomes (Madsen et al., 2001).
64741-46-4	Light aliphatic naphtha	In rats treated with mixtures of hydrocarbons, some nephrotoxicity was observed that was related to the alkane components. The kidney effects observed only in male rats are indicative of alpha-2u-globulin nephropathy. These kidney effects are specific to male rats and are not considered to be of biological relevance to humans (Halder et al., 1985).

CASRN	Chemical Name	Notes
74-87-3	Methyl Chloride	Methyl chloride is not assessed under IRIS for oral exposure and it is not classifiable as a human carcinogen. In water it is moderately soluble and decomposes to methanol and hydrogen chloride; this dissolution will reduce toxicity. Methanol is addressed in the set of chemicals of interest. Hydrogen chloride in produced water is likely to be found as a very weak solution of hydrochloric acid and likely much less corrosive than human stomach contents. See discussion in section 'Chemicals considered to be non-toxic or generally regarded as safe (GRAS)' (US EPA, 2001).
No CASRN	Methyl ester of sulfonated tannin	Methyl ester of sulfonated tannin is the primary component (60-80%) of the drilling mud additive Desco® Deflocculant. Desco® Deflocculant SDS lists an oral NOEL of methyl ester of sulfonated tannin as 1,000 mg/kg/day in rats in a 32-47 day study (SDS 1016805). The SDS also lists methyl ester of sulfonated tannin as negative for in vitro chromosome aberration test.
No CASRN	n-Alkanes	See Dodecane, registration dossier reports toxicologic data for mixed hydrocarbons with length of 10 or more carbons
7/1/52	n-Eicosene	No effects observed in a 90-day rat study with exposures up to 1000 mg/kg/day of multiple carbon number isomerized olefins and alkenes with length C20-24; also, no effects observed in 1000 mg/kg/day tetradec-1-ene (ECHA, Icos-1-ene)
544-76-3	n-Hexadecane	See Dodecane, registration dossier reports toxicologic data for mixed hydrocarbons with length of 10 or more carbons
593-45-3	n-Octadecane	See Dodecane, registration dossier reports toxicologic data for mixed hydrocarbons with length of 10 or more carbons

CASRN	Chemical Name	Notes
629-59-4	n-Tetradecane	See Dodecane, registration dossier reports toxicologic data for mixed hydrocarbons with length of 10 or more carbons
6419-19-8	Nitrilotris (methylene phosphonic acid)	No effects observed in a study with exposures up to 500 mg/kg/day, reported in the registration dossier for ECHA REACH program (ECHA, Nitrilotrimethylenetris(phosphonic acid)).
7631-86-9	Non-crystalline silica [amorphous silica]	The route of exposure of concern for amorphous silica is inhalation. The available data are insufficient to demonstrate an association for an adverse outcome with oral exposure (ATSDR, 2017).
56919-55-2	Pentadecane, 3-methylene	See Pentadecane, 7-methylene as a read-across compound
115146-98-0	Pentadecane, 5-methylene	See Pentadecane, 7-methylene as a read-across compound
13043-55-5	Pentadecane, 7-methylene	There is little indication of toxicity, only acute toxicity with an LD50 >10g/kg. No other indications of toxicity reported in ECHA REACH dossier (ECHA, Pentadecene, 7-methylene).
69011-36-5	Poly(oxy-1,2-ethanediyl), a-tridecyl-w-hydroxy-branched	No compound-related gross or histopathological lesions were identified at any dose level, the changes reported are considered minor and not of toxicological significance. NOAEL > 500 mg/kg/d (ECHA, Isotridecanol, ethoxylated).
9003-05-9	Polyacrylamide	Polymerized acrylamide is non-toxic, unlike its monomer (Klaassen and Watkins, 1996).
9003-79-8	Polyacrylate	Ben-X is a blend of polyacrylamide and polyacrylate polymers. (SDS 9033-79-8). See polyacrylamide (table 5) and sodium polyacrylate (table 9). COSMOS lists a chronic oral "Highest No Effect Level" of 500mg/kg/day in a 2-year rat study (COSMOS, 2013).

CASRN	Chemical Name	Notes
26100-51-6	Polyactide resin [Polylactic acid]	Polylactic acid (PLA) is insoluble in water, it is used to make biodegradable food and beverage containers and for cosmetic surgery. The L-isomer (PLLA) is biologically inert (Simamora and Chern, 2006). PLA was first used for degradable implants; upon hydrolysis, lactic acid is produced, which is an intermediate carbohydrate metabolite (Szycher et al., 2014).
25322-69-4	Polypropylene glycol	Polyethylene glycols (PEGs) are acutely toxic, with no known chronic effects. The probably lethal oral dose in adult humans is between 1 oz and 1 pint (Laurence, 1977). Using PEGs as a read-across compound, polypropylene glycol likely has similar toxicologic properties.
9002-89-5	Polyvinyl alcohol	Polyvinyl Alcohol (PVA) has been orally administered to mice at doses of up to 2000 mg/kg/d with no evidence of bone marrow or chromosomal damage (TOXNET, 2016); in a rat study, doses of up to 5000 mg/kg/day did not show any effect (Kelly et al., 2003); PVA is not absorbed well in the gastrointestinal tract and does not accumulate in the body when ingested (DeMerlis and Schoneker, 2003).
7646-93-7	Potassium bisulfate	Produces a weak acid with potassium and sulfate ions in water. Potassium is a dietary requirement and sulfate is a common ion in food additives, such as calcium sulfate
1310-58-3	Potassium hydroxide	Potassium hydroxide is a strong base whose main concern to health arises due to its caustic properties, where it will irritate skin and other tissues (TOXNET, 2015b).

CASRN	Chemical Name	Notes
123-38-6	Propionaldehyde	The EPA has identified that there are no directly applicable human or animal data available to make a determination as to the oral chronic toxicity of propionaldehyde (US EPA, 2008). The most similar compound to propionaldehyde is acetaldehyde, an identified human carcinogen by IARC (IARC, 2010b). Acetaldehyde is a product of ethanol metabolism and is presumed to be a likely agent responsible for the carcinogenicity of drinking alcoholic beverages (Brooks and Theruvathu, 2005)). It is postulated that the carcinogenic toxicity of acetaldehyde is related to it forming reactive DNA adducts that eventually block DNA synthesis and induce DNA damage (Brooks and Theruvathu, 2005; Mizumoto et al., 2017). Given propionaldehyde's similar structure to acetaldehyde, i.e., propionaldehyde's carbon chain is just one carbon atom longer, it will likely form a similarly reactive DNA adduct capable of causing similar DNA damage. Acetaldehyde has been quantitatively evaluated for carcinogenicity by OEHHA with a cancer slope factor of 0.001 per mg/kg/day, but only for the inhalation route. Evidence for the oral route of exposure is not sufficient to make that determination. It is known that as saturated aldehydes get longer, their toxicity decreases (Gosselin et al., 1984), which means that propionaldehyde is less toxic than acetaldehyde. In the context of the use of produced water for irrigation, acetaldehyde is evaluated here for non-cancer outcomes related to oral exposure, based on the available animal data. As the evidence suggests that propionaldehyde is less toxic than acetaldehyde, the surrogate RfD for the latter has been applied to propionaldehyde to provide an informed health protective value (Til et al., 1988).
68153-60-6	Salt of fatty acid polyamine	See Fatty alkyl amines

CASRN	Chemical Name	Notes
1338-43-8	Sorbitan, mono-(9Z)-9-octadecenoate [Sorbitan oleate]	There are no known human health effects observed with ingestion of sorbitan oleate. In a study where humans were given 6 grams of sorbitan oleate per day for 30 days, no effects were observed (Gosselin et al., 1976)
67784-80-9	Soybean oil, Me ester	See Fatty acid ester
61790-33-8	Tallow alkyl amines	See Fatty alkyl amines
629-59-4	Tetradecane	See Dodecane, registration dossier reports toxicologic data for mixed hydrocarbons with length of 10 or more carbons
7440-32-6	Titanium	Chronic toxicity of titanium and its alloys related to inhalation exposures (Stellman, 1998))
629-50-5	Tridecane	No effects observed in a study with exposures up to 5000 mg/kg/day, reported in the registration dossier for ECHA REACH program (ECHA, Tridecane).
112-27-6	Triethylene Glycol	No toxicologically relevant local or systemic effects were observed in a rat study with doses of up to 4360 mg/kg/d over 90 days (Van and Ballantyne, 2001). Later studies have also reported a similar lack of relevant local or systemic toxicity (Ballantyne and Snelling, 2007)
13573-18-7	Triphosphoric acid, sodium salt	Polyphosphates have low oral toxicity (Madsen et al., 2001). No mutagenicity or carcinogenicity was observed with the Ames Test and in a chromosomal aberration assay in vitro using a Chinese hamster fibroblast cell line (Ishidate et al. 1984). Sodium triphosphate was shown to have no reproductive effects with doses up to 238 mg/kg/day (IPCS 1982).

CASRN	Chemical Name	Notes
No CASRN	Triterpenes	Triterpenes are naturally occurring in plant, animals and fungi. The class of chemicals have been investigated as to their use as a chemotherapeutic agent and thought to have low toxicity to health cells (Chudik et al., 2015). In a study looking at the pharmacokinetics of a triterpenes after ingestion at a dose of 30-60 mg of total triterpenes from Centella asiatica—which mainly contain asiaticoside, madecassoside, asiatic and madecassic acids (Bylka et al., 2013)—no adverse systemic effects were observed (Grimaldi et al, 1990).
1120-21-4	Undecane	No effects observed in a rat study with exposures up to 1000 mg/kg/day, reported in the registration dossier for the ECHA REACH program (ECHA, Undecane).
57-13-6	Urea	No effects observed in a study with exposures up to 2250 mg/kg/d in the rat and 6750 mg/kg/d in the mouse (Fleischman et al., 1980). Also classified as GRAS (FDA, SCOGS).

Table 7: Chemicals with incomplete information related to chronic oral toxicity

CASRN	Chemical Name	Notes
479-66-3	1H, 3H-Pyrano (4,3-b)(1)benzopyran-9-carboxylic acid, 4,10-dihydro-3,7,8 trihydroxy-3-methyl-10-oxo (fulvic acid)	Fulvic acid is an organic acid structurally similar to humic acids. Fulvic acid is associated with Kashin-beck disease (KBD), a chronic osteoarthritic disease endemic to parts of china. Consumption of drinking water containing 211 ppm fulvic acid in conjunction with a low-selenium diet for 49 days resulted in reduced skeletal tissue structural integrity in mice (Yang et al., 1993). There is some evidence that fulvic acid could mechanistically be chronically toxic, as it alters immune response and has been shown to reduce thyroid function (Vucskits et al., 2010).
100-73-2	Acrolein dimer	Acrolein dimer is the polymerized version of acrolein; it has a free aldehyde group. There is some evidence that the polymer is less toxic than the monomers with LD50 of 4920mg/kg and 26mg/kg, respectively. Long-term oral exposure to acrolein, at an amount within the range of human unsaturated aldehyde intake, induces a phenotype of dilated cardiomyopathy in the mouse, i.e., 1mg/kg for 48 days. Human exposure to acrolein may have analogous effects and raise consideration of an environmental, aldehyde-mediated basis for heart failure (Ismahil et al., 2011). The literature suggests that the toxicity for most aldehydes are mediated through similar pathways and similar function groups (LoPachin and Gavin, 2014).
No CASRN	Aromatic Amine	Toxicity of aromatic amines is related to the form. See discussion in text.

CASRN	Chemical Name	Notes
38011-25-5	Disodium ethylenediaminetetraacetate	Sodium EDTA has been shown in some studies to be cytotoxic, a reproductive toxicant, and to demineralize teeth, bones and organs in animals. However, for these studies, identifying the mg/kg doses is not possible because exposure groups are categorized by percentage of EDTA in food. Other studies reported in the same EDTA assessment report show no toxicity in rats exposed to 375 mg/kg/day for 721 days; no effects in a multigeneration study where rats were exposed up to 250 mg/kg/day; and in a dog study, no effects were seen in exposures up to 250 mg/kg/day (Lanigan and Yamerick 2002).
No CASRN	Heavy catalytic reformed naptha	Heavy catalytic reformed naphtha is a complex combination of hydrocarbons formed through the catalytic reforming process. Heavy catalytic reformed naphtha is a component of full range catalytic reformed naphtha. Full range catalytic reformed naphtha is a broad molecular weight hydrocarbon mixture of various hydrocarbons. There is little evidence of acute toxicity, with an oral LD_{50} of > 5,000mg/kg in rats (SDS 0129MAR020). There are no studies looking at chronic oral exposure to heavy catalytic reformed naphtha. The SDS for full range catalytic reformed naphtha lists the mixture as a Category 1A carcinogen (known carcinogen) and a Category 2 reproductive toxicant (suspected reproductive toxicant). However, the full range catalytic reformed naphtha is known to contain benzene, toluene, ethylbenzene, xylene, and naphthalene; chemicals likely absent from heavy catalytic reformed naphtha(SDS 0129MAR020).

CASRN	Chemical Name	Notes
1415-93-6	Humic acids	There is some evidence that Humic Acid could mechanistically be chronically toxic, as it promotes lipid peroxidation (Ho et al., 2003); damage to vascular endothelial cells (Kihara et al., 2014); and damage to cultured human umbilical endothelial cells (Hseu, 2002). However, there are no studies looking at exposures in humans. Humic acids are naturally occurring and no dosage information is available.
85-01-8	Phenanthrene	There are no reliable human studies assessing chronic oral exposure to phenanthrene. The acute toxicity of phenanthrene has been determined for phenanthrene at 700 mg/kg (Lewis, 2004). It is not assessed under IRIS for oral exposure (US EPA, IRIS). It is also not classifiable as to its human carcinogenicity due to a lack of studies (IARC, 2010a). However, a test of human lymphoblast TK6 cells incubated with rat liver S9 (Arochlor) and 9 ug/mL phenanthrene yielded a forward mutation (US EPA, IRIS).
19019-43-3	Polycarboxlate salt [Trisodium ethylenediaminetetraacetate]	See Disodium ethylenediaminetetraacetate

CASRN	Chemical Name	Notes
74-84-0	Polyethylene	For this entry, “Polyethylene” in the list of chemical additives, a query of the CASRN number associated with the entry does not return polyethylene, but instead returns Ethane. Ethane is considered to be physiologically and toxicologically inert. At high concentration, risks are associated with the displacement of oxygen, which results in asphyxiation (Browning and Snyder, 1987). It is also possible that the CASRN is incorrect and this should be polyethylene glycol. Polyethylene glycols (PEGs) are acutely toxic, with no known chronic effects. The probably lethal oral dose in adult humans is between 1 oz and 1 pint (Laurence, 1977). However, PEG 3350 is used as a mild laxative in Miralax™, and other similar over-the-counter laxative products, with a dose of 17 g per day.
9038-95-3	Polyglycol ether	Comptox references 3 studies as available in COSMOS. COSMOS references 1964 studies by US FDA CFSAN. However, no additional report is available. The studies cannot be found electronically. Findings of the three studies area: Chronic oral "HNEL" in dog of 616 mg/kg-day for 714-day study; Chronic oral "HNEL" in rat of 500 mg/kg-day for 734-day study; Chronic oral "HNEL" in rat of 500 mg/kg-day for 793-day study. (COSMOS, CMS-14254)

CASRN	Chemical Name	Notes
91-63-4	Quinaldine	Unable to find studies looking at chronic exposure to quinaldine. LD50 is 1230mg/kg in rats. It has the weakest mutagenicity among methylquinoline, with some indication of mutagenicity in bacterial cultures. Different bacteria studies of genotoxicity report both mutagenic (Dong et al., 1978; Takahashi et al., 1988) and null effects (Bowden et al., 1976). These kinds of bacterial culture studies do not necessarily predict cancer in higher life forms well (Hakura et al., 1999). However, innocuous chemicals rarely give false positives (Priva et al 1991)
NP-SMO3_U1240	Sorbitan ester	There are three main esters of sorbitan (sorbitan monostearate, sorbitan tristearate, and sorbitan monolaurate). Each of these esters of sorbitan are food additives and act as emulsifiers or wetting agents. It is unclear from the entry if the sorbitan used in oil and gas production is the same as that which is used as a food additive. For this reason, it is unclear as to the toxic potential of this oil/gas field additive. For context, sorbitan monostearate is practically non-toxic with a probably human-lethal dose greater than 15 g/kg (Gosselin et al., 1976).
65996-69-2	Steel mill slag	TSCA Definition 2018: The fused substance formed by the action of a flux upon the gangue of the iron-bearing materials charged to a blast furnace and upon the oxidized impurities in the iron produced. Depending upon the particular blast furnace operation, the slag is composed primarily of sulfur and oxides of aluminum, calcium, magnesium, and silicon. Toxicity for steel mill slag will likely be attributable to metals discussed further in other sections of this report. There was no available literature directly assessing toxicity of steel mill slag contamination of waters.

CASRN	Chemical Name	Notes
8052-41-3	Stoddard Solvents	In general, ingestion of most petroleum distillates at doses less than 1,000 mg/kg causes little toxicity (Ellenhorn and Barceloux, 1988)
64-02-8	Tetrasodium ethylenediaminetetraacetate	See Disodium ethylenediaminetetraacetate

Table 8: List of aromatic amines with IARC carcinogenicity classification [1]

IARC Classification	Chemical Name
Group 1: Carcinogenic to humans	4-Aminobiphenyl Benzidine 4,4′-methylenebis(2-chloroaniline) 2-Naphthylamine ortho-Toluidine
Group 2B: Possibly carcinogenic to humans	Auramine 4-Chloro-ortho-toluidine

[1] This is the list of aromatic amines evaluated in the IARC monograph. It is unknown at this time which of these are used as additives in oil and gas development

Table 9: Chemicals with toxicity values that have been screened, based on toxicity level and biodegradability in water

CASRN	Chemical Name	Toxicity Screening Value (mg/kg/d)	Source of Toxicity Value[1]	OECD Biodegradation Category	Oil Field Additive ?	Is Naturally Occurring ?
53-70-3	Dibenzo(a,h)anthracene	0.000002	OPR	Poorly Biodeg.	N	Y
50-32-8	Benzo(a)pyrene	0.000003	OPR	Poorly Biodeg.	N	Y
119-65-3	Isoquinoline	0.000003	RA - OPR	Poorly Biodeg.	Y	N
111-44-4	Bis (2-chloroethyl) ether	0.000004	OPR	Poorly Biodeg.	N	Y
7440-38-2	Arsenic	0.000007	OPR	Inorganic	N	Y
205-99-2	Benzo(b)fluoranthene	0.000008	OPR	Poorly Biodeg.	N	Y
193-39-5	Indenopyrene	0.000008	OPR	Poorly Biodeg.	N	Y
56-55-3	Benzo(a)anthracene	0.000008	OPR	Poorly Biodeg.	N	Y
218-01-9	Chrysene	0.00008	OPR	Poorly Biodeg.	N	Y
123-91-1	1,4 Dioxane	0.0001	OPR	Non-biodeg.	Y	N
7440-43-9	Cadmium	0.0001	OPR	Inorganic	Y	Y
7439-97-6	Mercury	0.0002	OPR	Inorganic	Y	Y
7440-48-4	Cobalt	0.0003	OPR	Inorganic	N	Y
7439-92-1	Lead	0.0003	OPR	Inorganic	Y	Y

[1] OPR: Organizational Peer Reviewed Toxicity Value [usually agency derived]; RA – OPR: Read-across assessment using an Organizational Peer Reviewed Toxicity Value; STV: Project-specific Surrogate Toxicity Value; RA – STV: Read-Across assessment using a project-specific Surrogate Toxicity Value

CASRN	Chemical Name	Toxicity Screening Value (mg/kg/d)	Source of Toxicity Value[1]	OECD Biodegradation Category	Oil Field Additive ?	Is Naturally Occurring ?
7440-36-0	Antimony	0.0004	OPR	Inorganic	N	Y
1309-64-4	Antimony trioxide	0.0004	RA - OPR	Inorganic	Y	N
7439-93-2	Lithium	0.002	OPR	Inorganic	N	Y
1310-65-2	Lithium hydroxide	0.002	OPR	Inorganic	Y	N
13453-71-9	Lithium chlorate	0.002	OPR	Inorganic	Y	N
13840-33-0	Lithium hypochlorite	0.002	OPR	Inorganic	Y	N
554-13-2	Lithium carbonate	0.002	OPR	Inorganic	Y	N
7440-41-7	Beryllium	0.002	OPR	Inorganic	Y	Y
7447-41-8	Lithium chloride	0.002	RA - OPR	Inorganic	Y	N
7440-61-1	Uranium	0.003	OPR	Inorganic	N	Y
7440-47-3	Chromium	0.003	OPR	Inorganic	Y	Y
7439-98-7	Molybdenum	0.005	OPR	Inorganic	N	Y
7782-49-2	Selenium	0.005	OPR	Inorganic	N	Y
7440-22-4	Silver	0.005	OPR	Inorganic	N	Y
7440-50-8	Copper	0.01	OPR	Inorganic	Y	Y
7553-56-2	Iodine	0.01	OPR	Inorganic	Y	N

CASRN	Chemical Name	Toxicity Screening Value (mg/kg/d)	Source of Toxicity Value[1]	OECD Biodegradation Category	Oil Field Additive ?	Is Naturally Occurring ?
7758-99-8	Copper sulfate pentahydrate	0.01	OPR	Inorganic	Y	N
7440-02-0	Nickel	0.01	OPR	Inorganic	Y	Y
7786-81-4	Nickel sulfate	0.01	OPR	Inorganic	Y	N
108-90-7	Chlorobenzene	0.02	OPR	Poorly Biodeg.	N	Y
120-12-7	Anthracene	0.02	OPR	Poorly Biodeg.	N	Y
129-00-0	Pyrene	0.03	OPR	Poorly Biodeg.	N	Y
64742-95-6	Solvent naphtha, petroleum, light arom.	0.03	OPR	Poorly Biodeg.	Y	N
29868-05-1	Alkanolamine phosphate	0.04	RA - OPR	Poorly Biodeg.	Y	N
206-44-0	Fluoranthene	0.04	OPR	Poorly Biodeg.	N	Y
16984-48-8	Fluoride	0.05	OPR	Inorganic	N	Y
7664-39-3	Hydrofluoric acid	0.05	OPR	Inorganic	Y	N
83-32-9	Acenaphthene	0.06	OPR	No data	N	Y
14797-65-0	Nitrite	0.1	OPR	Inorganic	N	Y
7440-62-2	Vanadium	0.1	OPR	Inorganic	N	Y
7439-96-5	Manganese	0.1	OPR	Inorganic	N	Y
7446-09-5	Sulfur dioxide	0.1	OPR	Inorganic	Y	N

CASRN	Chemical Name	Toxicity Screening Value (mg/kg/d)	Source of Toxicity Value[1]	OECD Biodegradation Category	Oil Field Additive ?	Is Naturally Occurring ?
7440-42-8	Boron	0.2	OPR	Inorganic	N	Y
12179-04-3	Sodium tetraborate pentahydrate	0.2	OPR	Inorganic	Y	N
7440-39-3	Barium	0.2	OPR	Inorganic	Y	Y
7727-43-7	Barite	0.2	OPR	Inorganic	Y	N
7440-31-5	Tin	0.3	OPR	Inorganic	N	Y
7440-66-6	Zinc	0.3	OPR	Inorganic	Y	Y
7646-85-7	Zinc chloride	0.3	OPR	Inorganic	Y	N
60-24-2	2-mercaptoethanol	0.005	STV	Poorly Biodeg.	Y	N
64742-53-6	Distillates, hydrotreated light naphthenic	0.04	STV	No data, as mixture	Y	N
126-97-6	Ethanolamine thioglycolate	0.07	STV	Poorly Biodeg.	Y	N
115-19-5	2-methyl-3-Butyn-2-ol	0.2	STV	Poorly Biodeg.	Y	N
68308-87-2	Cottonseed, flour	0.2	STV	No data on gossypol	Y	N
26027-38-3	Ethoxylated 4- nonphenol	0.2	STV	Poorly Biodeg.	Y	N
No CASRN	Nonylphenol ethoxylates	0.2	RA - STV	Poorly Biodeg.	Y	N
127087-87-0	Nonylphenol polyethylene glycol ether	0.2	RA - STV	Poorly Biodeg.	Y	N

CASRN	Chemical Name	Toxicity Screening Value (mg/kg/d)	Source of Toxicity Value[1]	OECD Biodegradation Category	Oil Field Additive ?	Is Naturally Occurring ?
68412-54-4	Oxyalkylated alkylphenol	0.2	RA - STV	Poorly Biodeg.	Y	N
2809-21-4	Hydroxyethylidenediphosphonic acid	0.3	STV	Poorly Biodeg.	Y	N
68439-70-3	Alkyl amine	0.4	STV	Poorly Biodeg.	Y	N
61790-41-8	Quaternary ammonium compound	0.4	STV	Poorly Biodeg.	Y	N

Table 10: Proposed outline of Task 2 literature review

Section		Description
1.0	**INTRODUCTION**	Overarching introductory section of literature review describing project and purpose of review
2.0	**METHODS**	Methods section describing scope of review and sources of literature
3.0	**REVIEW OF PRODUCED WATER REUSE FOR AGRICULTURAL IRRIGATION**	Review of conventional and non-conventional produced water in the context of its use for agricultural irrigation
4.0	**CHEMICALS OF INTEREST**	A summary of the identification of the list of Chemicals of Interest
5.0	**REVIEW OF WATER QUALITY DATA FOR PRODUCED WATER**	A review of chemical analytic data available for produced water effluent and blended irrigation water used for food crop irrigation in the San Joaquin Valley in the context of the Chemicals of Interest
6.0	**KNOWN AMBIENT LEVELS OF CHEMICALS OF INTEREST**	Summary of reported levels of Chemicals of Interest in water, air, soil, and food
7.0	**OTHER SOURCES OF CHEMICALS OF INTEREST**	Summary of agricultural and other sources of the Chemicals of Interest
8.0	**FATE AND TRANSPORT**	A review of available fate and transport literature that reports on the factors that play a role in the ultimate fate of the Chemicals of Interest in agricultural environments
9.0	**DEGRADATION AND TRANSFORMATION PRODUCTS**	A review of the available literature that reports on the breakdown and transformation products related to the Chemicals of Interest within an agricultural environment
10.0	**PLANT UPTAKE**	A review of the available literature reporting on the plant uptake of the Chemicals of Interest in normal agricultural environments
11.0	**REVIEW OF TOXICITY OF CHEMICALS OF INTEREST**	A further review of the toxicity of Chemicals of Interest that focuses on identifying toxicity information for the larger classes of chemicals where specific toxicity data were unavailable for review in Task 1

Section	Description
12.0 RADIONUCLIDES	A review of identified radionuclides associated with produced water in the context of agricultural environments
13.0 SUMMARY AND CONCLUSIONS	Summary and conclusions based on review of the available literature presented
14.0 REFERENCES	Reference list

APPENDIX A

Appendix A: List of chemicals thought to be naturally occurring in produced water

CASRN	Chemical Name	Source
90-12-0	1-Methylnaphthalene	Hum et al., 2006
78-93-3	2-Butanone	Veil et al., 2004
91-57-6	2-Methylnaphthalene	Hum et al., 2006
105-67-9	2,4-Dimethylphenol	Veil et al., 2004
83-32-9	Acenaphthene	Manfra et al., 2010; OGP, 2002; OGP, 2005
208-96-8	Acenaphthylene	Manfra et al., 2010; OGP, 2002; OGP, 2005
7429-90-5	Aluminum	Guerra et al., 2011
7664-41-7	Ammonia	Liske and Leong, 2006
120-12-7	Anthracene	Manfra et al., 2010; OGP, 2002; OGP, 2005
7440-36-0	Antimony	Guerra et al., 2011
7440-38-2	Arsenic	Martel-Valles et al., 2013; OGP, 2005
7440-39-3	Barium	Veil et al., 2004; OGP, 2005; Dorea et al., 2006
71-43-2	Benzene	Manfra et al., 2010; OGP, 2002; OGP, 2005
56-55-3	Benzo(a)anthracene	Manfra et al., 2010; OGP, 2002; OGP, 2005
50-32-8	Benzo(a)pyrene	Veil et al., 2004; OGP, 2002; OGP, 2005
205-99-2	Benzo(b)fluoranthene	Manfra et al., 2010; OGP, 2002; OGP, 2005
191-24-2	Benzo(ghi)perylene	Hum et al., 2006; OGP, 2002; OGP, 2005
65-85-0	Benzoic acid	Veil et al., 2004

CASRN	Chemical Name	Source
7440-41-7	Beryllium	Guerra et al., 2011
111-44-4	Bis (2-chloroethyl) ether	Hum et al., 2006
7440-42-8	Boron	Guerra et al., 2011
7726-95-6	Bromine (Br)	Guerra et al., 2011
106-97-8	Butane	Hum et al., 2006
128-37-0	Butylhydroxytoluene	Hum et al., 2006
7440-43-9	Cadmium	Manfra et al., 2010; OGP, 2005
7440-70-2	Calcium	Veil et al., 2004; Dorea et al., 2006
124-38-9	Carbon dioxide	Martel-Valles et al., 2016
No CASRN	Carbonate	Martel-Valles et al., 2013; OGP, 2005; Dorea et al., 2006
16887-00-6	Chloride	OGP, 2002; OGP, 2005; Dorea et al. ,2006
108-90-7	Chlorobenzene	Veil et al., 2004
7440-47-3	Chromium	Manfra et al., 2010; OGP, 2005;
218-01-9	Chrysene	Manfra et al., 2010; OGP, 2002; OGP, 2005
7440-48-4	Cobalt	Guerra et al., 2011
7440-50-8	Copper	Guerra et al., 2011; OGP, 2005
84-74-2	di-n-Butylphthalate	Veil et al., 2004
53-70-3	Dibenzo(a,h)anthracene	Manfra et al., 2010; OGP, 2002; OGP, 2005
111-46-6	Diethylene glycol	Manfra et al., 2010
100-41-4	Ethylbenzene	Manfra et al., 2010; OGP, 2002; OGP, 2005

CASRN	Chemical Name	Source
206-44-0	Fluoranthene	Manfra et al., 2010; OGP, 2002; OGP, 2005
86-73-7	Fluorene	Manfra et al., 2010; OGP, 2002; OGP, 2005
16984-48-8	Fluoride	Guerra et al., 2011
110-54-3	Hexane	Hum et al., 2006
142-62-1	Hexanoic acid	Hum et al., 2006
7783-06-4	Hydrogen sulfide	Liske and Leong, 2006
193-39-5	Indenopyrene	Manfra et al., 2010; OGP, 2002; OGP, 2005
7439-89-6	Iron	Guerra et al., 2011; OGP, 2005
7439-92-1	Lead	Martel-Valles et al., 2013; OGP, 2005
7439-93-2	Lithium	Guerra et al., 2011
7439-95-4	Magnesium	Guerra et al., 2011
7439-96-5	Manganese	Guerra et al., 2011
7439-97-6	Mercury	Manfra et al., 2010; OGP, 2005
7439-98-7	Molybdenum	Guerra et al., 2011
No CASRN	n-Alkanes	Veil et al., 2004
124-18-5	n-Decane	Hum et al., 2006
3452-07-1	n-Eicosene	Hum et al., 2006
544-76-3	n-Hexadecane	Hum et al., 2006
593-45-3	n-Octadecane	Hum et al., 2006
629-59-4	n-Tetradecane	Hum et al., 2006

CASRN	Chemical Name	Source
91-20-3	Naphthalene	Veil et al., 2004; OGP, 2002; OGP, 2005
7440-02-0	Nickel	Manfra et al., 2010; OGP, 2005
14797-55-8	Nitrate	Martel-Valles et al., 2013; OGP, 2005
14797-65-0	Nitrite	Martel-Valles et al., 2013
7727-37-9	Nitrogen	Guerra et al., 2011
7631-86-9	Non-crystalline silica [amorphous silica]	Hum et al., 2006
95-48-7	o-Cresol	Hum et al., 2006
59-50-7	p-Chloro-m-cresol	Veil et al., 2004
106-44-5	p-Cresol	Hum et al., 2006
85-01-8	Phenanthrene	Manfra et al., 2010; OGP, 2002; OGP, 2005
108-95-2	Phenol	Veil et al., 2004; OGP, 2005
7723-14-0	Phosphorous	Martel-Valles et al., 2013
No CASRN	Polyhydroxyalkanoates (PHA)	Hum et al., 2006
7440-09-7	Potassium	Martel-Valles et al., 2013
129-00-0	Pyrene	Manfra et al., 2010; OGP, 2002; OGP, 2005
7440-14-4	Radium 226	Veil et al., 2004; Neff, 2002
15262-20-1	Radium 228	Veil et al., 2004; Neff, 2002
7782-49-2	Selenium	Guerra et al., 2011
7440-22-4	Silver	Guerra et al., 2011

CASRN	Chemical Name	Source
7440-23-5	Sodium	Guerra et al., 2011; Dorea et al., 2006
No CASRN	Steranes or cyclopentanoperhydrophenanthrene	Veil et al., 2004
7440-24-6	Strontium	Fillo et al., 1992; Dorea et al., 2006
No CASRN	Sulfate (SO_4^{2-})	Veil et al., 2004; OGP, 2005; Dorea et al., 2006
7704-34-9	Sulfur	Martel-Valles et al., 2016
7440-31-5	Tin	Fillo et al., 1992
7440-32-6	Titanium	Guerra et al., 2011; OGP, 2002
108-88-3	Toluene	Manfra et al., 2010; OGP, 2005
No CASRN	Triterpenes	Veil et al., 2004
7440-61-1	Uranium	Guerra et al., 2011
7440-62-2	Vanadium	Guerra et al., 2011
1330-20-7	Xylene	Manfra et al., 2010; OGP, 2002; OGP, 2005
7440-66-6	Zinc	Guerra et al., 2011; OGP, 2005

REFERENCES FOR APPENDIX A

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APPENDIX B

Appendix B: List of declared chemicals additives evaluated for toxicity

CASRN	Chemical Name
629-73-2	1-Hexadecene
2634-33-5	1,2 Benzisothiazol-3(2H)-one
526-73-8	1,2,3 Trimethylbenzene
95-63-6	1,2,4-Trimethylbenzene
108-67-8	1,3,5 Trimethylbenzene
123-91-1	1,4 Dioxane
479-66-3	1H, 3H-Pyrano (4,3-b)(1)benzopyran-9-carboxylic acid, 4,10-dihydro-3,7,8 trihydroxy-3-methyl-10-oxo
111-76-2	2-Butoxyethanol
104-76-7	2-Ethylhexanol
60-24-2	2-Mercaptoethanol
27646-80-6	2-Methylamino-2-methyl-1-propanol
67990-40-3	2-Propen-1-aminium, N,N-dimethyl-N-2-propenyl-, chloride, polymer with 2-hydroxypropyl 2-
145417-45-4	2-Propenoic acid, 2-methyl-, polymer with methyl 2-methyl-2-propenoate, octadecyl 2-methyl 2 propenoate and 2propenoic acid, sodium salt
25987-30-8	2-Propenoic acid, polymer with 2-propenamide, sodium salt
130800-24-7	2-Propenoic acid, telomer with 2-methyl-2-(1-oxo-2-propenyl)-1-propanesulfonic acid, sodium salt
115-19-5	3-Butyn-2-ol, 2-methyl
75-07-0	Acetaldehyde
64-19-7	Acetic acid
67-64-1	Acetone
107-02-8	Acrolein
100-73-2	Acrolein dimer
79-06-1	Acrylamide
79-10-7	Acrylic acid
124-04-9	Adipic Acid

CASRN	Chemical Name
68951-67-7	Alchohols, C14-15, ethoxylated
68439-45-2	Alcohol ethoxylate
66455-15-0	Alcohol ethoxylated, C-10-14
68439-46-3	Alcohols, C9-11, ethoxylated
90622-58-5	Alkanes, C11-15-iso
90622-46-1	Alkanes, C14-16
4719-04-4	Alkanolamine aldehyde condensate
29868-05-1	Alkanolamine phosphate
69011-36-5	Alkoxylated alcohol
68439-70-3	Alkyl amine
68081-81-2	Alkyl benzenesulfonate
68584-22-5	Alkyl benzenesulfonic acid
8001-54-5	Alkyl dimethyl benzyl ammonium chloride
68584-27-0	Alkylaryl sulfonate
68910-32-7	Alkylaryl sulfonates
90218-35-2	Alkylarylsulfonate amine salt
68648-87-3	Alkylbenzene mixture
90320-37-9	Almond shell
1344-28-1	Aluminium oxide
7446-70-0	Aluminum chloride
12042-91-0	Aluminum chloride hydroxide
300-92-5	Aluminum stearate
No CASRN	Amide surfactant acid salt
68140-01-2	Amides, Non Ionics
61791-24-0	Amine derivative
67924-33-8	Amine salt
NP-U2856	Amine salt
64346-44-7	Amine sulfate
926-39-6	Amine sulfate

CASRN	Chemical Name
6419-19-8	Aminotri (methylenephosphonic acid)
68910-31-6	Ammonium alkylaryl sulfonates
1863-63-4	Ammonium benzoate
10192-30-0	Ammonium bisulfate
12125-02-9	Ammonium chloride
1341-49-7	Ammonium fluoride
7783-20-2	Ammonium sulfate
7631-86-9	Amorphous silica
1309-64-4	Antimony trioxide
No CASRN	Aromatic amines
13462-86-7	Barite
7440-39-3	Barium
7727-43-7	Barium sulfate
1302-78-9	Bentonite
71-43-2	Benzene
65-85-0	Benzoic acid
100-44-7	Benzyl chloride
139-07-1	Benzyl Dimethyl Dodecyl Ammonium Chloride
122-18-9	Benzyl Dimethyl Hexadecyl Ammonium Chloride
122-19-0	Benzyl Dimethyl Octadecyl Ammonium Chloride
139-08-2	Benzyl Dimethyl Tetradecyl Ammonium Chloride
7440-41-7	Beryllium
68239-30-5	Bis(HMDA)- EPI Copolymer Hydrochloride
68411-32-5	Branched DDBSA
68551-19-9	C12-C14 Isoalkanes
68551-20-2	C12-C14 Isoalkanes
68855-24-3	C14-30 Alkyl Derivatives
7440-43-9	Cadmium
471-34-1	Calcium carbonate

CASRN	Chemical Name
1305-78-8	Calcium oxide
7778-18-9	Calcium sulfate
7440-44-0	Carbon
124-38-9	Carbon dioxide
9004-32-4	Carboxymethyl cellulose
69418-26-4	Cationic acrylamide copolymer
44992-01-0	Cationic acrylamide monomer
54076-97-0	Cationic polymer
681331-04-4	Causticized Lignite
11132-73-3	Cedar fiber
9005-81-6	Cellophane
9004-34-6	Cellulose
7440-47-3	Chromium
77-92-9	Citric acid
94266-47-4	Citrus terpenes
68155-07-7	Cocamide DEA
68603-42-9	Cocamide DEA
64743-05-1	Coke, petroleum, calcined
7440-50-8	Copper
7758-99-8	Copper sulfate pentahydrate
68308-87-2	Cotton seed hulls
129828-31-5	Crosslinked polyol ester
98-82-8	Cumene
108-93-0	Cyclohexanol
108-91-8	Cyclohexylamine
25155-15-1	Cymenes
5989-27-5	d-Limonene
No CASRN	DDBSA Salt
124-18-5	Decane

CASRN	Chemical Name
123-42-2	Diacetone Alcohol
2673-22-5	Diester of sulfosuccinic acid sodium salt
111-42-2	Diethanolamine
No CASRN	Dimethyl siloxane
9014-93-1	Dinonylphenyl polyoxyethylene
7722-88-5	Diphosphoric acid, sodium salt (1:4)
34590-94-8	Dipropylene glycol methyl ether
38011-25-5	Disodium ethylenediaminediacetate
125005-87-0	Diutan gum
112-40-3	Dodecane
No CASRN	Drilling paper
56449-05-9	EO PO Sorbitol
64-17-5	Ethanol
126-97-6	Ethanolamine thioglycolate
26027-38-3	Ethoxylated 4 Nonylphenol
61791-26-2	Ethoxylated amine
68002-97-1	Ethoxylated C10-16 Alcohols
34398-01-1	Ethoxylated C11 alcohol
61791-12-6	Ethoxylated Castor Oil
No CASRN	Ethoxylated octylphenol
9005 67 8	Ethoxylated sorbitan monostearate
9005-67-8	Ethoxylated Sorbitan Monostearate
141-78-6	Ethyl acetate
140-88-5	Ethyl acrylate
5877-42-9	Ethyl octynol
100-41-4	Ethylbenzene
107-21-1	Ethylene glycol
143-07-7	Fatty acid
67762-38-3	Fatty acid ester

CASRN	Chemical Name
70142-34-6	Fatty acid oxyalkylate
61790-45-2	Fatty acids, tall-oil, sodium salts
61788-91-8	Fatty alkylamines
17375-41-6	Ferrous sulfate
50-00-0	Formaldehyde
75-12-7	Formamide
64-18-6	Formic acid
98-00-0	Furfuryl alcohol
111-30-8	Glutaral
97722-02-6	Glycerides, tall oil mono-, di, and tri
56-81-5	Glycerine
139-33-3	Glycine, N,N, 1,2- ethanediylbis (N-(carboxymethyl)-disodium salt
79-14-1	Glycolic acid
107-22-2	Glyoxal
7782-42-5	Graphite
13397-24-5	Gypsum
64742-94-5	Heavy aromatic naphtha
64741-68-0	Heavy catalytic naphtha
108-74-7	Hexahydro 1,3,5 Trimethyl S Triazine
1415-93-6	Humic acids
7647-01-0	Hydrochloric acid
7664-39-3	Hydrofluoric acid
7722-84-1	Hydrogen peroxide
61790-59-8	Hydrogenated Tallow-Amine Acetate
123-31-9	Hydroquinone
64742-48-2	Hydrotreated heavy naphtha
64742-48-9	Hydrotreated Heavy Naphtha
64742-47-8	Hydrotreated light distillate
9004-62-0	Hydroxyethyl cellulose

CASRN	Chemical Name
2809-21-4	Hydroxyethylidenediphosphonic acid
7783-18-8	Inorganic sulfer compound
20461-54-5	Iodide
7553-56-2	Iodine
No CASRN	Ionic surfactants
124-68-5	Isobutanolamine
67-63-0	Isopropanol
119-65-3	Isoquinoline
8008-20-6	Kerosene
68648-89-5	Kraton G1702H
7439-90-9	Krypton
13983-27-2	Krypton 85
7439-92-1	Lead
64742-89-8	Light aliphatic naphtha
64742-95-6	Light aromatic naphtha
129521-66-0	Lignite
1317-65-3	Limestone
554-13-2	Lithium carbonate
13453-71-9	Lithium chlorate
7447-41-8	Lithium chloride
1310-65-2	Lithium hydroxide
13840-33-0	Lithium hypochlorite
6806-10-0000	Magma fiber
7439-97-6	Mercury
67-56-1	Methanol
74-87-3	Methyl chloride
No CASRN	Methyl ester of sulfonated tannin
PE-M2464	Methyl oxirane polymer
26172-55-4	Methylchloroisothiazolinone

CASRN	Chemical Name
8012-95-1	Mineral oil
141-43-5	Monoethanolamine
74-89-5	Monomethylamine
1302-93-8	Mullite
689391-01-5	n-Alkyl dimethyl benzyl ammonium chlorides
91-20-3	Naphthalene
7440-02-0	Nickel
7786-81-4	Nickel sulfate
9016-45-9	Non phenol ethoxylates
127087-87-0	Nonylphenol polyethylene glycol ether
No CASRN	Nutshell
112-80-1	Oleic acid
68647-72-3	Orange terpenes
104-55-2	Organic acids ethoxylated alcohols
577-11-7	Organic surfactant
68412-54-4	Oxyalkylated alkylphenol
30704-64-4	Oxyalkylated alkylphenolic resin
30846-35-6	Oxyalkylated alkylphenolic resin
63428-92-2	Oxyalkylated alkylphenolic resin
68171-44-8	Oxyalkylated alkylphenolic resin
26316-40-5	Oxyalkylated Ethylenediamine
67939-72-4	Oxyalkylated polyamine
68910-19-0	Oxyalkylated polyamine
64742-55-8	Paraffinic petroleum distillate
56919-55-2	Pentadecane, 3-methylene
115146-98-0	Pentadecane, 5-methylene
13043-55-5	Pentadecane, 7-methylene
140-01-2	Pentasodium diethylenetriamine pentaacetate
79-21-0	Peroxyacetic acid

CASRN	Chemical Name
64742-53-6	Petrolleum distillates
68425-75-2	Phosphate ester salt
P-84-470	Phosphonate salt
13598-36-2	Phosphonic acid
55566-30-8	Phosphonium, tetrakis (hydroxymethyl)-, sulfate (2:1), salt
7664-38-2	Phosphoric acid
No CASRN	Phosphoric acid ester salt
2008-9-3	Pine Oil
110-85-0	Piperazine
9005-70-3	POE (20) Sorbitan trioleate
68938-70-5	Poly (triethanolamine.MCQ)
9003-05-8	Polyacrylamide
9003-79-8	Polyacrylate
9003 01 4	Polyacrylic acid
64114-46-1	Polyamine
68955-69-1	Polyamine salts
19019-43-3	Polycarboxlate salt
26062-79-3	PolyDADMAC
No CASRN	Polydimethylsiloxane emulsion
25038-59-9	Polyethylene
25322-68-3	Polyethylene glycol
68036-92-0	Polyglycol diepoxide
68036-95-3	Polyglycol diepoxide
PE-M2481	Polyglycol ester
9038-95-3	Polyglycol ether
9051-89-2	Polylactide resin
9033-79-8	Polymer sodium acrylate
64741-71-5	Polymers (petroleum) viscous
68123-18-2	Polyoxyalklene glycol

CASRN	Chemical Name
68551-12-2	Polyoxyalkylene
36484-54-5	Polyoxyalkylene glycol
61790-86-1	Polyoxyalkylenes
78330-21-9	Polyoxyalkylenes
68412-53-3	Polyoxyethylene nonylphenyl ether phosphate
25322-69-4	Polypropylene glycol
42751-79-1	Polyquaternary amine
9002-89-5	Polyvinyl alcohol
127-08-2	Potassium acetate
7646-93-7	Potassium bisulfate
7447-40-7	Potassium chloride
1310-58-3	Potassium hydroxide
12136-45-7	Potassium Oxide
16068-46-5	Potassium Phosphate
107-19-7	Propargl alcohol
123-38-6	Propionaldehyde
57-55-6	Propylene glycol
14808-60-7	Quartz crystalline silica
61790-41-8	Quaternary ammonium compound
68424-85-1	Quaternary ammonium compound
68609-18-7	Quaternized condensed alkanolamines
91-63-4	Quinaldine
P-88-1256	Salt of an organic sulfur compound
68153-60-6	Salt of fatty acid polyamine
1319-41-1	Saponite
64742-62-7	Severely hydrotreated paraffinic
15468-32-3	Silica crystalline tridymite
14464-46-1	Silica, crystalline, cristoballite
63148-62-9	Siloxanes and silicones

CASRN	Chemical Name
1318-93-0	Smectite
127-09-3	Sodium acetate
7758-16-9	Sodium acid pyrophosphate
532-32-1	Sodium benzoate
144-55-8	Sodium bicarbonate
7631-90-5	Sodium bisulfite
497-19-8	Sodium carbonate
9063-38-1	Sodium carboxymethylstarch
7775-09-9	Sodium chlorate
7647-14-5	Sodium chloride
4647-14-5	Sodium chloride
2893-78-9	Sodium dichloroisocyanurate
64-02-8	Sodium edetate
6381-77-7	Sodium erythorbate
2836-32-0	Sodium glycolate
1310-73-2	Sodium hydroxide
7681-52-9	Sodium hypochlorite
7681-82-5	Sodium Iodide
68439-57-6	Sodium olefin sulfonate
1313-59-3	Sodium Oxide
9003-04-7	Sodium polyacrylate
9003-79-3	Sodium polyacrylate
7757-82-6	Sodium sulfate
12179-04-3	Sodium tetraborate pentahydrate
10102-17-7	Sodium thiosulfate pentahydrate
7772-98-7	Sodium thiosulfate pentahydrate
7785-84-4	Sodium trimetaphosphate
64742-65-0	Solvent dewaxed heavy paraffinic

CASRN	Chemical Name
NP-SMO3_U1240	Sorbitan ester
9005-65-6	Sorbitan mono-9-Octadecenoate
1338-43-8	Sorbitan monooleate
67784-80-9	Soybean oil, me ester
57-11-4	Stearic acid
65996-69-2	Steel mill slag
8052-41-3	Stoddard solvents
7446-09-5	Sulfur dioxide
7664-93-9	Sulfuric acid
61790-12-3	Tall oil fatty acids
68140-11-4	Tall Oil, DETA Imidazoline Acetates
61790-33-8	Tallow alkylamines
68201-64-9	Tannins, sulfomethylated
72480-70-7	Tar bases, quinoline derivatives, benzyl chloride- quaternized
8002-09-3	Terpene hydrocarbon
629-59-4	Tetradecane
25265-78-5	Tetrapropylenebenzene
68527-49-1	Thiourea, polymer with formaldehyde and 1-phenylethanone
13463-67-7	Titanium dioxide
108-88-3	Toluene
629-50-5	Tridecane
112-27-6	Triethylene Glycol
25551-13-7	Trimethyl benzene
7758-29-4	Triphosphoric acid, sodium salt (1:5)
5064-31-3	Trisodium nitrilotriacetic acid
1120-21-4	Undecane
57-13-6	Urea
84012-43-1	Walnut shell

CASRN	Chemical Name
7732-18-5	Water
No CASRN	Wood dust
11138-66-2	Xanthan gum
7440-63-3	Xenon
14932-42-4	Xenon radionuclide
1330-20-7	Xylene
7440-66-6	Zinc
7646-85-7	Zinc chloride

APPENDIX C

Appendix C: Biodegradability memo from Dr. Will Stringfellow, PHD sent to GSI as reference material

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To: Bernard Beckerman, GSI Environmental
From: William T. Stringfellow
Date: June 25, 2019 (Final Draft)
Subject: Interpretation of standard biodegradation screening tests
Cc: Clay Rogers, Dale Harvey

The Food Safety Panel agrees that "biodegradability" can be considered as a criteria for establishing a priority list of chemicals of interest (COI). In the context of using produced water for irrigated agriculture, COI that are "biodegradable" are expected to be less persistent in the environment and therefore less of a health or environmental risk than COI that are not biodegradable. Given the large number of chemicals that could potentially be found in produced water, it is important and necessary to establish a short list of priority COI for detailed investigation. In this memo I am providing some background on standardized testing for biodegradation and some guidance for interpretation of standard biodegradation screening tests in the context of the environmental fate of industrial chemicals in agricultural ecosystems and the reuse of produced water for irrigated agriculture.

Biodegradation of organic compounds in agricultural ecosystems and other environments is a complicated process that involves interactions between bacteria or other microorganism and their physical environment, and chemical factors, including the properties of the compound being biodegraded (Belanger et al., 2002; Chishti et al., 2013; Liu et al., 2019). Factors that may influence biodegradation in environmental systems include nutrient availability, pH, salinity, and the concentration of oxygen (e.g. Belanger et al., 2002; Karpuzcu et al., 2013; Pomies et al., 2013). Absorption and adsorption influence bioavailability and are known to retard degradation rates (Grimberg et al., 1996; Stringfellow and Alvarez-Cohen, 1999; Rogers and Stringfellow, 2009). Since all of the physical, chemical, and biological factors cannot be know specifically for all scenarios of exposure or release, simplified tests are often conducted to establish first principals that can be applied to complex scenarios.

The first principle of biodegradation is to demonstrate the ability of a microorganism to enzymatically transform a larger molecule to a smaller molecule. If sufficient enzymatic degradation can be shown to occur, a molecule is then classified as biodegradable. Complete biodegradation or "mineralization" occurs when microorganisms decompose organic molecules into carbon dioxide, water, and inorganic products such as ammonia. Microorganisms can also biologically catalyze or "transform" chemicals, especially metals and inorganic chemicals, from one form to another in reactions are reversible. Transformation of inorganic chemicals is not typically considered biodegradation, since the reactions are reversible, but they are important reactions to consider in risk assessments. For example, microbial catalysis of metals can change metal properties such as solubility, bioavailability, and toxicity. The concept of biodegradation discussed in this memo is applied to the degradation of organic chemicals.

It is possible for organic compounds to be transformed only partially to products that may not be further degraded (e.g. Pan et al., 2015; Lobo et al., 2018). It is also possible for microorganisms

to form intermediate products that are more toxic than the parent compound (e.g. Scheutz et al., 2011). However, the formation of stable, toxic products is unusual, especially in open aerobic systems with mixed bacterial communities, as are found in agricultural ecosystems.

There has been long standing interest in developing reproducible methods for measuring the biodegradability of individual industrial chemicals (e.g. Mills and Stack, 1955; Ott et al., 2019). Standard methods for measuring biodegradation potential of chemicals were developed initially to address water pollution by synthetic detergents that were not degraded in regional biological sewage treatment plants and were causing foaming and other water pollution in receiving waters (Borstlap and Kooijman, 1963; Cohn, 1963; Wayman and Robertson, 1963; Coughlin, 1965; Procter & Gamble, 2008; Cowan-Ellsberry et al., 2014). Standardized biodegradation testing is now applied widely and has been used to characterize many categories of industrial chemicals (United States Environmental Protection Agency, 1979; Fushiwaki and Urano, 1988; Okuda et al., 1991; Calmon-Decriaud et al., 1998; Vazquez-Rodriguez and Beltran-Hernandez, 2004; Ericson, 2010; Ericson et al., 2014; Dick et al., 2016; Martin et al., 2017a).

Early biodegradation screening tests focused on predicting chemical fate in activated sludge and other biological wastewater treatment plans and therefore used aerobic conditions, high to intermediate chemical concentrations, and activated sludge as a source of the microbial inoculum (Organization for Economic Co-operation and Development (OECD), 1986, 1995). Initial test protocols were also limited to water soluble chemicals (Organization for Economic Co-operation and Development (OECD), 1995). Over time, numerous modification of standard biodegradation screening tests have been considered, evaluated, and used (Okuda et al., 1991; Organization for Economic Co-operation and Development (OECD), 1995; Vazquez-Rodriguez and Beltran-Hernandez, 2004; Ericson, 2007, 2010; Kowalczyk et al., 2015; Dick et al., 2016; Martin et al., 2017a; Martin et al., 2017b; Corada-Fernandez et al., 2018; Ott et al., 2019).

Most standardized biodegradation screening tests are batch tests, where the removal of the test chemical over time is measured by aggregate methods, such as removal of dissolved organic carbon (DOC) or oxygen consumption over time. Tests where the removal of the "parent" test compound is measured are often referred to as "die-away" tests (Wylie et al., 1982; Fushiwaki and Urano, 1988; Okpokwasili and Olisa, 1991; Okuda et al., 1991; Yamaguchi et al., 1997; Ericson, 2010). Various modifications of the basic die-away test include using specialize bacteria; using river water or soils as test medium or inoculum; and measuring carbon dioxide to demonstrate complete mineralization of the test compound (Quiroga et al., 1992; Struijs and Stoltenkamp, 1994; Ingerslev and Nyholm, 2000; Corada-Fernandez et al., 2018; Ott et al., 2019).

Although standard biodegradation screening tests were originally developed over 30 years ago, the results of tests used today are consistent with earlier test results and a significant body of knowledge concerning the biodegradability of industrial chemicals and other pollutants has been developed using standardized biodegradability screening tests (Dick et al., 2016; Martin et al., 2017a; Menzies et al., 2017; Corada-Fernandez et al., 2018; Ott et al., 2019). There is general agreement that if a compound is degraded microbially in a standardized biodegradability screening tests, then the compound will be degraded in sewage treatment systems, open bodies of

water, and other well aerated systems with active microbial populations (Dick et al., 2016; Martin et al., 2017a; Menzies et al., 2017; Corada-Fernandez et al., 2018; Ott et al., 2019).

The most common and consistent criticism of standardized biodegradability screening tests is that they will yield false-negatives, i.e. chemicals that are not demonstrating biodegradation in the standardized test would be biodegraded in nature, under circumstances not reflected in the test conditions. A common reason for false-negative results is that the microbial inoculum does not contain bacteria or other microorganisms capable of degrading the test compound (Mills and Stack, 1955; Thouand and Block, 1993; Kowalczyk et al., 2015; Dick et al., 2016; Martin et al., 2017b; Ott et al., 2019). It is also recognized that standardized biodegradability screening tests are best suited for water soluble compounds and higher substrate concentrations (>10 mg/L) and may not accurately measure biodegradation of poorly soluble (hydrophobic) chemicals or compounds that exhibit microbial inhibition (Organization for Economic Co-operation and Development (OECD), 1986, 1995; Dick et al., 2016; Timmer et al., 2019).

I found no evidence in the literature of false-positive results from standardized biodegradability screening tests. It can be concluded that standardized biodegradability screening tests are conservative tests, in that they can yield false-negative, but not false-positive, results. Therefore, as a conservative test, it is entirely appropriate to the use standardized biodegradability screening tests as a criteria for selection of COIs in the context of food safety.

The United Stated Environmental Protection Agency (USEPA) has utilized standardized biodegradation screening tests as part of regulatory requirements since at least the 1970s (United States Environmental Protection Agency, 1979, 1998a, 2008; David Markell, 2010). Biodegradation testing is required for the registration of pesticides and toxic substances under the Toxic Substances Control Act (United States Environmental Protection Agency, 1998b). In federal regulations, the USEPA requires the use of standard biodegradation testing protocols published by the Organization for Economic Co-operation and Development (OECD) or equivalent methods published by the National Institute of Standards and Technology (United States Environmental Protection Agency, 1998b, a, 2008).

The OECD has developed and approved a series of standardized biodegradability screening tests that include testing for chemical biodegradation under both aerobic and anaerobic conditions (Table 1). The OECD guidelines organize the examination of the biodegradability of chemicals into a tiered strategy, applying tests of increasing complexity and environmental realism (and costs) as needed to establish biodegradability of a test compound (Organization for Economic Co-operation and Development (OECD), 2003, 2005). This tiered approach includes screening tests for "ready" biodegradability, which are simple batch experiments conducted under closely defined conditions. Organic chemicals that are not found to degrade sufficiently in screening tests can be further tested in "inherent" biodegradation tests that allow testing under more flexible conditions, where variables such as inoculum and incubation time can be changed. In addition, OECD guidelines also allow for "simulation" or higher tiered tests which were developed as confirmatory studies for compounds that may be yielding false-negatives in simpler tests (Organization for Economic Co-operation and Development (OECD), 2003; Ott et al., 2019). The use of OECD biodegradation tests to identify potentially persistent compounds is

considered fundamental to an effective environmental risk assessment strategy (United States Environmental Protection Agency, 1998a; Ott et al., 2019).

Ready biodegradability tests are stringent screening tests, conducted under aerobic conditions, over a defined period of time (up to 28 days, typically), in which a high concentration of the test substance (in the range of 2 to 100 mg/L) is used and the biodegradation rate is measured by non-specific parameters like DOC, biochemical oxygen demand, and CO_2 production (Organization for Economic Co-operation and Development (OECD), 1986, 2003). The tests which can be used to determine the ready biodegradability of organic chemicals are identified as screening methods in Table 1. The be classified as "readily" biodegradable, the compound must be degraded by 70% as measured by DOC or 60% as measured by theoretical CO_2 production ($ThCO_2$) or theoretical oxygen demand (ThOD) within 28 days (Organization for Economic Co-operation and Development (OECD), 2003). In these tests, a positive result can be considered as indicative of rapid ultimate degradation in most environments (Organization for Economic Co-operation and Development (OECD), 2003).

Two of the ready biodegradability screening tests identified in Table 1 are conducted under special conditions, but are modifications of various 301 series tests. OECD Test Number 306: Biodegradability in Seawater was developed to address degradation of organic chemicals in seawater, which has generally been found to be slower than that experienced in freshwater, activated sludge and sewage effluent. Positive result obtained during 28 days in a Biodegradability in Seawater test (>60% ThOD; >70% DOC) can normally be regarded as an indication of ready biodegradability. OECD Test Number 311 includes biodegradability screening test conducted under anoxic conditions, in which a high concentration of the test substance (mg/L) is used and the biodegradation rates are measured by non-specific parameters like total inorganic carbon formation or CO_2 and CH_4 production. These tests are used for the evaluation of potential anaerobic biodegradability in an anaerobic digester at a given range of concentration of microorganisms (Organization for Economic Co-operation and Development (OECD), 2003).

Inherent biodegradability tests (Table 1) are tests that allow for more favorable conditions for degradation than screening tests (Organization for Economic Co-operation and Development (OECD), 2003). Inherent test procedures allow prolonged exposure of the test substance to microorganisms and a low test substance to biomass ratio, which makes the tests powerful (Organization for Economic Co-operation and Development (OECD), 2003). Some of these tests may be conducted using microorganisms that have previously been exposed to the test substance, which frequently results in adaptation leading to a significantly more extensive degradation of the chemical (Kowalczyk et al., 2015; Dick et al., 2016; Martin et al., 2017b). Because of the favorable conditions employed in these tests, it can not be assumed that "inherently biodegradable" chemicals will rapidly biodegrade in all environments or conditions (Organization for Economic Co-operation and Development (OECD), 2003).

Simulation tests are tests that provide data for the rate of degradation under specified environmentally relevant conditions (Organization for Economic Co-operation and Development (OECD), 1995, 2001, 2003; Ericson, 2007; Menzies et al., 2017). These tests simulate the

degradation in a specific environment by use of indigenous biomass, relevant solids (i.e. soil, sediment or other surfaces) to allow sorption of the chemical, and a typical temperature which represents the particular environment (Organization for Economic Co-operation and Development (OECD), 2003). A low concentration of the test substance is used in tests designed to determine the biodegradation rate whereas higher concentrations are normally used for identification and quantification of major transformation products. A low concentration of chemical in this type of tests means a concentration of less than 1 μg/L to 100 μg/L, which is low enough to ensure that the biodegradation kinetics obtained in the test reflect those expected in the environment being simulated. The degradation rates are measured either by ^{14}C-radiolabelling techniques or by specific chemical analyses (Organization for Economic Co-operation and Development (OECD), 2003). Simulations tests are designed to simulate specific environments including soils, aquatic sediments, surface water, and sewage treatment plants (Organization for Economic Co-operation and Development (OECD), 2003). Simulations tests are identified in Table 1. The criteria for determining biodegradability vary, but all tests require demonstration of extensive degradation or transformation to qualify a test substance as biodegradable.

In summary, standardized biodegradation tests are based on well established science that have been developed over several decades. Standardized biodegradation tests are conservative tests, in that the tests may yield false-negative results, but are not known to produce false-positive results. The procedures for conducting and interpreting biodegradation tests have been formalized to the extent that they are now a routine part of environmental regulations in the United States, Europe, and elsewhere. Compounds that are classified as “readily biodegradable” by OECD guidelines can be considered to degrade rapidly in any environment. Compounds classified as “inherently biodegradable” will degrade in the environment, but may not rapidly degrade under all conditions. Compounds that do not meet the criteria for classification as either readily or inherently biodegradable, may still be biodegradable in the environment, since the standardized biodegradation tests are conservative.

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Table 1. Approved standardized biodegradation assessment methods from the Organization for Economic Co-operation and Development (OECD). These guidelines are now used as reference tests for federal regulation in the United States.

No.	Title	Type
301	Ready Biodegradability (301 A-F) DOC Die-Away Test (301 A) CO2 Evolution Test (301 B) Modified MITI Test (I) (301 C) Closed Bottle Test (301 D) Modified OECD Screening Test (301 E) Manometric Respirometry Test (301 F)	Screening
302	Inherent Biodegradability (302 A-C) Modified SCAS Test (302 A) Zahn-Wellens/EMPA Test (302 B) Modified MITI Test (II) (302 C)	Inherent
303	Simulation Test - Aerobic Sewage Treatment -- A: Activated Sludge Units; B: Biofilms	Simulation
304A	Inherent Biodegradability in Soil	Inherent
306	Biodegradability in Seawater	Screening
307	Aerobic and Anaerobic Transformation in Soil	Simulation
308	Aerobic and Anaerobic Transformation in Aquatic Sediment Systems	Simulation
309	Aerobic Mineralization in Surface Water – Simulation Biodegradation Test	Simulation
310	Ready Biodegradability - CO2 in sealed vessels (Headspace Test)	Screening
311	Anaerobic Biodegradability of Organic Compounds in Digested Sludge: by Measurement of Gas Production	Screening
314	Simulation Tests to Assess the Biodegradability of Chemicals Discharged in Wastewater	Simulation

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APPENDIX D

Appendix D: List of Chemicals of Interest to be reviewed in Task 2

CASRN	Chemical Name	Oil Field Additive?	Naturally Occurring?	Reason for Inclusion in Chemicals of Interest[1]
479-66-3	1H, 3H-Pyrano (4,3-b)(1)benzopyran-9-carboxylic acid, 4,10-dihydro-3,7,8 trihydroxy-3-methyl-10-oxo (fulvic acid)	Y	N	Insufficient Tox. Data
100-73-2	Acrolein dimer	Y	N	Insufficient Tox. Data
No CASRN	Aromatic Amine	Y	N	Insufficient Tox. Data
38011-25-5	Disodium ethylenediaminetetraacetate	Y	N	Insufficient Tox. Data
No CASRN	Heavy catalytic reformed naptha	Y	N	Insufficient Tox. Data
1415-93-6	Humic acids	Y	N	Insufficient Tox. Data
85-01-8	Phenanthrene	N	Y	Insufficient Tox. Data
19019-43-3	Polycarboxlate salt	Y	N	Insufficient Tox. Data
74-84-0	Polyethylene	Y	N	Insufficient Tox. Data
9038-95-3	Polyglycol ether	Y	N	Insufficient Tox. Data
91-63-4	Quinaldine	Y	N	Insufficient Tox. Data

[1] OPR: Organizational Peer Reviewed Toxicity Value [usually agency derived]; RA – OPR: Read-across assessment using an Organizational Peer Reviewed Toxicity Value; STV: Project-specific Surrogate Toxicity Value; RA – STV: Read-Across assessment using an project-specific Surrogate Toxicity Value

CASRN	Chemical Name	Oil Field Additive?	Naturally Occurring?	Reason for Inclusion in Chemicals of Interest[1]
NP-SMO3_U1240	Sorbitan ester	Y	N	Insufficient Tox. Data
65996-69-2	Steel mill slag	Y	N	Insufficient Tox. Data
8052-41-3	Stoddard Solvents	Y	N	Insufficient Tox. Data
64-02-8	Tetrasodium ethylenediaminetetraacetate	Y	N	Insufficient Tox. Data
27646-80-6	2-Methylamino-2-methyl-1-propanol	Y	N	No Tox. Data
67990-40-3	2-Propen-1-aminium, N,N-dimethyl-N-2-propenyl-, chloride, polymer with 2-hydroxypropyl 2-propenoate and 2-propenoic acid	Y	N	No Tox. Data
145417-45-4	2-Propenoic acid, 2-methyl-, polymer with methyl 2-methyl-2-propenoate, octadecyl 2-methyl 2 propenoate and 2propenoic acid, sodium salt	Y	N	No Tox. Data
9033-79-8	2-propenoic acid, polymer with sodium 2-propenoate	Y	N	No Tox. Data
130800-24-7	2-Propenoic acid, telomer with 2-methyl-2-(1-oxo-2-propenyl)-1-propanesulfonic acid, sodium salt	Y	N	No Tox. Data
300-92-5	Aluminum distearate	Y	N	No Tox. Data

CASRN	Chemical Name	Oil Field Additive?	Naturally Occurring?	Reason for Inclusion in Chemicals of Interest[1]
No CASRN	Amide surfactant acid salt	Y	N	No Tox. Data
No CASRN	Amides, Non Ionics	Y	N	No Tox. Data
61791-24-0	Amine derivative	Y	N	No Tox. Data
67924-33-8	Amine salt	Y	N	No Tox. Data
NP-U2856	Amine salt	Y	N	No Tox. Data
64346-44-7	Amine sulfate	Y	N	No Tox. Data
68239-30-5	Bis (HDMA) EPI Copolymer hydrochloride	Y	N	No Tox. Data
69418-26-4	Cationic acrylamide copolymer	Y	N	No Tox. Data
44992-01-0	Cationic acrylamide monomer	Y	N	No Tox. Data
54076-97-0	Cationic polymer	Y	N	No Tox. Data
681331-04-4	Causticized Lignite	Y	N	No Tox. Data
64743-05-1	Coke (petroleum), calcined	Y	N	No Tox. Data
25987-30-8	Copolymer of acrylamide and sodium acrylate	Y	N	No Tox. Data
129828-31-5	Crosslinked polyol ester	Y	N	No Tox. Data
2673-22-5	Diester of sulfosuccinic acid sodium salt	Y	N	No Tox. Data
No CASRN	Drilling paper	Y	N	No Tox. Data

CASRN	Chemical Name	Oil Field Additive?	Naturally Occurring?	Reason for Inclusion in Chemicals of Interest[1]
61791-26-2	Ethoxylated amine	Y	N	No Tox. Data
9081-83-8	Ethoxylated octylphenol	Y	N	No Tox. Data
5877-42-9	Ethyl octynol	Y	N	No Tox. Data
63428-92-2	Formaldehyde, polymer with 2-methyloxirane, 4-nonylphenol and oxirane	Y	N	No Tox. Data
30704-64-4	Formaldehyde, polymer with 4-(1,1-dimethylethyl)phenol, 2-methyloxirane and oxirane	Y	N	No Tox. Data
30846-35-6	Formaldehyde, polymer with 4-nonylphenol and oxirane	Y	N	No Tox. Data
No CASRN	Heavy catalytic reformed naptha	Y	N	No Tox. Data
61790-59-8	Hydrogenated tallow amine acetone	Y	N	No Tox. Data
68648-89-5	Kraton G1702H	Y	N	No Tox. Data
129521-66-0	Lignite	Y	N	No Tox. Data
PE-M2464	Methyl oxirane polymer	Y	N	No Tox. Data
No CASRN	Organic acid ethoxylated alcohols	Y	N	No Tox. Data
68171-44-8	Oxyalkylated alkylphenolic resin	Y	N	No Tox. Data
68910-19-0	Oxyalkylated polyamine	Y	N	No Tox. Data
67939-72-4	Oxyalkylated polyamine	Y	N	No Tox. Data

CASRN	Chemical Name	Oil Field Additive?	Naturally Occurring?	Reason for Inclusion in Chemicals of Interest[1]
68123-18-2	Phenol, 4,4'-(1-methylethylidene) bis-, polymer with 2-(chloromethyl)oxirane, 2-methyloxirane and oxirane	Y	N	No Tox. Data
68425-75-2	Phosphate ester salt	Y	N	No Tox. Data
9005-70-3	POE (20) Sorbitan Trioleate	Y	N	No Tox. Data
68938-70-5	Poly (triethanolamine.mce)	Y	N	No Tox. Data
68955-69-1	Polyamine salts	Y	N	No Tox. Data
26062-79-3	Polydimethyl diallyl ammonium chloride	Y	N	No Tox. Data
68036-92-0	Polyglycol diepoxide	Y	N	No Tox. Data
68036-95-3	Polyglycol diepoxide	Y	N	No Tox. Data
No CASRN	Polyhydroxyalkanoates (PHA)	N	Y	No Tox. Data
64741-71-5	Polymers (petroleum) viscous	Y	N	No Tox. Data
36484-54-5	Polyoxyalkylene glycol	Y	N	No Tox. Data
61790-86-1	Polyoxyalkylenes	Y	N	No Tox. Data
9014-93-1	Polyoxyethylene dinonylphenol	Y	N	No Tox. Data
12068-19-8	Polyoxyethylene nonyl phenyl ether phosphate	Y	N	No Tox. Data
70142-34-6	Polyoxyl 15 hydroxystearate	Y	N	No Tox. Data

CASRN	Chemical Name	Oil Field Additive?	Naturally Occurring?	Reason for Inclusion in Chemicals of Interest[1]
42751-79-1	Polyquaternary amine	Y	N	No Tox. Data
68609-18-7	Quaternized condensed alkanolamines	Y	N	No Tox. Data
No CASRN	Steranes or cyclopentanoperhydrophenanthrene	N	Y	No Tox. Data
68140-11-4	Tall oil, DETA/ midazoline acetates	Y	N	No Tox. Data
72480-70-7	Tar bases, quinoline derivatives, quaternized benzyl chloride	Y	N	No Tox. Data
68527-49-1	Thiourea, polymer with formaldehyde and 1-phenylethanone	Y	N	No Tox. Data
64114-46-1	Triethanolamine homopolymer	Y	N	No Tox. Data
53-70-3	Dibenzo(a,h)anthracene	N	Y	OPR=0.000002 mg/kg/d
50-32-8	Benzo(a)pyrene	N	Y	OPR=0.000003 mg/kg/d
111-44-4	Bis (2-chloroethyl) ether	N	Y	OPR=0.000004 mg/kg/d
7440-38-2	Arsenic	N	Y	OPR=0.000007 mg/kg/d
56-55-3	Benzo(a)anthracene	N	Y	OPR=0.000008 mg/kg/d
205-99-2	Benzo(b)fluoranthene	N	Y	OPR=0.000008 mg/kg/d
193-39-5	Indenopyrene	N	Y	OPR=0.000008 mg/kg/d
218-01-9	Chrysene	N	Y	OPR=0.00008 mg/kg/d

CASRN	Chemical Name	Oil Field Additive?	Naturally Occurring?	Reason for Inclusion in Chemicals of Interest[1]
123-91-1	1,4 Dioxane	Y	N	OPR=0.0001 mg/kg/d
7440-43-9	Cadmium	Y	Y	OPR=0.0001 mg/kg/d
7439-97-6	Mercury	Y	Y	OPR=0.0002 mg/kg/d
7440-48-4	Cobalt	N	Y	OPR=0.0003 mg/kg/d
7439-92-1	Lead	Y	Y	OPR=0.0003 mg/kg/d
7440-36-0	Antimony	N	Y	OPR=0.0004 mg/kg/d
7440-41-7	Beryllium	Y	Y	OPR=0.002 mg/kg/d
7439-93-2	Lithium	N	Y	OPR=0.002 mg/kg/d
554-13-2	Lithium carbonate	Y	N	OPR=0.002 mg/kg/d
13453-71-9	Lithium chlorate	Y	N	OPR=0.002 mg/kg/d
1310-65-2	Lithium hydroxide	Y	N	OPR=0.002 mg/kg/d
13840-33-0	Lithium hypochlorite	Y	N	OPR=0.002 mg/kg/d
7440-47-3	Chromium	Y	Y	OPR=0.003 mg/kg/d
7440-61-1	Uranium	N	Y	OPR=0.003 mg/kg/d & Radionuclide
7439-98-7	Molybdenum	N	Y	OPR=0.005 mg/kg/d
7782-49-2	Selenium	N	Y	OPR=0.005 mg/kg/d
7440-22-4	Silver	N	Y	OPR=0.005 mg/kg/d
7440-50-8	Copper	Y	Y	OPR=0.01 mg/kg/d

CASRN	Chemical Name	Oil Field Additive?	Naturally Occurring?	Reason for Inclusion in Chemicals of Interest[1]
7758-99-8	Copper sulfate pentahydrate	Y	N	OPR=0.01 mg/kg/d
7553-56-2	Iodine	Y	N	OPR=0.01 mg/kg/d
7440-02-0	Nickel	Y	Y	OPR=0.01 mg/kg/d
7786-81-4	Nickel sulfate	Y	N	OPR=0.01 mg/kg/d
120-12-7	Anthracene	N	Y	OPR=0.02 mg/kg/d
108-90-7	Chlorobenzene	N	Y	OPR=0.02 mg/kg/d
129-00-0	Pyrene	N	Y	OPR=0.03 mg/kg/d
64742-95-6	Solvent naphtha, petroleum, light arom.	Y	N	OPR=0.03 mg/kg/d
206-44-0	Fluoranthene	N	Y	OPR=0.04 mg/kg/d
16984-48-8	Fluoride	N	Y	OPR=0.05 mg/kg/d
7664-39-3	Hydrofluoric acid	Y	N	OPR=0.05 mg/kg/d
83-32-9	Acenaphthene	N	Y	OPR=0.06 mg/kg/d
7439-96-5	Manganese	N	Y	OPR=0.1 mg/kg/d
14797-65-0	Nitrite	N	Y	OPR=0.1 mg/kg/d
2025884	Sulfur dioxide	Y	N	OPR=0.1 mg/kg/d
7440-62-2	Vanadium	N	Y	OPR=0.1 mg/kg/d
7727-43-7	Barite	Y	N	OPR=0.2 mg/kg/d
7440-39-3	Barium	Y	Y	OPR=0.2 mg/kg/d

CASRN	Chemical Name	Oil Field Additive?	Naturally Occurring?	Reason for Inclusion in Chemicals of Interest[1]
7440-42-8	Boron	N	Y	OPR=0.2 mg/kg/d
12179-04-3	Sodium tetraborate pentahydrate	Y	N	OPR=0.2 mg/kg/d
7440-31-5	Tin	N	Y	OPR=0.3 mg/kg/d
7440-66-6	Zinc	Y	Y	OPR=0.3 mg/kg/d
7646-85-7	Zinc chloride	Y	N	OPR=0.3 mg/kg/d
119-65-3	Isoquinoline	Y	N	RA - OPR=0.000003 mg/kg/d
1309-64-4	Antimony trioxide	Y	N	RA - OPR=0.0004 mg/kg/d
7447-41-8	Lithium chloride	Y	N	RA - OPR=0.002 mg/kg/d
29868-05-1	Alkanolamine phosphate	Y	N	RA - OPR=0.04 mg/kg/d
60-24-2	2-mercaptoethanol	Y	N	STV=0.005 mg/kg/d
64742-53-6	Distillates, hydrotreated light naphthenic	Y	N	STV=0.04 mg/kg/d
126-97-6	Ethanolamine thioglycolate	Y	N	STV=0.07 mg/kg/d
115-19-5	2-methyl-3-Butyn-2-ol	Y	N	STV=0.2 mg/kg/d
68308-87-2	Cottonseed, flour	Y	N	STV=0.2 mg/kg/d
26027-38-3	Ethoxylated 4- nonphenol	Y	N	STV=0.2 mg/kg/d
2809-21-4	Hydroxyethylidenediphosphonic acid	Y	N	STV=0.3 mg/kg/d
68439-70-3	Alkyl amine	Y	N	STV=0.4 mg/kg/d

CASRN	Chemical Name	Oil Field Additive?	Naturally Occurring?	Reason for Inclusion in Chemicals of Interest[1]
61790-41-8	Quaternary ammonium compound	Y	N	STV=0.4 mg/kg/d
No CASRN	Nonylphenol ethoxylates	Y	N	RA - STV=0.2 mg/kg/d
127087-87-0	Nonylphenol polyethylene glycol ether	Y	N	RA - STV=0.2 mg/kg/d
68412-54-4	Oxyalkylated alkylphenol	Y	N	RA - STV=0.2 mg/kg/d
13983-27-2	Krypton-85	Y	N	Radionuclide
7440-14-4	Radium-226	N	Y	Radionuclide
15262-20-1	Radium-228	N	Y	Radionuclide
14932-42-4	Xenon-133	Y	N	Radionuclide