CHEMICAL ALTERNATIVES ASSESSMENT: CLEANING SOLUTIONS FORMULATIONS

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Abstract

On behalf of a cleaning solutions formulator, the Toxics Use Reduction Institute (TURI) investigated the relative chemical hazards of five enzymatic detergent formulations, which included 21 individual chemicals. The analysis used two chemical hazard assessment tools: the Pollution Prevention Options Assessment System (P2OASys) developed by TURI and the GreenScreen™ for Safer Chemicals (GreenScreen) developed by Clean Production Action. Comprehensive P2OASys analyses, which consider 11 different hazard areas with 61 total hazard characteristics, and unverified GreenScreen analyses for each of the individual chemicals is provided. There is evidence of limited correlation between the P2OASys scores and the GreenScreen™ scores. Based on our investigation, TURI identified several ingredients that should be avoided within the basic elements of these formulations (i.e., the base detergent, the enzyme components and the stabilizer package). This research also indicates that while the primary component of the formulations – the base detergent – dominates the formulation's overall P2OASys derived hazard profile, the use of boron-containing stabilizers can increase the formulation's overall hazard profile. Significant data gaps were found for most of the chemical ingredients. Therefore, the formulator would benefit from conducting additional hazard testing to better guide their choice of safer formulation ingredients.

The Toxics Use Reduction Institute is a multi-disciplinary research, education, and policy center established by the Massachusetts Toxics Use Reduction Act of 1989. The Institute sponsors and conducts research, organizes education and training programs, and provides technical support to promote the reduction in the use of toxic chemicals or the generation of toxic chemical byproducts in industry and commerce. Further information can be obtained by writing the Toxics Use Reduction Institute, University of Massachusetts Lowell, 600 Suffolk Street, Wannalancit Mills, Suite 501, Lowell, MA 01854-2866

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Overview

A cleaning solutions formulator requested assistance from the Toxics Use Reduction Institute (TURI) to assess the chemicals in various detergent formulations using available assessment tools. The company is committed to reducing or eliminating their use of non-biodegradable chemicals in their detergent formulations, as well as identifying safer new detergent formulations. Ideally, these safer formulations will be comprised of the chemical ingredients that demonstrate the best results based on a careful application of robust, scientifically-based chemical hazard evaluation tools.

This Chemical Alternatives Assessment report addresses the chemical hazard profiles for the chemicals in the detergent formulations; however, the cleaning solutions formulator was unable to provide any related cost and performance information associated with the formulations at the time this report was published.

TURI analyzed chemical hazard information for the chemicals that comprise the following five detergent formulations:

- **Formulation 1:** No stabilizer included in this formulation.
- **Formulation 2:** Common stabilizer package with higher pH for industrial detergent applications – stabilizer contains sodium formate.
- **Formulation 3:** Common stabilizer package with lower pH for residential detergent applications – stabilizer contains boric acid and propylene glycol.
- **Formulation 4:** Newer stabilizer (4-FPBA) with significantly less boron than Formulation #3.
- **Formulation 5:** Peptide-based stabilizer chemistry with no boron included in this formulation.

Table 1 lists the twenty-two chemicals that are found in one or more of the five detergent formulations and are included in the scope of this chemical alternatives assessment:

Table 1. Chemicals Included in the Chemical Alternatives Assessment

Formulation Component	Chemical	CAS #
Stabilizers	Boric Acid	10043-35-3
	DSAA (disubstituted alaninamide)	*Confidential*
	4-FPBA (4 formylphenyl boronic acid)	87199-17-5
	Glycerol[1]	56-81-5
	Sodium formate	141-53-7
Enzyme Product Components	Alpha-amylase	9000-90-2
	Calcium chloride, anhydrous	10043-52-4
	Cellulase	9012-54-8
	Ethoxylated fatty alcohol, C_{11}-C_{15} (Softanol 90)	68131-40-8

[1] Based on the original formulation information provided by the cleaning solutions formulator in the "Enzyme Product Ingredients Matrix", glycerol is listed as a component of the Conventional Stabilization System B.

Formulation Component	Chemical	CAS #
	Lipase	9001-62-1
	Mannanase, endo-1,4-beta	37288-54-3
	Phenoxy ethanol	122-99-6
	Propylene glycol	57-55-6
	Protease (Subtilisin)	9014-01-1
	Proxel, containing: 10-20% 1,2-benzisothiazolin-3-one 5-10% Sodium hydroxide	 2634-33-5 1310-73-2
	Sorbitol (crystalline) – 70%	50-70-4
Base Detergent Components	Alcohols, C_{12}-$_{15}$, ethoxylated	68131-39-5
	Sodium laureth sulfate	9004-82-4
	Sodium citrate, anhydrous	68-04-2
	Calcium chloride, dihydrate	10035-04-8
	Water	7732-18-5

The five detergent formulations included minor variations in the base detergent composition consisting of:

- 58 – 63 wt% water
- 20.0 wt% ethoxylated alcohols C12-15, the primary nonionic surfactant
- 10.0 wt% sodium laureth sulfate, the primary anionic surfactant
- 5.0 wt% sodium citrate, a mild chelant and buffer
- 0.10 wt% calcium chloride dihydrate, a detergent stabilizer and buffer.

The enzymes used in the detergent formulations include a mixture of five enzyme types[2]. The enzyme ingredients were consistent for all detergent formulations with the exception of the protease enzyme systems, which varied dependent upon the stabilizers used.

The stabilization systems for the various formulations were:

- No stabilizer
- Conventional System A – 3.0 wt% sodium formate
- Conventional System B – 2.0 wt% boric acid + 3.0 wt% glycerol
- Optimized System C – 0.0085 wt% 4-formylphenyl boronic acid (4-FPBA)
- Optimized System D – 0.0007 wt% sodium disubstituted alaninamide sulfonate (DSAA)

Chemical Hazard Assessment Approach

TURI used the two chemical hazard assessment tools (i.e., the Pollution Prevention Options Analysis System – P2OASys and the GreenScreen™ for Safer Chemicals) for this assessment, to accomplish a

[2] As provided by the cleaning solutions formulator.

quicker screening level assessment and a more in-depth chemical hazard assessment of the various chemicals in the formulations.

P2OASys – Screening Level Assessment

The Pollution Prevention Options Analysis System (P2OASys) was developed by TURI as a tool to help companies assess the potential environmental, worker, and public health impacts of alternative technologies that could be implemented to reduce toxic chemical use. In this project, P2OASys is used as a screening tool for a rapid assessment of environmental, health, and safety hazards. The use of the tool requires the examination of limited data sources (i.e., safety data sheets and relevant technical bulletins and data sheets for each product used in the formulations) and can be completed in a relatively short period of time.

Embedded formulae in P2OASys generate a numerical hazard score for the current formulation and the identified options, which can then be combined with other information sources and professional judgment to make decisions on the implementation of preferred alternatives. The tool evaluates chemicals and/or processes in the following key hazard areas:

1. Acute human effects
2. Chronic human effects
3. Physical hazards
4. Aquatic hazards
5. Persistence/bioaccumulation
6. Atmospheric hazards
7. Disposal hazards
8. Other Chemical hazards
9. Energy and resource use
10. Product hazards
11. Exposure potential

Each hazard area includes one or more hazard characteristics[3] which can be evaluated. When the necessary data is not found using these sources, the user of the P2OASys tool either leaves it blank or applies professional judgment to determine the qualitative values (e.g. H, M, L) for those characteristics. The values for the characteristics for each chemical are then entered into an Excel spreadsheet, which computes a corresponding score. The hazard characteristic scores range from 2 to 10, with a score of 2 being the best or safest, and a score of 10 being the worst or least safe. The average of the two least safe hazard characteristics within each hazard area is then used to generate the hazard area score. The eleven hazard area scores are then averaged to generate an overall P2OASys score for the chemical.

GreenScreen™ – Chemical Hazard Assessment Level

The GreenScreen™ for Safer Chemicals is a comparative chemical hazard assessment method that builds on the U.S. Environmental Protection Agency's Design for Environment (now Safer Choice) approach and other national and international precedents, including the Globally Harmonized System of Classification

[3] Note that the P2OASys tool is undergoing modification and the newer revision will likely have slightly fewer hazard areas and hazard characteristics within each hazard area.

and Labelling of Chemicals (GHS). The GreenScreen™ for Safer Chemicals methodology, developed by Clean Production Action, provides a much greater level of effort, detail, and rigor than using the P2OASys screening tool. The GreenScreen™ tool uses all relevant and available data, has a different evaluation methodology from P2OASys, does not evaluate process changes, and typically requires more time to complete than P2OASys. Therefore, the final results obtained using the GreenScreen™ and P2OASys tools will most likely exhibit some differences.

GreenScreen™ Hazard Endpoints

In this tool, there are 20 human health, environmental toxicity, fate, and physical hazard endpoints that must be evaluated for each chemical, as shown in Table 2.

Table 2. Groupings of GreenScreen™ Hazard Endpoints

Hazard Grouping	Hazard Endpoint (Abbreviation)
Human Health Group I	Carcinogenicity (C) Mutagenicity and Genotoxicity (M) Reproductive Toxicity (R) Developmental Toxicity, including Neurodevelopmental Toxicity (D) Endocrine Activity (E)
Human Health Group II	Acute Toxicity (AT) Systemic Toxicity & Organ Effects (ST-single) Neurotoxicity (N-single) Skin Irritation (IrS) Eye Irritation (IrE)
Human Health Group II*	Systemic Toxicity & Organ Effects, Repeated Exposure sub-endpoint (ST-repeated) Neurotoxicity – Repeated Exposure sub-endpoint (N-repeated) Skin Sensitization (SnS) Respiratory Sensitization (SnR)
Environmental Toxicity & Fate	Acute Aquatic Toxicity (AA) Chronic Aquatic Toxicity (CA) Persistence (P) Bioaccumulation (B)
Physical Hazards	Reactivity (Rx) Flammability (F)

Group I Human Health

These endpoints reflect priorities that are consistent with national and international governmental regulations, and cover hazards that can lead to chronic or life threatening effects or adverse impacts that are potentially induced at low doses and transferred between generations.

Group II and II Human Health*

These endpoints reflect hazards that are also important for understanding and classifying chemicals. Typically, Group II hazards may be mitigated. Group II and II* are differentiated from one another in the Benchmarking system because Group II endpoints have four hazard levels (i.e., vH, H, M and L) and are evaluated on single exposure, while Group II* endpoints have only three hazard levels (i.e., H, M and L) and are evaluated based on repeated exposure.

Environmental Toxicity and Fate

Environmental Toxicity and Fate includes Acute and Chronic Aquatic Toxicity, Persistence and Bioaccumulation potential. Additional Ecotoxicity endpoints such as Avian or Bee Toxicity may be included when available and relevant. There are five hazard levels possible for environmental toxicity and fate (i.e., vH, H, M, L and vL).

Physical Hazards

Physical hazards include Flammability and Reactivity and are based on GHS criteria.

GreenScreen™ Process Steps

The GreenScreen™ assessments for this project were conducted in 8 steps:

Step 1 – Determine Chemicals to Assess

The cleaning solutions formulator provided a list of twenty-two chemicals to include in the GreenScreen chemical hazard assessment.

Step 2 – Research and Collect Data

Assessing chemicals is accomplished by examining comprehensive toxicological data, checking GreenScreen™ specified lists, and using estimated data from suitable analogs or modeled data where measured data are lacking for the parent chemical. For this study, we used data provided by the cleaning solutions formulator, data that is publicly available, and data provided by ToxServices[4] (and in one case by SciVera, LLC[5]) for evaluations that they had previously conducted for some of the chemicals in this study. The data sources used to conduct the GreenScreen™ assessment are provided in Appendix D: GreenScreen™ Data Sources.

Step 3 – Classify Hazard Level for each Hazard Endpoint (e.g., vH, H, M, L, vL)

TURI used the Hazard Criteria resource provided by the GreenScreen™ guidance to classify the hazard level as very High (vH), High (H), Moderate (M), Low (L) or in some cases very Low (vL) for each hazard endpoint. The following color scheme was used to indicate the hazard score assigned for each hazard endpoint:

Hazard Score	
Very High	vH
High	H
Moderate	M
Low	L
Very Low	vL
Data gap	DG

[4] ToxServices is a woman owned and operated small business focused on toxicological and risk assessment consultancy. Based in Washington D.C., ToxServices provides expert, professional services to industrial, commercial and public sector clients and is a Licensed GreenScreen™ Provider.

[5] SciVera, LLC develops and delivers web-based B2B software solutions and professional services to manufacturers, their trade customers (retailers) and suppliers. SciVera provides its SciVera Lens™ Chemical Safety Assessment Platform and SciVera Lens Secure Supplier Platform to clients to enable efficient, secure and reliable toxicological hazard and risk assessment of products and their chemical ingredients and is a Licensed GreenScreen™ Provider.

Step 4 – Determine Level of Confidence for Each Hazard Score Assigned

This step was not included in TURI's assessment. If we were to take the GreenScreen™ assessment to the point of being authorized by Clean Production Action, the level of confidence of the data used to assign hazard scores would be determined in accordance with GreenScreen™ guidance.

Step 5 – Assign a Data Gap to Each Hazard Endpoint with Insufficient Information

It is unusual to have complete data for all 18 hazard endpoints. Therefore, it is necessary to have a consistent approach to dealing with data gaps. For this assessment, a Data Gap (DG) classification was assigned to any hazard endpoint where there was insufficient information to assess the hazard using measured data on the parent chemical, measured data on a suitable analog, or estimated data on the parent chemical or suitable analog chemical.

Step 6a – Document Findings and Conclusions

It is essential to provide detailed documentation of the supporting data and rationale for all hazard classifications in an assessment report. The actual data values collected for each of the twenty-two chemicals are provided in Appendix C: GreenScreen™ Hazard Summary Tables, as part of each chemical's assessment.

Step 6b – Fill in the Hazard Summary Table

The designated hazard classification level for each hazard endpoint is filled into the respective box of the hazard summary table. The hazard summary tables are provided for each of the twenty-two chemicals in Appendix C: GreenScreen™ Hazard Summary Tables.

Step 7 – Determine the Relative Benchmark Score

Using criteria established by Clean Production Action, the relative Benchmark Score for each of the twenty-two chemicals is determined. The following are the four Benchmark Levels:

Benchmark 1: Chemical of High Concern - Avoid
Benchmark 2: Use but Search for Safer Substitutes
Benchmark 3: Use but Still Opportunity for Improvement
Benchmark 4: Prefer – Safer Chemical

The criteria used to determine the GreenScreen™ Benchmark Levels are provided in Figure 1.

Step 8 – Conduct a Data Gap Analysis to Assign a Final Benchmark Score

Data requirements become more stringent with higher Benchmark scores. With solid information on as few as a single endpoint, one may be able to confidently assess a chemical and assign a Benchmark score of 1. However, additional data are needed to assess a chemical and confidently assign it a higher Benchmark score (e.g., Benchmark 2, 3, or 4). The number and type of data gaps present must be considered when assigning a Benchmark score to a chemical. If a chemical does not achieve the minimum data requirements for the corresponding Benchmark level, then it is assigned a "U" for unspecified.

TURI used the GreenScreen™ Chemical Hazard Assessment Procedure V1.2 Final, developed by Clean Production Action as its primary guidance for the GreenScreen™ methodology. In addition, we have provided information on Benchmark scores prior to applying the data gap analysis as well as the final Benchmark score.

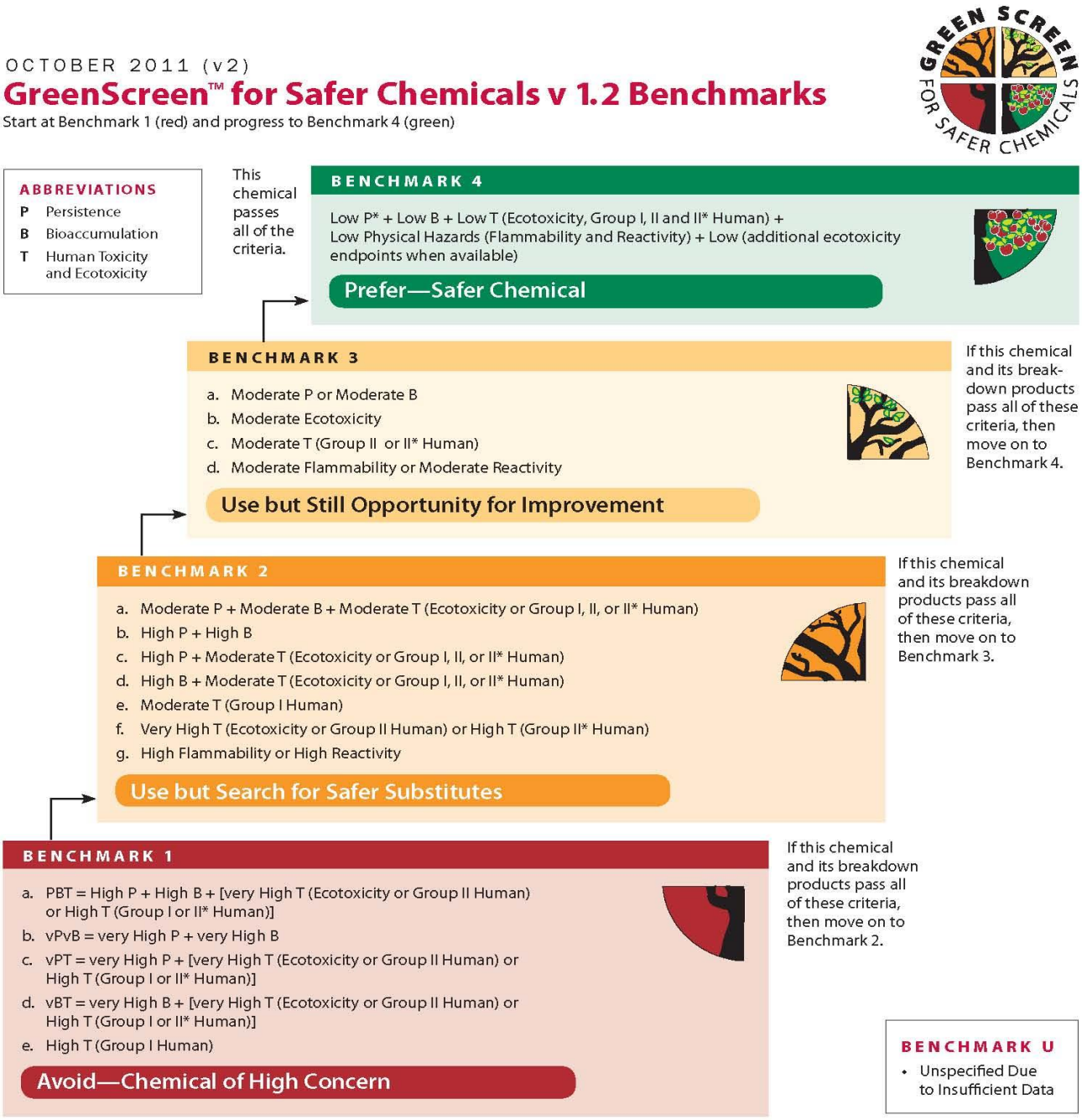


Figure 1: Criteria for GreenScreen™ Benchmark Levels

While the GreenScreen™ Chemical Hazard Assessment Procedure is transparent and freely available, all GreenScreen™ assessments are considered non-verified unless they have gone through the GreenScreen™ Verification Process. The GreenScreen™ Verification Program is performed by Licensed Profilers or by Authorized GreenScreen™ Practitioners and then verified by a Licensed Profiler. All GreenScreen™ results in this report are non-verified, as such these results may not be used to make public promotional or product claims.

Chemical Hazard Comparison Results

P2OASys Chemical Hazard Screening Results

The individual P2OASys hazard rating values for each of the twenty-two chemicals are provided in Appendix A. The populated cells with no color indicate data values that were obtained from MSDS or other data sources. The populated cells with a brown color indicate data values that were determined using professional judgment. The non-populated cells with no color indicate data gaps. Appendix B provides the professional judgment scoring methodology for the P2OASys tool.

Table 3 provides the aggregate P2OASys score generated for each of the twenty-two chemicals included in the Chemical Alternatives Assessment. The chemicals are sorted from most safe (lowest value) to least safe (highest value) based upon their P2OASys score within each of the three major component functions: stabilization, base detergent, and enzyme products.

Table 3. P2OASys Scores

Component Function	Chemical	P2OASys Score[6]
Stabilizers	DSAA (disubstituted alaninamide)	2.64
	Glycerol	3.18
	4-FPBA (4 formylphenyl boronic acid)	3.36
	Sodium formate	3.82
	Boric Acid	4.64
Base Detergent Components	Water	2.18
	Sodium citrate, anhydrous	3.36
	Calcium chloride, dihydrate	3.91
	Sodium laureth sulfate	4.27
	Alcohols, $C_{12\text{-}15}$, ethoxylated	4.55
Enzyme Product Components	Sorbitol (crystalline) – 70%	2.27
	Alpha-amylase	2.64
	Mannanase, endo-1,4-beta	2.64
	Lipase	2.73
	Cellulase	2.91
	Protease (Subtilisin)	3.09

[6] The results here are not meant to imply accuracy. Three significant figures have been included to help differentiate between substances with similar profiles.

Component Function	Chemical	P2OASys Score[6]
	Phenoxyethanol	3.27
	Propylene glycol	3.45
	Calcium chloride, anhydrous	3.82
	Ethoxylated fatty alcohol, C_{11}-C_{15}	4.00
	Proxel (includes 1,2-benzisothiazolin-3-one and sodium hydroxide)	4.91

Not surprisingly, water (2.18) and sorbitol (2.27) had the lowest P2OASys scores and are considered the safest of the chemicals included in the assessment. Boric acid (4.64) and Proxel (4.91) had the highest P2OASys scores and are therefore considered the least safe of the chemicals included in the assessment.

For the stabilizer components of the formulations, the safest stabilizer components were DSAA (2.64), glycerol (3.18), and 4-FPBA (3.36), while the less safe stabilizer components were sodium formate (3.82) and boric acid (4.64).

Green Screen™ Chemical Hazard Results

As shown in Appendix C, TURI utilized additional data sources to assess the various chemicals using the GreenScreen™ method as compared to the limited data sources relied on for the P2OASys. Specifically, REACH dossier data were used when the research received a reliability score of 1 (without restrictions[7]) or 2 (with restrictions[8]). TURI also found relevant data from authoritative sources, which are provided in Appendix D. Each of the twenty-two GreenScreen™ Hazard Summary Tables is provided in Appendix C: GreenScreen™ Hazard Summary Tables. GreenScreen™ Benchmark Level scores were checked using the GreenScreen™ Inspector functionality available at the ToxServices website at http://toxservices.com/. Appendix E provides a summary of the criteria used to make the hazard score determination.

Upon checking the data sources and completing the GreenScreen™ assessment, there were numerous data gaps for many endpoints for the twenty-two chemicals evaluated. Consequently, fifteen chemicals did not achieve the minimum data requirements for the corresponding Benchmark level, and were assigned a "U" for unspecified hazard. Since there were many chemicals with a "U" rating, this does not provide useful information for the cleaning solutions formulator to assess and prioritize the chemicals in their detergent formulations. For the purposes of this study, therefore, we have provided an anticipated Benchmark level by ignoring the data gaps and generating a Benchmark score based upon only the obtained data values. It is important to note that chemicals with a "U" benchmark are considered to be less reliable with respect to determining relative hazard as compared to chemicals with a numbered benchmark score.

Table 4 provides a list of the actual GreenScreen™ Benchmark scores as well as the GreenScreen™ Benchmark scores assigned when data gaps are ignored. The chemicals are sorted from safest

[7] Testing upon which the results are based have been conducted in compliance with applicable OECD guidance.

[8] Testing upon which the results are based is comparable to relevant OECD guidance with some acceptable restrictions.

(Benchmark 4) to least safe (Benchmark 1) for each of the three major component functions of the formulations: stabilizer system, base detergent, and enzyme products.

Table 4. GreenScreen™ Scores

Component Function	Chemical	GreenScreen™ Benchmark Score	GreenScreen™ Score Ignoring Data Gaps
Stabilizer System Components	DSAA	U	3
	Glycerol	3	3
	4-FPBA	U	2
	Sodium formate	2	2
	Boric Acid	1	1
Base Detergent Components	Water	U	4
	Sodium citrate, anhydrous	U	3
	Alcohols, C_{12}-$_{15}$, ethoxylated	U	2
	Calcium chloride, dihydrate	1	1
	Sodium laureth sulfate	U	2
Enzyme Product Components	Sorbitol	U	4
	Propylene glycol	3	3
	Phenoxyethanol	U	3
	Mannanase, endo-1,4-beta	U	3
	Cellulase	U	2
	Protease (Subtilisin)	U	2
	Alpha-amylase	U	2
	Calcium chloride, anhydrous	U	2
	Lipase	2	2
	Proxel (5-10% sodium hydroxide)	U	2
	Proxel (10-20% 1,2 benzisothiazolin-3-one)	U	2
	Ethoxylated fatty alcohol, C_{11}-C_{15}	2	2

Overall for all chemicals in the five formulations, water (benchmark 4), sorbitol (benchmark 4), phenoxy ethanol (benchmark 3), DSAA (benchmark 3), mannanase, endo-1,4-beta (benchmark 3), propylene glycol (benchmark 3) and sodium citrate (benchmark 3) had the best GreenScreen™ benchmarks and would therefore be considered the safest of the chemicals included in the assessment. Boric acid (benchmark 1) and calcium chloride dihydrate (benchmark 1) had the worst Green Screen™ benchmarks and would therefore be considered the least safe of the chemicals included in the assessment.

When considering only the stabilizer components of the formulations, the safest stabilizer components were DSAA (benchmark 3), glycerol (benchmark 3), sodium formate (benchmark 2), and 4-FPBA

(benchmark 2). However, if the data gaps are considered then 4-FPBA and DSAA would receive a benchmark score of U. Boric acid was the least safe stabilizer component with a benchmark 1.

P2OASys and GreenScreen™ Chemical Hazard Comparison

Table 5 provides a summary of the P2OASys score, and GreenScreen™ benchmark ignoring data gaps for all twenty-two chemicals contained in the five formulations. The results obtained using P2OASys and GreenScreen™ were not expected to be exactly equivalent. P2OASys was applied as a screening tool for a rapid assessment using limited data sources, whereas the GreenScreen™ was used for a deeper evaluation of each chemical. The two tools have different evaluation and scoring methodologies and, as described, utilize different data sources. Further, higher numerical scores for Green Screen evaluations indicate safer chemicals, while lower numerical scores for P2OASys evaluations indicate safer chemicals.

Table 5. Comparison of P2OASys and GreenScreen™ Chemical Hazard Scores

Component Function	Chemical	P2OASys Score[9]	GreenScreen™ Benchmark Score Ignoring Data Gaps[10]
Stabilizer System Components	DSAA	2.64	3
	Glycerol	3.18	3
	4-FPBA	3.36	2
	Sodium formate	3.82	2
	Boric Acid	4.64	1
Base Detergent Components	Water	2.18	4
	Sodium citrate, anhydrous	3.36	3
	Calcium chloride, dihydrate	3.91	1
	Sodium laureth sulfate	4.27	2
	Alcohols, $C_{12\text{-}15}$, ethoxylated	4.55	2
Enzyme Product Components	Sorbitol	2.27	4
	Alpha-amylase	2.64	2
	Mannanase, endo-1,4-beta	2.64	3
	Lipase	2.73	2
	Cellulase	2.91	2
	Protease (Subtilisin)	3.09	2
	Phenoxyethanol	3.27	3
	Propylene glycol	3.45	3
	Calcium chloride, anhydrous	3.82	2
	Ethoxylated fatty alcohol, C_{11}-C_{15}	4.00	2
	Proxel	4.91	2

[9] The hazard characteristic scores range from 2 to 10, with a score of 2 being the best or safest, and a score of 10 being the worst or least safe.

[10] Benchmark scores range from 1 (avoid) to 4 (safe to use).

There is evidence of limited correlation between the P2OASys scores and the GreenScreen™ scores. For all of the eleven chemicals that received a P2OASys score from 2.5 through 3.5, the corresponding GreenScreen™ Benchmark was either Benchmark 2 or 3. For all of the eight chemicals that received an overall P2OASys score above 3.5, the corresponding score was either a GreenScreen™ Benchmark 1 (three chemicals) or Benchmark 2 (five chemicals). Further, water and sorbitol received the best scores for both P2OASys (2.18 and 2.27 respectively) and GreenScreen™ (Benchmark 4 for both).

A more detailed discussion of the results from the two tools used is provided in the following sections.

P2OASys Results for Enzyme and Stabilizer Systems

One advantage of using the P2OASys tool is that it allows for an assessment of an overall formulation as well as for each individual chemical component of each formulation. Using P2OASys, TURI developed the scores for the five formulations. The P2OASys results for the five overall detergent formulations are provided in Appendix A.

Since the base detergent ingredients represent the dominant component of each overall formulation, it is difficult to differentiate between the P2OASys scores for the five full formulations. To better understand the difference made by using alternative stabilizers in the formulations, P2OASys scores were derived for the five formulations with only the stabilizer and enzyme components included[11].

Tables 11 through 15 provide information for the calculation of the P2OASys scores for the stabilizer and enzyme components for the five different detergent formulations identified above.

Table 11. P2OASys Score for the Stabilizer and Enzyme Components of Formulation #1

Formulation #1 Enzyme & Stabilizer Chemicals	% Weight	P2OASys Score	Weighted Score
Alpha-amylase*	2.8	2.64	0.073
Cellulase*	2.2	2.91	0.063
Glycerol	47.8	3.18	1.5
Lipase*	1.1	2.73	0.029
Mannanase, endo-1,4-beta *	0.3	2.64	0.008
Phenoxyethanol	0.9	3.27	0.030
Propylene Glycol	14.4	3.45	0.50
Protease (Subtilisin)*	1.2	3.09	0.038
Proxel	0.1	4.91	0.006
Sodium Formate	0.9	3.82	0.035
Sorbitol	28.3	2.27	0.64
Total	**100**		**2.9**

**Defined as enzyme concentrate, dry matter basis.*

[11] Note that as weighted averages, the overall scores are still dominated by the substances with the largest weight percentage in the formulation.

Table 12. P2OASys Score for the Stabilizer and Enzyme Components of Formulation #2

Formulation #2 Enzyme & Stabilizer Chemicals	% Weight	P2OASys Score	Weighted Score
Sodium formate	65.15	3.82	2.5
Alpha-amylase*	0.97	2.64	0.026
Cellulase*	0.76	2.91	0.022
Glycerol	16.81	3.18	0.54
Lipase*	0.38	2.73	0.010
Mannanase, endo-1,4-beta *	0.11	2.64	0.003
Phenoxyethanol	0.32	3.27	0.011
Propylene Glycol	5.08	3.45	0.18
Protease (Subtilisin)*	0.43	3.09	0.013
Proxel	0.04	4.91	0.002
Sorbitol	9.94	2.27	0.23
Total	**100**		**3.5**

**Defined as enzyme concentrate, dry matter basis.*

Table 13. P2OASys Score for the Stabilizer and Enzyme Components of Formulation #3

Formulation #3 Enzyme & Stabilizer Chemicals	% Weight	P2OASys Score	Weighted Score
Boric Acid	30.18	4.64	1.4
Glycerol	57.01	3.18	1.8
Alpha-amylase*	0.68	2.64	0.018
Cellulase*	0.53	2.91	0.015
Lipase*	0.26	2.73	0.007
Mannanase, endo-1,4-beta *	0.08	2.64	0.002
Phenoxyethanol	0.23	3.27	0.007
Propylene Glycol	3.55	3.45	0.12
Protease (Subtilisin)*	0.30	3.09	0.009
Proxel	0.03	4.91	0.001
Sodium Formate	0.23	3.82	0.009
Sorbitol	6.94	2.27	0.16
Total	**100.0**		**3.6**

**Defined as enzyme concentrate, dry matter basis.*

Table 14. P2OASys Score for the Stabilizer and Enzyme Components of Formulation #4

Formulation #4 Enzyme & Stabilizer Chemicals	% Weight	P2OASys Score	Weighted Score
4-FPBA - 4-formylphenyl boronic acid	0.54	3.36	0.018
Alpha-amylase*	2.84	2.64	0.075

Formulation #4 Enzyme & Stabilizer Chemicals	% Weight	P2OASys Score	Weighted Score
Calcium Chloride, anhydrous	0.06	3.82	0.002
Cellulase*	2.21	2.91	0.064
Ethoxylated fatty alcohol, C_{11}-C_{15}	0.06	4.00	0.003
Glycerol	49.10	3.18	1.6
Lipase*	1.10	2.73	0.030
Mannanase, endo-1,4-beta *	0.32	2.64	0.008
Phenoxyethanol	0.09	3.27	0.003
Propylene Glycol	13.25	3.45	0.46
Protease (Subtilisin)*	1.26	3.09	0.039
Proxel	0.13	4.91	0.006
Sorbitol	29.03	2.27	0.66
Total	**100**		**2.9**

**Defined as enzyme concentrate, dry matter basis.*

Table 15. P2OASys Score for the Stabilizer and Enzyme Components of Formulation #5

Formulation #5 Enzyme & Stabilizer Chemicals	% Weight	P2OASys Score	Weighted Score
DSAA	0.04	2.64	0.001
Alpha-amylase*	2.78	2.64	0.073
Calcium Chloride, anhydrous	0.06	3.82	0.002
Cellulase*	2.16	2.91	0.063
Glycerol	47.12	3.18	1.5
Lipase*	1.08	2.73	0.030
Mannanase, endo-1,4-beta *	0.31	2.64	0.008
Phenoxyethanol	0.93	3.27	0.030
Propylene Glycol	14.82	3.45	0.51
Protease (Subtilisin)*	1.24	3.09	0.038
Proxel	0.12	4.91	0.006
Sodium Formate	0.93	3.82	0.035
Sorbitol	28.41	2.27	0.65
Total	**100**		**2.9**

**Defined as enzyme concentrate, dry matter basis.*

Table 16 provides the weighted P2OASys score for the stabilizer and enzyme components and the percentage of stabilizer/enzyme components for each of the five formulations.

Table 16. Stabilizer and Enzyme Component Scores and Percent Composition

Formulation	Enzyme Stabilizer System	Enzyme and Stabilizer Weighted P2OASys score	Percentage in Detergent	Enzyme and Stabilizer Contribution to Weighted P2OASys Score for the Formulation
1	No stabilizer	2.9	1.67%	0.049
2	Sodium formate stabilizer	3.5	4.6%	0.16
3	Boric acid and glycerol stabilizer	3.6	6.6%	0.23
4	4-FPBA stabilizer	2.9	1.67%	0.049
5	DSAA stabilizer	2.9	1.67%	0.049

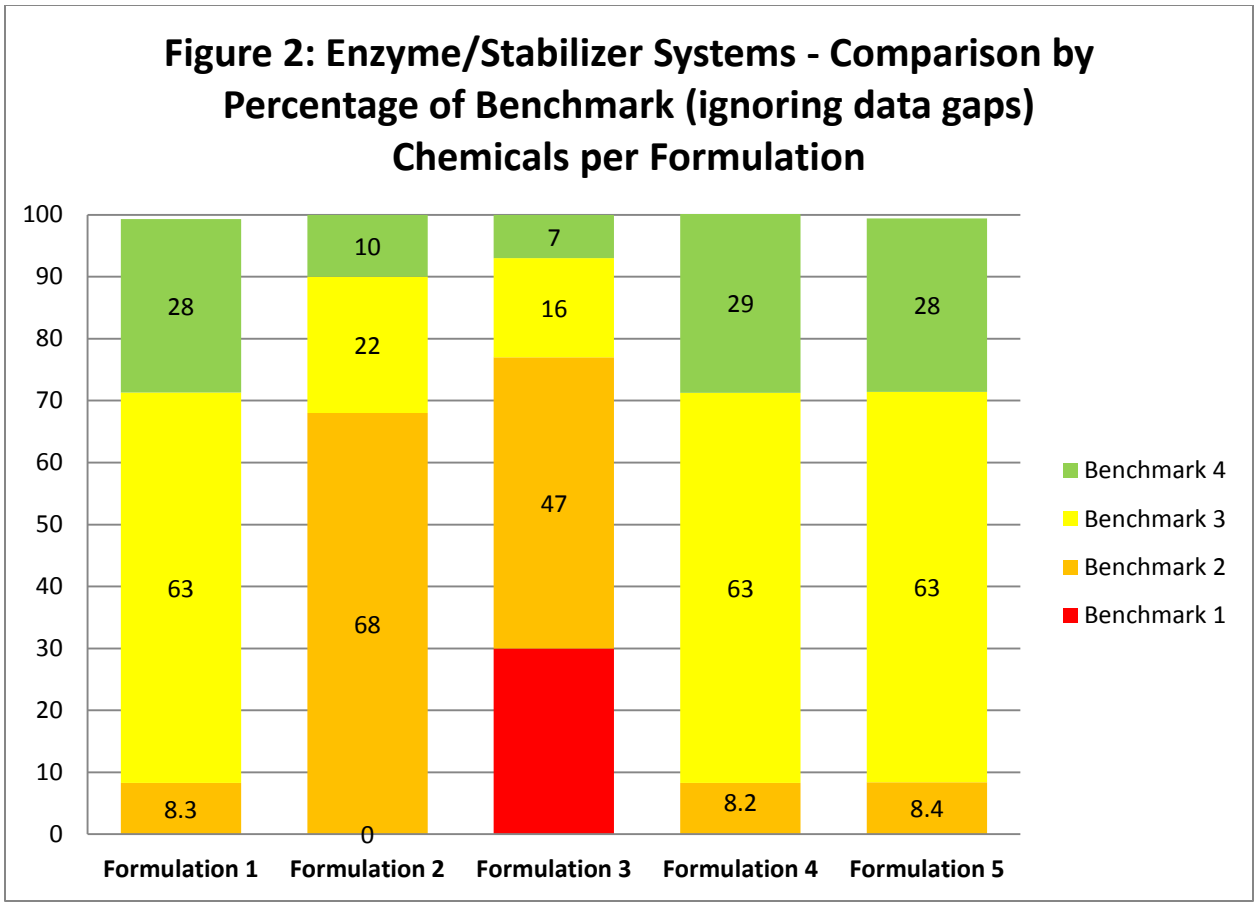
GreenScreen Analysis of Enzymes and Stabilizers

Unlike with P2OASys, the GreenScreen™ is not designed to evaluate overall formulations, but rather focuses on assessing the hazards associated with individual chemicals. As discussed above, detergent components dominate the overall formulation hazard profile. Therefore, as with the P2OASys analysis, the impact of the individual enzyme and stabilizer components provides the most insight into the impact of modifying the stabilizer system on the overall formulation.

Figure 2 illustrates the breakdown (by weight percentage) of chemicals by GreenScreen™ benchmark (ignoring data gaps) for the enzyme and stabilizer systems of each of the five formulations.

As illustrated in Figure 2, the use of boric acid in the stabilizer package for Formulation 3 creates a significantly less desirable formulation from a chemical hazard perspective. The difference between Formulations 1, 4 and 5, on the other hand, is relatively insignificant when focusing on the GreenScreen™ benchmarks that ignore data gaps. Based on the GreenScreen™ analysis, the preferred stabilizer package is the DSAA formulation, which does not contain any benchmark 1[12] chemicals, and has an overall hazard profile similar to the formulation that uses no stabilizer. In addition, it appears that, with the limited data available, the benchmark for DSAA is likely a preferable alternative to 4-FPBA.

[12] This relates only to the benchmark scores that ignore data gaps. This assessment could change if data gaps were able to be adequately addressed.



Performance and Cost Evaluation

Chemical alternatives assessments include an assessment of the technical performance and cost considerations for the chemicals under evaluation. The technical performance and cost information necessary for this evaluation, which was to be developed by the cleaning solutions formulator, was not available at the time this report was finalized. Therefore, this chemical alternatives assessment, including the conclusions and recommendations, is only based upon the chemical hazard evaluation. However, we can assume that the company did an initial assessment of both the performance and cost implications of the various formulas, and found them to be acceptable enough to warrant further consideration.

Conclusions and Recommendations

TURI evaluated the various detergent formulations using two chemical hazard comparison tools – P2OASys and GreenScreen™. These tools were helpful in determining if the optimized stabilization systems are safer than the conventional stabilization systems.

The P2OASys tool relies on information available from material safety data sheets (MSDS) and product technical data sheets along with professional judgment for the 61 hazard characteristics addressed. This

tool is used by the TURI Cleaning Laboratory to evaluate various cleaning products and processes and their alternatives. It is worth noting that the P2OASys methodology is typically conducted at the formulation level, and the final aggregated score is heavily dependent upon the weight percentage of each of the individual chemicals in the formulation. With this in mind, it is helpful to consider the stabilizer/enzyme component of the overall formulation separately. Based on the P2OASys analysis of the various stabilizer/enzyme packages, the two optimized stabilizer systems (associated with Formulations #4 and #5) did, in fact, result in an overall stabilizer/enzyme score that was approximately equivalent to that of Formulation #1 which uses no stabilizer (e.g., an aggregate weighted P2OASys score of 2.9). In contrast, the aggregated stabilizer/enzyme weighted scores for the conventional stabilizer systems were higher (less favorable) – with scores of 3.5 (Formulation #2) and 3.6 (Formulation #3).

The GreenScreen™ tool and methodology is fundamentally different than the weighted average approach of the P2OASys tool. Specifically, a high hazard score for a critical (e.g., Group 1 Human Health) endpoint always results in the least favorable (Benchmark 1) overall score. In order to generate reproducible results, it also requires a more thorough review of the individual components of the various formulations. This process facilitates a comprehensive data gathering effort to better understand the relevant hazards associated with the chemicals used in the various formulations. The GreenScreen™ analyses include data from authoritative scientific and government sources (see Appendix D), as well as from company dossiers (as part of the European Union REACH registration process) and MSDSs. The results of this analysis (presented in detail in Appendix C) demonstrate that one of the primary components of the conventional stabilization systems (boric acid) is categorized as a Benchmark 1 chemical, and should therefore be avoided[13]. These components receiving a Benchmark 1 should be the focus of substitution efforts to identify safer ingredients.

It is important to note, however, that the presence of significant data gaps for both the DSAA and 4-FPBA stabilizers limits the reliability of these conclusions. The cleaning solutions formulator would therefore benefit from conducting additional toxicology testing to better characterize both 4-FPBA and DSAA. Specifically, testing for carcinogenicity and reproductive and developmental toxicity are priority needs. Additional testing for Group II Human health hazards, particularly systemic toxicity, neurotoxicity and respiratory sensitization, should also be conducted.

Based on our analysis of the various chemicals and formulations used by the cleaning solutions formulator, the following recommended actions should be considered as part of an overall strategy for creating safer detergent formulations:

- Avoid using stabilizer systems that contain boric acid.
- Consider conducting additional testing to fill data gaps, particularly associated with chemicals for which a Benchmark U was assigned. Working with complete Benchmarks will allow the cleaning solutions formulator to make more informed decisions on potential reformulations.

[13] In addition, the base detergent ingredient calcium chloride dihydrate was identified as a Benchmark 1 chemical. Components receiving a Benchmark 1 should be the focus of substitution efforts to identify safer ingredients.

- Investigate the feasibility of using safer enzyme product ingredients. Specifically, try to move away from the use of Proxel (highest P2OASys score) by identifying well characterized alternatives that provide the needed functionality.
- Calcium chloride dihydrate is identified as a Benchmark 1 chemical. This is largely because of limited data indicating high hazard associated with mutagenic impacts. Conducting additional mutagenicity testing on this chemical could provide better evidence of an effect.
- Obtain performance and cost data so that a full chemical alternatives assessment can be conducted for the chemicals contained in the five detergent formulations.

Appendix A: P2OASys Hazard Screening Ratings

The populated cells with no color indicate data values that were obtained from material safety data sheets or relevant technical data sheets. The populated cells with a brown color denote values that were determined using professional judgment. The non-populated cells with no color indicate data gaps on the MSDS. A score of "NA" indicates that the hazard characteristic is not applicable for the particular chemical.

Table A1: P2OASys Scoring for Water, Alcohols C12 - 15 ethyoxylated, Sodium laureth sulfate, Sodium citrate anhydrous, and Calcium chloride dihydrate

Endpoint	Unit	Water	Alcohols, C12 - 15, ethoxylated	Sodium Laureth Sulfate	Sodium citrate, anhydrous	Calcium chloride, dihydrate
		7732-18-5	68131-39-5	9004-82-4	68-04-2	10035-04-8
Acute human effects						
Inhalation LC_{50}	ppm					
PEL/TLV	ppm					
PEL/TLV (dusts/particles)	mg/m3					
IDLH	ppm					
Respiratory irritation	L/M/H	L	L/M	M	L/M	M
Oral LD_{50}	mg/kg		500	>5000		
Dermal irritation	L/M/H	L	M	M	L/M	M
Skin absorption	L/M/H	L	M	M	L	L/M
Dermal LD_{50}	mg/kg					
Eye irritation	L/M/H	L	M/H	L/M	L/M	M/H
Chronic human effects						
Reference Dose RfD	mg/kg/day					
Carcinogen	IARC/EPA Class	L	L	L	L	L
Mutagen	L/M/H	L	L	L	L	L/M
Reproductive effects	L/M/H	L	L	L/M	L	L
Neurotoxicity	L/M/H	L	L	L	L	L
Developmental effects	L/M/H	L	L	L	L	L
Respir sensitivity/disease	L/M/H	L	L	M	L	L
Other chronic organ effects	L/M/H	L	L	L	L	M
Physical hazards						
Heat	WBGT, °C					
Noise generation	dBA					
Vibration	m/S^2					
Ergonomic hazard	L/M/H	L	M	L/M	M	M
Psychosocial hazard	L/M/H	L	M	L/M	L	L/M
Aquatic hazards						
Water Quality Criteria (HWQC)	mg/l					
Aquatic LC_{50}	mg/l		0.4			
Fish NOAEC	mg/l					
Plant EC_{50}	mg/l					

Endpoint	Unit	Water	Alcohols, C12 - 15, ethoxylated	Sodium Laureth Sulfate	Sodium citrate, anhydrous	Calcium chloride, dihydrate
		7732-18-5	68131-39-5	9004-82-4	68-04-2	10035-04-8
Observed ecological effects	L/M/H	L	M	L/M	L/M	L
Persistence/bioaccumulation						
Persistence	L/M/H	L	L	L	L	
BOD half-life	days					
Hydrolysis half-life	days					
Bioconcentration	log kow					
Bioconcentration factor (BCF)	kg/l					
Atmospheric hazard						
Greenhouse gas	Y/N	N	N	N	N	N
Ozone depletor	ODP units	N	N	N	N	N
Acid rain formation	Y/N	N	N	N	N	N
NESHAP	Y/N	N	N	N	N	N
Disposal hazard						
Landfill	L/M/H	L	M	L/M	L	L
EPCRA reportable quantity	lbs	no value	no value			no value
Incineration	L/M/H	L	M	L/M	L	L
Recycling	L/M/H	L	M	M	M	M
Chemical hazard						
Vapor pressure	mm Hg					0.01
Solubility in water	mg/L					
Specific gravity	no units					
Flammability	0,1,2,3,4	0	1		1	0
Flash point	°C	>100	> 93.9	25		
Reactivity	0,1,2,3,4	0	0		0	0
pH	pH units	7	6.75	8.11	8	6.5
Corrosivity	L/M/H	L	L	L	L/M	L
High pressure system	L/M/H	L	L	L	L	L
High temperature system	L/M/H	L	L	L	L	L
Mixture/reaction potential	L/M/H	L	L/M	L	L	L
Odor threshold	L/M/H	L	L/M	L	L	L
Volatile organic compound	L/M/H	L	L	M	L	L
Energy & resource use						
Non renewable resource	L/M/H	L	L/M	L/M	L/M	L/M
Water use	L/M/H	L/M	M	M	M	M
Energy use	L/M/H	L/M	L	L	L	L
Product hazard						
Upstream effects	L/M/H	L	L/M	L/M	L	L
Consumer hazard	L/M/H	L	L	L/M	L	L
Disposal hazard	L/M/H	L	M	L	L	L
Exposure potential						
Exposure potential	L/M/H	L	L/M	L/M	L/M	L/M

Table A2: P2OASys Scoring for Calcium Chloride, anhydrous, Sodium Formate, Boric Acid, Glycerol, and Propylene Glycol

Endpoint	Unit	Calcium Chloride, anhydrous	Sodium Formate	Boric Acid	Glycerol	Propylene Glycol
		10043-52-4	141-53-7	10043-35-3	56-81-5	57-55-6
Acute human effects						
Inhalation LC_{50}	ppm					
PEL/TLV	ppm					
PEL/TLV (dusts/particles)	mg/m3			2	10	10
IDLH	ppm					
Respiratory irritation	L/M/H		L/M	L/M	L/M	L/M
Oral LD_{50}	mg/kg	2,301	11,200	2,660	12,600	> 20,000
Dermal irritation	L/M/H	L	L/M	L/M	L/M	L/M
Skin absorption	L/M/H	M	L/M	M		L
Dermal LD_{50}	mg/kg				10000	> 2,000
Eye irritation	L/M/H	H	L/M	L/M	L/M	L/M
Chronic human effects						
Reference Dose RfD	mg/kg/day					
Carcinogen	IARC/EPA Class	L	L	L	L	L
Mutagen	L/M/H	L/M	L	M	L	L
Reproductive effects	L/M/H	L	L	M	L	L
Neurotoxicity	L/M/H	L	L	L	L	L
Developmental effects	L/M/H	L	L	M	L	L
Respir sensitivity/disease	L/M/H	L	L		L	L
Other chronic organ effects	L/M/H	M	M	M	L/M	L/M
Physical hazards						
Heat	WBGT, °C					
Noise generation	dBA					
Vibration	m/S^2					
Ergonomic hazard	L/M/H	M	M	M	M	L/M
Psychosocial hazard	L/M/H	L/M	L	M	L	L
Aquatic hazards						
Water Quality Criteria (HWQC)	mg/l					
Aquatic LC_{50}	mg/l	10,650	954	279	55	40,613
Fish NOAEC	mg/l					
Plant EC_{50}	mg/l		790			19,000
Observed ecological effects	L/M/H	L/M		L/M	L	L
Persistence/bioaccumulation						
Persistence	L/M/H	L	M	L	L/M	L
BOD half-life	days					28
Hydrolysis half-life	days					
Bioconcentration	log kow					<3
Bioconcentration factor (BCF)	kg/l					0.09

Endpoint	Unit	Calcium Chloride, anhydrous	Sodium Formate	Boric Acid	Glycerol	Propylene Glycol
		10043-52-4	141-53-7	10043-35-3	56-81-5	57-55-6
Atmospheric hazard						
Greenhouse gas	Y/N	N	N	N	N	N
Ozone depletor	ODP units	N	N	N	N	N
Acid rain formation	Y/N	N	N	N	N	N
NESHAP	Y/N	N	N	N	N	N
Disposal hazard						
Landfill	L/M/H	L	L	L/M	L/M	L/M
EPCRA reportable quantity	lbs		no value			
Incineration	L/M/H	L	L	L	L	L/M
Recycling	L/M/H	L/M	L/M	L/M	L/M	L/M
Chemical hazard						
Vapor pressure	mm Hg	0.01		2.6	0	0.15
Solubility in water	mg/L					
Specific gravity	no units					
Flammability	0,1,2,3,4	0	1	0	1	1
Flash point	°C				160	104
Reactivity	0,1,2,3,4	0	0	0	0	0
pH	pH units		7.7	5.1		
Corrosivity	L/M/H	L	L	L/M	L	L
High pressure system	L/M/H	L	L	L	L	L
High temperature system	L/M/H	L	L	L	L	L
Mixture/reaction potential	L/M/H	L	L	M	L/M	L
Odor threshold	L/M/H	L	L/M	L	L/M	
Volatile organic compound	L/M/H	L	L	L	L	L/M
Energy & resource use						
Non renewable resource	L/M/H	L/M	L/M	L/M	L	L/M
Water use	L/M/H	M	M	M	L/M	L
Energy use	L/M/H	L	L	L	L	L
Product hazard						
Upstream effects	L/M/H	L	L	M	L	L
Consumer hazard	L/M/H	L/M	L/M	M	L	L
Disposal hazard	L/M/H	L	L	M	L	L/M
Exposure potential						
Exposure potential	L/M/H	L/M	L/M	L/M	L	L/M

Table A3: P2OASys Scoring for Protease, Ethoxylated fatty alcohol C11 – C15, Sorbitol, Alpha-Amylase, Phenoxy ethanol, and Mannanase, endo-1,4-beta

Endpoint	Unit	Protease (Subtilisin)	Ethoxylated fatty alcohol, C11 - C15 (Softanol 90)	Sorbitol	Alpha-amylase	Phenoxy ethanol	Mann-anase, endo-1,4-beta
		9014-01-1	68131-40-8	50-70-4	9000-90-2	122-99-6	37288-54-3
Acute human effects							
Inhalation LC_{50}	ppm						
PEL/TLV	ppm						
PEL/TLV (dusts/particles)	mg/m3	0.00006					
IDLH	ppm						
Respiratory irritation	L/M/H	L/M	L/M	L	L/M	L/M	L/M
Oral LD_{50}	mg/kg	2,000	1,800	17,800		1,840	
Dermal irritation	L/M/H	M		L	L/M	L	L/M
Skin absorption	L/M/H	L/M	M	L	L/M	L/M	L/M
Dermal LD_{50}	mg/kg			7,100		14,391	
Eye irritation	L/M/H	M/H	M/H	L	L/M	M	L/M
Chronic human effects							
Reference Dose RfD	mg/kg/day						
Carcinogen	IARC/EPA Class	L	L	L	L	L	L
Mutagen	L/M/H	L	L	L	L	L	L
Reproductive effects	L/M/H	L	L	L	L	L	L
Neurotoxicity	L/M/H	L	L	L	L	L	L
Developmental effects	L/M/H	L	L	L	L	L	L
Respir sensitivity/disease	L/M/H	M	L	L	L/M	L/M	L
Other chronic organ effects	L/M/H	L	L	L	L	L/M	L/M
Physical hazards							
Heat	WBGT, °C						
Noise generation	dBA						
Vibration	m/S^2						
Ergonomic hazard	L/M/H	M	M	L/M	M	M	M
Psychosocial hazard	L/M/H	L	L/M	L	L/M	L/M	L
Aquatic hazards							
Water Quality Criteria (HWQC)	mg/l						
Aquatic LC_{50}	mg/l	>100	0.1			345	
Fish NOAEC	mg/l						
Plant EC_{50}	mg/l					> 500	
Observed ecological effects	L/M/H		M	L	L	L	L
Persistence/ bioaccumulation							
Persistence	L/M/H	L		L	L	L	L
BOD half-life	days		28			10	
Hydrolysis half-life	days						

Endpoint	Unit	Protease (Subtilisin)	Ethoxylated fatty alcohol, C11 - C15 (Softanol 90)	Sorbitol	Alpha-amylase	Phenoxy ethanol	Mann-anase, endo-1,4-beta
		9014-01-1	68131-40-8	50-70-4	9000-90-2	122-99-6	37288-54-3
Bioconcentration	log kow						
Bioconcentration factor (BCF)	kg/l					<100	
Atmospheric hazard							
Greenhouse gas	Y/N	N	N	N	N	N	N
Ozone depletor	ODP units	N	N	N	N	N	N
Acid rain formation	Y/N	N	N	N	N	N	N
NESHAP	Y/N	N	N	N	N	N	N
Disposal hazard							
Landfill	L/M/H	L	L/M	L	L	L	L
EPCRA reportable quantity	lbs						
Incineration	L/M/H	L	L/M	L	L	L	L
Recycling	L/M/H	L/M	L/M	L	L	L	L
Chemical hazard							
Vapor pressure	mm Hg		0.01			0.0043	
Solubility in water	mg/L						
Specific gravity	no units						
Flammability	0,1,2,3,4	0	0	0	0	0	1
Flash point	°C		193			119	
Reactivity	0,1,2,3,4	0	0	0	0	0	0
pH	pH units		6.5				
Corrosivity	L/M/H	L	L	L	L	L	L
High pressure system	L/M/H	L	L	L	L	L	L
High temperature system	L/M/H	L	L	L	L	L	L
Mixture/reaction potential	L/M/H	L	L	L	L	L	L
Odor threshold	L/M/H	L	L/M	L/M	L	L	L
Volatile organic compound	L/M/H	L	L/M	L	L	L	L
Energy & resource use							
Non renewable resource	L/M/H	L	L/M	L	L	L	L
Water use	L/M/H	L	L	L/M	L/M	L/M	L/M
Energy use	L/M/H	L	L	L	L	L	L
Product hazard							
Upstream effects	L/M/H	L	L	L	L	L	L
Consumer hazard	L/M/H	L	L	L	L	L	L
Disposal hazard	L/M/H	L	L	L	L	L	L
Exposure potential							
Exposure potential	L/M/H	L	L	L	L	L	L

Table A4: P2OASys Scoring for Proxel, Lipase, Cellulose, DSAA, and 4-FPBA

Endpoint	Unit	Proxel	Lipase	Cellulase	DSAA - DiSubstituted Alaninamide	4-FPBA - 4-formylphenyl boronic acid *(MSDS supplied by* the cleaning solutions company*)*
		2634-33-5	9001-62-1	9012-54-8	*confidential*	87199-17-5
Acute human effects						
Inhalation LC_{50}	ppm					
PEL/TLV	ppm					
PEL/TLV (dusts/particles)	mg/m3	2				
IDLH	ppm					
Respiratory irritation	L/M/H	L/M	L/M	M		L/M
Oral LD_{50}	mg/kg				> 2,000	> 2,000
Dermal irritation	L/M/H	L/M	L/M	M	L	L
Skin absorption	L/M/H	L/M	L/M	L/M		L/M
Dermal LD_{50}	mg/kg					> 2,000
Eye irritation	L/M/H	M/H	L/M	M	L	L
Chronic human effects						
Reference Dose RfD	mg/kg/day					
Carcinogen	IARC/EPA Class	L	L	L		
Mutagen	L/M/H	L	L	L	L	L
Reproductive effects	L/M/H	L	L	L		L
Neurotoxicity	L/M/H	L	L	L		L
Developmental effects	L/M/H	L	L	L		L
Respir. sensitivity/disease	L/M/H	L/M	L/M	L/M	L	L
Other chronic organ effects	L/M/H	L/M	L/M	L	M	M/H
Physical hazards						
Heat	WBGT, °C					
Noise generation	dBA					
Vibration	m/S^2					
Ergonomic hazard	L/M/H	M	M	M	L	M
Psychosocial hazard	L/M/H	M/H	L/M	L/M	L	L
Aquatic hazards						
Water Quality Criteria (HWQC)	mg/l					
Aquatic LC_{50}	mg/l	5			>88.4	64
Fish NOAEC	mg/l					64
Plant EC_{50}	mg/l	0.6			>101	>10.7
Observed ecological effects	L/M/H	H	L	L	L	L
Persistence/ bioaccumulation						
Persistence	L/M/H	L	L	L	L	L
BOD half-life	days					
Hydrolysis half-life	days					
Bioconcentration	log kow				1.8	1.36
Bioconcentration factor (BCF)	kg/l					

Endpoint	Unit	Proxel	Lipase	Cellulase	DSAA - DiSubstituted Alaninamide	4-FPBA - 4-formylphenyl boronic acid *(MSDS supplied by* the cleaning solutions company*)*
		2634-33-5	9001-62-1	9012-54-8	*confidential*	87199-17-5
Atmospheric hazard						
Greenhouse gas	Y/N	N	N	N	N	N
Ozone depletor	ODP units	N	N	N	N	N
Acid rain formation	Y/N	N	N	N	N	N
NESHAP	Y/N	N	N	N	N	N
Disposal hazard						
Landfill	L/M/H	L	L	L	L	L
EPCRA reportable quantity	lbs					
Incineration	L/M/H	L	L	L	L	L
Recycling	L/M/H	L	L	L	M	L/M
Chemical hazard						
Vapor pressure	mm Hg					2.48E-07
Solubility in water	mg/L				1,400	810
Specific gravity	no units				1.17	1.4021 at 20 °C
Flammability	0,1,2,3,4	0	0	1	1	1
Flash point	°C	>100				207
Reactivity	0,1,2,3,4	0	0	0	0	
pH	pH units	10				
Corrosivity	L/M/H	H	L	L	L	H
High pressure system	L/M/H	L	L	L	L	L
High temperature system	L/M/H	L	L	L	L	L
Mixture/reaction potential	L/M/H	L	L	L	L	L
Odor threshold	L/M/H	L	L	L		L
Volatile organic compound	L/M/H	L	L	L	L	L
Energy & resource use						
Non renewable resource	L/M/H	L	L	L	L	L
Water use	L/M/H	L/M	L/M	L/M	L	L
Energy use	L/M/H	L	L	L	L/M	L
Product hazard						
Upstream effects	L/M/H	L	L	L	L	L
Consumer hazard	L/M/H	L/M	L	L	L	L
Disposal hazard	L/M/H	L	L	L	L	L
Exposure potential						
Exposure potential	L/M/H	M	L	L	L	L

P2OASys Results for Overall Formulations

Using P2OASys, TURI derived the scores for the overall formulations:

- **Formulation 1:** No stabilizer included in this formulation.
- **Formulation 2:** Conventional Stabilization System A, with higher pH for industrial detergent applications – stabilizer contains sodium formate.
- **Formulation 3:** Conventional Stabilization System B, with lower pH for residential detergent applications – stabilizer contains boric acid and propylene glycol.
- **Formulation 4:** Optimized Stabilization System C, using 4-FPBA, with significantly less boron than Conventional System B.
- **Formulation 5:** Optimized Stabilization System D, using peptide-based DSAA chemistry with no boron in this formulation.

Table A5. P2OASys Score for Formulation #1

Formulation #1 Chemicals	% Weight	P2OASys Score	Weighted Score**
Water	63.25	2.18	1.4
Alcohols, C_{12-15}, ethoxylated	20.00	4.55	0.91
Sodium laureth sulfate	10.00	4.27	0.43
Sodium citrate, anhydrous	5.00	3.36	0.17
Calcium chloride, dihydrate	0.101	3.91	0.004
Alpha-amylase*	0.045	2.64	0.001
Cellulase*	0.035	2.91	0.001
Glycerol	0.778	3.18	0.025
Lipase*	0.0175	2.73	0.000
Mannanase, endo-1,4-beta *	0.005	2.64	0.000
Phenoxyethanol	0.015	3.27	0.000
Propylene Glycol	0.235	3.45	0.008
Protease (Subtilisin)*	0.0202	3.09	0.001
Proxel	0.002	4.91	0.000
Sodium Formate	0.015	3.82	0.001
Sorbitol	0.46	2.27	0.010
Total	**100**		**2.9**

**Defined as enzyme concentrate, dry matter basis.*

*** Weighted score = % Weight * P2OASys Score*

Table A6. P2OASys Score for Formulation #2

Formulation #2 Chemicals	% Weight	P2OASys Score	Weighted Score**
Water	60.25	2.18	1.3
Alcohols, C_{12-15}, ethoxylated	20.00	4.55	0.91
Sodium laureth sulfate	10.00	4.27	0.43
Sodium citrate, anhydrous	5.00	3.36	0.17
Calcium chloride, dihydrate	0.10	3.91	0.004
Sodium formate	3.015	3.82	0.12
Alpha-amylase*	0.045	2.64	0.001
Cellulase*	0.035	2.91	0.001
Glycerol	0.778	3.18	0.025
Lipase*	0.0175	2.73	0.000
Mannanase, endo-1,4-beta *	0.005	2.64	0.000
Phenoxyethanol	0.015	3.27	0.000
Propylene Glycol	0.235	3.45	0.008
Protease (Subtilisin)*	0.0202	3.09	0.001
Proxel	0.002	4.91	0.000
Sorbitol	0.46	2.27	0.010
Total	100		**3.0**

**Defined as enzyme concentrate, dry matter basis.*

*** Weighted score = % Weight * P2OASys Score*

Table A7. P2OASys Score for Formulation #3

Formulation #3 Chemicals	% Weight	P2OASys Score	Weighted Score**
Water	58.25	2.18	1.30
Alcohols, C_{12-15}, ethoxylated	20.00	4.55	0.91
Sodium laureth sulfate	10.00	4.27	0.43
Sodium citrate, anhydrous	5.00	3.36	0.17
Calcium chloride, dihydrate	0.10	3.91	0.004
Boric Acid	2.00	4.64	0.093
Glycerol***	3.778	3.18	0.12
Alpha-amylase*	0.045	2.64	0.001
Cellulase*	0.035	2.91	0.001
Lipase*	0.0175	2.73	0.000
Mannanase, endo-1,4-beta *	0.005	2.64	0.000
Phenoxyethanol	0.015	3.27	0.000
Propylene Glycol	0.235	3.45	0.008
Protease (Subtilisin)*	0.0202	3.09	0.001
Proxel	0.002	4.91	0.000

Formulation #3 Chemicals	% Weight	P2OASys Score	Weighted Score**
Sodium Formate	0.015	3.82	0.001
Sorbitol	0.46	2.27	0.010
Total	**100**		**3.0**

**Defined as enzyme concentrate, dry matter basis.*

*** Weighted score = % Weight * P2OASys Score*

****Provides the aggregate weight for all glycerol subtotals.*

Table A8. P2OASys Score for Formulation #4

Formulation #4 Chemicals	% Weight	P2OASys Score	Weighted Score**
Water	63.30	2.18	1.4
Alcohols, C_{12-15}, ethoxylated	20.00	4.55	0.91
Sodium laureth sulfate	10.00	4.27	0.43
Sodium citrate, anhydrous	5.00	3.36	0.17
Calcium chloride, dihydrate	0.10	3.91	0.004
4-FPBA - 4-formylphenyl boronic acid	0.0085	3.36	0.000
Alpha-amylase*	0.045	2.64	0.001
Calcium Chloride, anhydrous	0.001	3.82	0.000
Cellulase*	0.035	2.91	0.001
Ethoxylated fatty alcohol, C_{11}-C_{15}	0.001	4.00	0.000
Glycerol	0.778	3.18	0.025
Lipase*	0.0175	2.73	0.000
Mannanase, endo-1,4-beta *	0.005	2.64	0.000
Phenoxyethanol	0.0015	3.27	0.000
Propylene Glycol	0.21	3.45	0.007
Protease (Subtilisin)*	0.0202	3.09	0.001
Proxel	0.002	4.91	0.000
Sorbitol	0.46	2.27	0.010
Total	**100**		**2.9**

**Defined as enzyme concentrate, dry matter basis.*

*** Weighted score = % Weight * P2OASys Score*

Table A9. P2OASys Score for Formulation #5

Formulation #5 Chemicals	% Weight	P2OASys Score	Weighted Score**
Water	63.26	2.18	1.4
Alcohols, C_{12-15}, ethoxylated	20.00	4.55	0.91
Sodium laureth sulfate	10.00	4.27	0.43

Formulation #5 Chemicals	% Weight	P2OASys Score	Weighted Score**
Sodium citrate, anhydrous	5.00	3.36	0.17
Calcium chloride, dihydrate	0.10	3.91	0.004
DSAA - Disubstituted Alaninamide	0.0007	2.64	0.000
Alpha-amylase*	0.045	2.64	0.001
Calcium Chloride, anhydrous	0.001	3.82	0.000
Cellulase*	0.035	2.91	0.001
Glycerol	0.763	3.18	0.024
Lipase*	0.0175	2.73	0.000
Mannanase, endo-1,4-beta *	0.005	2.64	0.000
Phenoxyethanol	0.015	3.27	0.000
Propylene Glycol	0.24	3.45	0.008
Protease (Subtilisin)*	0.0202	3.09	0.001
Proxel	0.002	4.91	0.000
Sodium Formate	0.015	3.82	0.001
Sorbitol	0.46	2.27	0.010
Total	**100**		**2.9**

**Defined as enzyme concentrate, dry matter basis.*

*** Weighted score = % Weight * P2OASys Score*

There is limited difference (2.9 to 3.0) between the overall P2OASys scores for the five different formulations. However this is not unexpected, as the five ingredients of the base detergent (water, alcohols, sodium laureth sulfate, sodium citrate anhydrous, and calcium chloride dihydrate) are included in each of the five formulations assessments and comprise a majority of the formulation weight (approximately 92% to 97% of the total formulation weight).

Formulations #1, #4, and #5 have the best P2OASys formulation scores (all three formulations are approximately 2.9). This is because they either have no stabilizer (Formulation #1) or they have very low concentrations of stabilizer components that have a P2OASys score very close to the Formulation #1 overall score of 2.9. Formulation #4 has a low concentration (0.0085%) of stabilizer 4-FPBA with a P2OASys score of 3.36. Formulation #5 has a low concentration (0.0007%) of stabilizer DSAA with a P2OASys score of 2.64.

In contrast, Formulations #2 and #3 had higher overall P2OASys scores of 3.5 and 3.6, respectively. These formulations have relatively high stabilizer concentrations, and the P2OASys scores for these stabilizer components are in general higher than the other formulation components. Formulation #2 had stabilizer component sodium formate at 3% concentration with a P2OASys score of 3.82. Formulation #3 had stabilizer component boric acid at 2% concentration with a P2OASys score of 4.64.

Appendix B: P2OASys Professional Judgment Scoring Methodology

Hazard	Characteristics	L (2)	L/M (4)	M (6)	M/H (8)	H (10)
Acute human effects	Inhalation LC_{50} (ppm)	> 10,000	≥ 1,000	≥ 150	≥ 15	<15
	PEL/TLV (ppm)	200	100	25	5	<5
	PEL/TLV (mg/m^3) (dusts/particles)	10	5	1	0.1	<0.1
	IDLH (ppm)	1,000	500	50	10	<10
	Respiratory irritation	Non-irritating	Evidence in humans and animals shows slight or minor reversible respiratory irritation effects	Evidence in humans or animals shows mild reversible respiratory irritation effects	Evidence in humans or animals shows reversible respiratory irritation effects	Existing human and animal data, in vitro data or information from structurally related compounds shows irreversible damage to the respiratory system
	Oral LD_{50} (mg/kg bw)	5,000	500	50	5	<5
	Dermal irritation	Non-irritating	Evidence in humans and animals shows slight or minor reversible skin irritation effects	Evidence in humans or animals shows mild reversible skin irritation effects; GHS category 3	Evidence in humans or animals shows reversible skin irritation effects; GHS category 2	Existing human and animal data, in vitro data or information from structurally related compounds shows irreversible skin burns; GHS category 1A, 1B or 1C
	Skin absorption	Not expected to be absorbed through skin	Repeated skin exposure may result in absorption of harmful amounts	Harmful if absorbed through skin; skin absorption is of moderate concern	Evidence show potential to be absorbed through skin; toxic if absorbed through skin	Evidence shows skin absorption is very likely and a major exposure route of concern; fatal if absorbed through skin
	Dermal LD_{50} (mg/kg bw)	5,000	500	50	5	<5
	Eye irritation	Non-irritating	Evidence in humans and animals shows slight or minor reversible eye irritation effects	Evidence in humans or animals shows mild reversible eye irritation effects	Evidence in humans or animals show reversible irritation effects on the eyes from single or repeated exposure; GHS category 2A or 2B	Existing human and animal data, in vitro data or information from structurally related compounds shows irreversible eye damage; GHS category 1A, 1B or 1C

Hazard	Characteristics	L (2)	L/M (4)	M (6)	M/H (8)	H (10)
Chronic human effects	Reference Dose RfD (mg/kg bw/d)	0.1	0.05	0.01	0.001	<0.001
	Carcinogen	Not classified as a carcinogen; IARC Group 3 or 4; EPA Group D or E			Suspected to be carcinogenic to humans; GHS category 2; IARC 2B, EU category 3; EPA Group C	Known or presumed to have carcinogenic potential in humans; GHS category 1A or 1B; IARC Group 1 or 2A; California Proposition 65; NIOSH Carcinogen List; NTP known or reasonably anticipated to be human carcinogen; EU category 1 or 2; EPA Groups A, B1 or B2
	Mutagen	Not classified as a mutagen			Evidence show possibility of inducing heritable mutations in the germ cells of humans; GHS category 2; EU category 3	Known or regarded to induce heritable mutations in the germ cells of humans; GHS category 1A or 1B; EU category 1 or 2
	Reproductive effects	Not expected to cause reproductive effects			Suspected human reproductive toxicant (damaging fertility or unborn child); GHS category 2; EU category 3	Known or presumed human reproductive toxicant (damaging fertility or unborn child); GHS category 1A or 1B; California Proposition 65; NTP Center for the Evaluation of Risks to Human Reproduction; EU category 1 or 2
	Neurotoxicity	Not classified or known to be neurotoxic		Relevant chemical class known to produce neurotoxic effects	Animal studies and analog data on chemical suggest neurotoxic effects	Evidence in humans shows potential neurotoxic effects of exposure to chemical
	Developmental effects	Not expected to cause developmental effects		Chemical class known to produce developmental effects	Animal studies and analog data suggest developmental effects	Evidence in humans shows developmental effects

Hazard	Characteristics	L (2)	L/M (4)	M (6)	M/H (8)	H (10)
	Respiratory sensitivity/ disease	Professional judgment				
	Other chronic organ effects	Not expected to cause chronic organ effects or systemic toxicity		Evidence shows temporary organ or systemic effects from which humans can recover following a reasonable period of time without significant alteration of structure or function; GHS category 3	Evidence from studies in experimental animals presumed to have the potential to be harmful to human health following single or repeated exposure; GHS category 2	Evidence in humans show significant toxicity from single or repeated exposure; Studies from experimental animals can be presumed to have the potential to produce significant toxicity in humans from single or repeated exposure; GHS category 1
Physical hazards	Heat (°C)	25	27	30	32	>32
	Noise generation (dBA)	80		85		>90
	Vibration (m/S^2)	4	6	8	12	>12
	Ergonomic hazard	Professional judgment				
	Psychosocial hazard	Water-based or materials/processes which presents very low or no safety concerns to workers; workers motivated to develop and utilize skills on the job; opportunities for workers to be involved in work-related decision making; low stress work environment		Moderate safety concerns about work materials/processes; moderate job demands; workers involvement in decision making but with certain limitations; opportunity to develop and utilize skills but not to full potential; some work-related stress		Solvent-based or materials/processes which presents significant safety concerns to workers; high job demands and low or no decision making opportunities for workers; inability to develop or utilize acquired skills to full potential; high stress work environment
Aquatic hazards	Water Quality Criteria (HWQC) (mg/L)	>10	6-8	4-6	1-4	<1
	Aquatic LC_{50} (mg/L)	1,000	50	1	0.1	<0.1
	Fish NOAEC (mg/L)	0.2	0.02	0.002	0.0002	<0.0002
	Plant EC_{50} (mg/L)	1,000	10	1	0.1	<0.1
	Observed ecological effects	Not harmful to aquatic organisms		May cause harm		Harmful

Hazard	Characteristics	L (2)	L/M (4)	M (6)	M/H (8)	H (10)
Persistence/ bioaccumulation	Persistence	Not classified as being persistent	Soil, sediment < 30 days; water < 7 days; or ready biodegradability	Soil, sediment 30 to 60 days; or water 7 to 40 days	Soil, sediment > 60 to 180 days; water > 40 to 60 days; or potential for long-range environmental transport	Soil, sediment > 180 days; or water > 60 days
	BOD half-life (day)	4	10	100	500	>500
	Hydrolysis half-life (day)	4	10	100	500	>500
	Bioconcentration/log Kow	1	2	4	5	>5
	Bioconcentration factor (BCF); Bioaccumulation factor (BAF)	BCF/BAF < 10; or absent such data	BCF/BAF ≥10 - 100	BCF/BAF ≥ 100 to 200; absent such data, log Kow > 4 to 4.5; or suggestive evidence of bioaccumulation in humans or wildlife	BCF/BAF > 200 to 1,000; absent such data, log Kow > 4.5 to 5; or weight of evidence demonstrates bioaccumulation in humans or wildlife	BCF/BAF > 1,000; or absent of such data, log Kow > 5
Atmospheric hazard	Greenhouse gas	Not listed as a greenhouse gas		Listed as a greenhouse gas with global warming potential similar to that of carbon dioxide (CO_2)		Listed as a greenhouse gas with global warming potential greater than that of carbon dioxide (CO_2)
	Ozone depletor	Not listed as an ozone depletor				Listed as an ozone depletor; Class I or II ozone depleting substances
	Acid rain formation	Not listed as a precursor of acid rain				Listed as a precursor of acid rain
	NESHAP	Not listed as a Hazardous Air Pollutant				Listed as a Hazardous Air Pollutant
Disposal hazard	Landfill	Recyclable; filterable				Limited use/emulsifier
	EPCRA reportable quantity (lb)	5,000	1,000	100	10	1
	Incineration	Incinerable with no hazardous byproducts				Hazardous decomposition
	Recycling	Recyclable; filterable				Limited use/emulsifier

Hazard	Characteristics	L (2)	L/M (4)	M (6)	M/H (8)	H (10)
Chemical hazard	Vapor pressure (mm Hg)	0.1	1	10	100	>100
	Flammability	Minimal flammability hazard; will not burn; NFPA or HMIS rating number 0	Slight flammability hazard; must be preheated before ignition can occur; NFPA or HMIS rating number 1	Moderate flammability hazard; must be preheated or high ambient temperature to burn; NFPA or HMIS rating number 2	Serious flammability hazard; can be ignited under all ambient temperatures; NFPA or HMIS rating number 3	Severe flammability hazard; will vaporize and readily burn at normal temperatures; NFPA or HMIS rating number 4
	Flash point (°C)	100	75	25	10	<10
	Reactivity	Minimal hazard; stable; NFPA or HMIS rating number 0	Slight hazard; normally stable but high temperatures make unstable; NFPA or HMIS rating number 1	Moderate hazard; violent chemical change at high temperatures or pressures; NFPA or HMIS rating number 2	Serious hazard; may explode at high temperatures or shock; NFPA or HMIS rating number 3	Severe hazard; may explode at normal temperatures and pressures; NFPA or HMIS rating number 4
	pH	Non corrosive (neutral pH)				Existing human and animal data, in vitro data or information from structurally related compounds shows irreversible skin burns or eye damage; pH ≤ 2 or pH ≥ 11.5; GHS category 1A, 1B or 1C
	High pressure system	Immersion system				High pressure system; media blasting
	High temperature system	Temperature > 68 to 77 °F; cold temperature; cold cleaning	Temperature > 77 to 100 °F	Temperature > 100 to 150 °F	Temperature > 150 to 170 °F	Temperature > 170 °F; vapor degreasing
	Mixture/reaction potential	No hazardous byproducts formed when mixed with other chemicals used				Hazardous decomposition or mixtures formed when mixed with chemicals used
	Odor threshold	Odorless		Mild odor; faint odor; characteristic odor; citrus odor		Pungent odor; irritating odor; strong citrus smell; solvent smell

Hazard	Characteristics	L (2)	L/M (4)	M (6)	M/H (8)	H (10)
	Volatile organic compound	No VOC to 24 g/l	25-49	50-99	100-300	>300
Energy and resource use	Non-renewable resource	Bio-based substance; biomass; renewable resource		Aqueous-based solvents; semi-renewable resource		Petroleum-based solvents; fossil fuels; nuclear power; non-renewable resource
	Water use	Solvents used; no rinsing; little to no water used	Cascade rinsing	Semi-aqueous; multi stage rinsing without reuse; moderate quantities of water used	Dump rinsing	Aqueous; continuous flow rinsing; significant quantities of water used
	Energy use	Temperature > 68 to 77 °F for cleaning; cold/room temperature cleaning; manual cleaning	Temperature > 77 to 100 °F for cleaning; immersion cleaning system	Temperature ≥ 100 to 150 °F for cleaning; low pressure spray	Temperature > 150 to 170 °F for cleaning; heated cleaning; mechanical agitation	Temperature > 170 °F for cleaning; vapor degreasing; ultrasonic; high pressure cleaning
Product hazard	Upstream effects	Professional judgment				
	Consumer hazard	Aqueous; green cleaners, renewable materials				Solvent
	Disposal hazard	Resources conserved; waste reduction	Materials re-used more than once	Recyclable; compostable	Recovery; incineration to convert waste to energy (power and/or heat)	Landfill disposal; incineration; disposal without any value recovered
Exposure potential	Exposure potential	Low dustiness; low volatility; no control equipment required; no exposure concerns		Medium dustiness; medium volatility; control equipment recommended; concerns over potential exposure		High dustiness; high volatility; control equipment required; exposure very likely

Appendix C: GreenScreen™ Chemical Hazard Assessment Summary Tables

This Appendix provides the data, hazard score and benchmarks for each of the components of the various detergent formulations used by the cleaning solutions company. The following table indicates the order of the various chemicals assessed, as presented in this Appendix. The colors indicate the preliminary benchmark score for each chemical (ignoring data gaps). More detail is provided in the individual hazard score tables.

Component Function	Chemical	GreenScreen™ Benchmark Score	GreenScreen™ Score Ignoring Data Gaps
Stabilizer Package Components	Glycerol	3	3
	DSAA	U	3
	4-FPBA	U	2
	Sodium formate	2	2
	Boric Acid	1	1
Base Detergent Components	Water	4	4
	Sodium citrate, anhydrous	U	3
	Alcohols, C_{12-15}, ethoxylated	U	2
	Calcium chloride, dihydrate	1	1
	Sodium laureth sulfate	U	2
Enzyme Product Components	Sorbitol	U	4
	Propylene glycol	3	3
	Lipase	2	2
	Mannanase, endo-1,4-beta	U	3
	Cellulase	U	2
	Protease (Subtilisin)	U	2
	Alpha-amylase	U	2
	Calcium chloride, anhydrous	U	2
	Ethoxylated fatty alcohol, C_{11}-C_{15}	2	2
	Proxel ≥10-20% 1,2-Benzisothiazolin-3-one	U	2
	Proxel 5-10% Sodium hydroxide	U	2
	Phenoxyethanol	U	3

In the following data tables, the hazard scores are indicated as follows:

Hazard Score	
Very High	vH
High	H
Moderate	M
Low	L
Very Low	vL
Data gap	DG

Stabilizers Package Components

Boric acid, CAS# 10043-35-3

	Group I Human					Group II and II* Human								Ecotox		Fate		Physical	
	C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
							Single	Repeated *	Single	Repeated *										
Data from Scientific Sources or MSDS			May damage fertility or unborn child; H360; Repro Cat 1B	R61	EU Community Strategy for Endocrine Disrupters - Priority List - Category 1 - In vivo evidence of endocrine disruption activity; Potential (On TEDX list[14])	Rat oral,LD_{50} = 2,660 mg/kg bw	Hepatotoxin [HazMap]; H370	H372		CNS effects noted [HazMap]			High Skin Irritant; Cat 2; H315	Eye irritant	LC_{50} (*p.lucias*) = 279 mg/L LC_{50} (*daphnia*) = 53.2 mg/L EC_{50} (*daphnia*) = 133 mg/L		DSL list of substances that are persistent		Explodes when heated	NFPA = 0
Data from REACH Dossier§	NOEL > 5,000 mg/l, not carcinogenic	Multiple tests indicate Negative effects, *in vivo* and *in vitro*	Repro Cat 1B (oral) when conc ≥ 5.5%; H360	Some evidence		LD_{50} (rabbit, dermal) >2,000 mg/kg; LD_{50} (Rat,Oral)> 2,600 mg/kg: LC_{50} (rat, inh) > 2.03 mg/L		NOAEL (oral, rat) = 17.5-26 mg (B)/kg-bw/d; NOAEC (inh, rat) = 470 mg (B)/m3			Not sensitizer		Irritatation Index = 0.1, fully reversible (72 hr)	Overall irritation 13.6, fully rev; Eye Irritant	Numerous studies LC_{50} ≥64 mg/L for fish, water flea and algae	NOEC ≤5.6mg/L for *danio rerio*		BCF < 0.1		
Hazard Level	L	L	H	H	H	L	vH	M	DG	M	L	DG	H	H	M	M	H[15]	vL	M	L

§ REACH Dossier information available at: http://apps.echa.europa.eu/registered/data/dossiers/DISS-9c85f941-5dd4-6d9c-e044-00144f67d249/DISS-9c85f941-5dd4-6d9c-e044-00144f67d249_DISS-9c85f941-5dd4-6d9c-e044-00144f67d249.html

Benchmark = BM 1e[16]

[14] Research supporting this finding: Linder RE, Strader LF, Slott VL, Suarez JD. 1992. Endpoints of spermatotoxicity in the rat after short duration exposures to fourteen reproductive toxicants. *Reprod Toxicol* **6(6):**491-505.

[15] As an inorganic substance, the persistence is considered in combination with chronic hazards.

[16] This benchmark level is based on the High hazard score for reproductive and developmental toxicity and endocrine disruption. This is a non-verified GreenScreen™ assessment and may not be used to make public promotional or product claims.

DSAA (disubstituted alaninamide) CAS # *Confidential*

	Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
	C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
							Single	Repeated*	Single	Repeated*										
Data from Scientific Sources or MSDS		Not mutagenic (Ames test)				Oral, rat LD_{50} >2,000 mg/kg bw					GHS: Cat 1B H317, R43		Not irritating, corrosive	Not irritating	EC_{50} (*daphnia*) >88.4 mg/l[17], EC_{50} (algae) >101 mg/l		Readily biodegrades	Log Kow = 1.8	Not explosive	
Data from NICNAS Risk Evaluation (2014)		Non mutagenic to bacteria (Ames test)				LD_{50} (oral, rat) > 2,000 mg/kg bw					Evidence of sensitization, with reported stimulation indices of 3.9, 7.3 and 4.1 at 10, 25 and 50% concentration, respectively (EC_3 = 3.6%)		not classifiable as skin irritant (*in vitro* assessment)	Not classifiable for serious eye damage/eye irritation (*in vitro* assessment)	EC_{50} (*daphnia*) >88.4 mg/L; EC_{50} (algae) >101 mg/l		Expected to be mobile in soil based on its high water solubility and low potential to partition to the organic phase (log Pow = 1.8). No significant hydrolysis expected to occur in the environmental pH range of 4-9.	Classified as readily biodegradable and the notified chemical is not expected to bioaccumulate due to the low n-octanol/water partition coefficient (log Pow 1.8)	Not expected to be explosive based on structure, Not expected to be oxidising based on structure	Solid Flammability Not highly flammable Autoignition Temperature>400 °C
Hazard Level	DG	L	DG	DG	DG	L	DG	DG	DG	DG	M	DG	L	L	M	DG	L	vL	L	L

Benchmark = BM U

Ignoring Data Gaps, Benchmark = BM 3b, c [18]

[17] *Daphnia* are identified as the most sensitive species, therefore the hazard score is based on this data.

[18] This benchmark level is based on the Moderate hazard scores for acute aquatic toxicity and skin sensitization. This is a non-verified GreenScreen™ assessment and may not be used to make public promotional or product claims.

4-FPBA (4 Formylphenyl boronic acid), CAS# 87199-17-5

	Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
	C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
							Single	Repeated*	Single	Repeated*										
Data from Scientific Sources or MSDS			Not listed on Prop 65			Oral rat LD_{50}>2,000 mg/kg bw					H317		GHS Cat 1 (H314)	GHS Cat 1	EC_{50} (*daphnia*) = 64 mg/l/48 hr; EC_{50} (fish) =3.7/72 hr		93% degraded in 28d		Not explosive	FP>100°C
REACH Dossier data§		Gene mutation test: mammalian cell line, other: mus. Lymphomazellen (L5178Y): cytotoxicity exhibited at 1.000 ug/ml and 600 ug/ml (with and without metabolic activation); Chromosome aberration (mammalian cell line, other: Human lymphozyten) cytotoxicity at 734.6 ug/ml. These data indicate possibility it may induce heritable mutations, therefore classifiable as Cat 2				Oral rat LD_{50}>2,000 mg/kg bw; Dermal rat LD_{50}>2,000 mg/kg bw		Repeat dose oral rat: NOAEL = 250 mg/kg bw/d			Sens. Testing on gpg, Dunkin-Hartley (dose not indicated) indicates positive reaction to 4-FPBA (negative controls also indicate reaction, at half the rate of 4-FPBA); Results indicate GHS Cat 1B; H317		Rabbit tests: Erythema and edema score = 0 Results indicate GHS Cat 3	Rabbit tests: Max conjunctivae score = 2; max chemosis score = 4; max cornea score = 1; max iris score = 0 Results indicate GHS Cat 2 (data not available to det. if reversible within 7 days) therefore Cat 2A	R52 - Harmful to aquatic organisms LC_{50} (fish) = 56.7 mg/l: EC_{50} (*daphnia*) = 80.2 mg/l; NOEC = 48.9 mg/l	NOEC (fish) = 22.3 mg/l	Readily biodegradable (92% in 28 d) Solubility = 810.1 mg/L at 20 °C, pH ca. 4.8		Not explosive under flame, or more sensitive to shock or friction than m-dnb	
Hazard Level	DG	M	DG	DG	DG	L	DG	L	DG	DG	M	DG	M	H	M	L	L	DG	L	L

§ REACH Dossier information available at: http://apps.echa.europa.eu/registered/data/dossiers/DISS-eb89223b-3fe9-5b87-e044-00144f67d031/DISS-eb89223b-3fe9-5b87-e044-00144f67d031_DISS-eb89223b-3fe9-5b87-e044-00144f67d031.html

Benchmark = BM U

Ignoring Data Gaps, Benchmark = BM 2f [19]

[19] This benchmark level is based on the High hazard score for eye sensitization. This is a non-verified GreenScreen™ assessment and may not be used to make public promotional or product claims.

Glycerol, CAS# 56-81-5

	Group I Human					Group II and II* Human								Ecotox		Fate		Physical	
	C	M	R	D	E	AT	ST Single	ST Repeated*	N Single	N Repeated*	SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
Data from Scientific Sources or MSDS			Not on Prop 65			Oral rat LD_{50} = 12,600 mg/kg bw Oral mse LD_{50} = 4,090 mg/kg bw		Resp system is target organ						Strong eye irritant	LC_{50} = 10,000 mg/l LC_{50} = 5,000 mg/l	ChV = 9,500 mg/l	Water: 8.7 Soil/Sed.: 17/78 Air: 0.88	BCF: 3.2	Explosion hazard with halogens and strong oxidizing agents	FP= 177C (closed cup)
Data from ToxServices assessment	ECHA 2013: 2 year rat study, showed no increase in tumor formation	ECHA 2013: negative results in several studies	ECHA 2013: no effects	ECHA 2013: no effects				ECHA 2013: low NOEL levels from several sub-chronic and chronic studies			UNEP 2002: low hazard based on data from non-standard tests and expert judgment		ECHA 2013 : rabbit studies with trace or no irritation	ECHA 2013 : rabbit studies with trace or no irritation		Ecosar, EPA 2012: modeled data with algae ChV value of 1,334.4 mg/l	ECHA, 2013: sludge test with 94% degradation in 24 hours		EC 2000: not explosive	ECHA 2013: FP = 199 C (open cup)
REACH Dossier data [§]	no tumor formation noted in 2 yr study	several studies indicate negative results	no effect noted in 2 gen rat, oral study	NOAEL >1,180 mg/kg bw (no effects noted during study)		LD_{50} (oral, mse) >23,000 mg/kg; LC_{50} (inh, rat) >2.75 mg/L; LD_{50} (dermal, g.pig) = 56,700 mg/kg bw		NOAEL (oral) >8,000 mg/kg; NOAEL (inh) = 167 mg/m3; NOEL (dermal) = 5,040 mg/kg d					not irritating	irritation index ≤ 2 (fully rev); slightly irritating	LC_{50} (fish, 96h) > 885 mg/l; LC_{50} (daphnia, 48 h) = 1,955 mg/L			readily biodegradable		
Hazard Level	L	L	L	L	DG	L	DG	L	DG	DG	L	DG	L	M	L	L	vL	vL	L	L

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Benchmark = BM 3c [20]

[20] This benchmark level is based on the Moderate hazard score for eye irritation. This is a non-verified GreenScreen™ assessment and may not be used to make public promotional or product claims.

Sodium formate[21], CAS#: 141-53-7

	Group I Human					Group II and II* Human								Ecotox		Fate		Physical	
	C	M	R	D	E	AT	ST		N		SnS*	Sn R*	IrS	IrE	AA	CA	P	B	Rx	F
							Single	Repeated*	Single	Repeated*										
Data from Scientific Sources or MSDS	Experimental data indicates neoplasia not observed in rats; epidemiologic data indicates low chance for developing cancer.	EPA HPV and OECD SIDS studies conclude genetic toxicity for formates is low	Studies of formic acid (AN APPROPRIATE analog for sodium formate) conclude low hazard for repro tox; HazMap: Listed as reproductive toxicant	Weight of evidence, incl. 2008 SIDS studies, indicates low hazard.		LD_{50} (Oral) >3,000 mg/kg bw; LD_{50} (dermal) >2,000 mg/kg bw; LC_{50} (inh) undeterminable for sodium formate, =7.4 mg/L for formic acid (analog)	Large doses may cause cardiac depression; High concentrations may cause respiratory irritation rabbit studies indicate minimal systemic effect	may cause hemolytic anemia; NOAEL for formic acid (inh, rat) =60 mg/m3	one study indicates minor (rev) behavior effects (cat, subcut); analog data (formic acid) indicates high hazard[22]	some data suggests direct action on the brain by exposure to formate ions; formic acid data indicates neurologic impacts	not expected to act as skin sensitizer (OECD SIDS assessment)		Rabbit studies indicate no skin irritation after 72 hr	Rabbit studies indicate moderate to severe conjunctival irritation and conjunctival necrosis (rev)	EC_{50} = 954 mg/l	LC_{50} = >5,000 mg/L (fish, *daphnids*)	modeled data indicates low persistence in relevant media (Water=15 d; Soil=30 d)	BAF = 3.2	Not explosive; NFPA = 0	NFPA = 0
Data from REACH dossier §	Assume similar non-carcinogenic characteristics as potassium formate (read across method)							NOAEL (oral) calculated to be 3,138 mg/kg bw			Assumed similar to potassium formate, which is not sensitizing to skin				LC_{50} (fish, *daphnia*) > 1,000 mg/L;		tests indicate >70% degradation w/in 28 d			Not flammable
Data from ToxServices assessment		US EPA 2009: negative for mutagenicity in multiple tests		US EPA 2009: *in vitro* incubation tests indicate multiple developmental impacts		U.S. EPA 2009: Oral rat LD_{50} > 3,000 mg/kg-bw Oral mice LD_{50} >4,700-11,200 mg/kg-bw			US EPA 2009: Specific neurotoxicity seen at concentrations up to 60 mM (equal to 2,760 µg/mL)	US EPA 2009: no repeat dose toxicity observed in animal testing					US EPA 2009: L/EC_{50} values > 1,050 mg/L (*Daphnia magna*, 48 hr)		US EPA 2009: readily biodegradable			
Hazard Level	L	L	M	M	DG	L (oral); L (derm): H (inh)	L	M	H	L	L	DG	L	M	L	L	vL	vL	L	L

§ REACH dossier available at: http://apps.echa.europa.eu/registered/data/dossiers/DISS-9d836a42-eb75-1b31-e044-00144f67d249/AGGR-9ffd21d5-9cd7-44be-a8ca-b184d2bcfd41_DISS-9d836a42-eb75-1b31-e044-00144f67d249.html#AGGR-9ffd21d5-9cd7-44be-a8ca-b184d2bcfd41

Benchmark = BM 2e [23]

[21] Where data gaps are found, data for formic acid and calcium formate were considered as suitable analogs.

[22] The presence of minimal data for sodium formate coupled with more data from formic acid elevates the hazard score from Low to Moderate.

[23] This benchmark level is based on the moderate hazard score for reproductive and developmental toxicity. This is a non-verified GreenScreen™ assessment and may not be used to make public promotional or product claims.

Enzyme Product Components

Alpha-amylase (solid), CAS #9000-90-2

	Group I Human					Group II and II* Human								Ecotox		Fate		Physical	
	C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
							Single	Repeated*	Single	Repeated*										
Data from Scientific Sources or MSDS						Oral rat LD_{50}>7,500 mg/kg; Oral mse LD_{50}> 15,000 mg/kg (ChemID Plus)						GHS Cat 1, H334, A and Rs class. (AOEC)	May cause skin or eye irritation						Not explosive, NFPA rating =0	HMIS and NFPA =0
Data from Tox Services Assessment												R42					HERA, 2005 - readily biode-gradable			
Data from REACH Dossier §		Negative (*in vitro* mutagenic, chromosomal aberration, Ames, clastogenic and aneuploidy tests) at ≤5,000 µg/ml				Oral (rat) LD_{50} > 1,911 mg TOS/kg Inhalation LC_{50} > 4.96 mg/L GHS Cat 5		Oral NOAEL ≤ 1,320 mg TOS/kg bw/d		No behavioral effects observed	SI <1.23 at conc ≥25%, Not sensitizer		Erythema score = 0.3 (fully rev), edema score = 0.0, at 60 mg aep/L Not irritating	Conjunctivae score = 1 (fully rev), chemosis score = 0, Not irritating	NOEC (fish) >58.3 mg aep/LEC_{50} (*daphnia*) = 212 mg aep/L 48 h EC_{50} (alg, 72hr) = 2.5 mg aep L		Not PBT or vPvB			
Hazard Level	DG	L	DG	DG	DG	H[24]	DG	L	DG	L	*L*	H	*L*	*L*	L	DG	*L*	*L*	*L*	*L*

§ REACH Dossier information available at: http://apps.echa.europa.eu/registered/data/dossiers/DISS-d38d7b3c-e207-43e4-e044-00144f67d249/DISS-d38d7b3c-e207-43e4-e044-00144f67d249_DISS-d38d7b3c-e207-43e4-e044-00144f67d249.html

Benchmark = BM U

Ignoring Data Gaps, Benchmark = BM 2f [25]

[24] Based on inhalation values for test material as a gas or vapor.

[25] This benchmark level is based on the hazard score for High acute toxicity (inhalation) and respiratory sensitization. This is a non-verified GreenScreen™ assessment and may not be used to make public promotional or product claims.

Cellulase, CAS# 9012-54-8

	Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
	C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
							Single	Repeated*	Single	Repeated *										
Data from Scientific Sources or MSDS												Asthmagen H334, R42; A and Rs classification (AOEC)							Not explosive, NFPA rating =0	HMIS and NFPA =0
Data from REACH Dossier §		Conclusion: Non-clastogenic to human lymphocytes *in vitro*. Cellulase is not mutagenic in the Ames assay in both the presence and absence of metabolic activation				Oral LD_{50} > 2,880 mg/kg bw inh LC_{50} ≥ 4.86 mg/L		Based on the results of this study, the NOEL as well as the NOAEL for the test item ß-Glucanase was set at 1,000 mg/kg/day TOS		No behavioral effects observed		H334	Erythema score =1 (fully rev), no edema observed; Classified as "Non Irritant".	No ocular effects noted, overall irritation score =0; Classified as "Non Irritant".	LC_{50} (fish, 96 hr) > 100 mg TOC/L, >52.1 mg aep/L; EC_{50} (*daphnia*, 48hr) > 100 mg TOC/L, >52.1 mg aep/L		The enzyme substance is readily biodegradable and has no bioaccumulation potential, thus cellulase has no PBT or vPvB properties.			
Hazard Level	DG	L	DG	DG	DG	H	DG	L	DG	L	DG	H	L	L	L	DG	L	L	L	L

§ REACH dossier information available at: http://apps.echa.europa.eu/registered/data/dossiers/DISS-d6b29c08-a036-58eb-e044-00144f67d031/DISS-d6b29c08-a036-58eb-e044-00144f67d031_DISS-d6b29c08-a036-58eb-e044-00144f67d031.html

Benchmark = BM U

Ignoring Data Gaps, Benchmark = BM 2f [26]

[26] This benchmark level is based on the High hazard score for acute toxicity (inhalation) and respiratory sensitization. This is a non-verified GreenScreen™ assessment and may not be used to make public promotional or product claims.

Lipase, CAS# 9001-62-1

	Group I Human					Group II and II* Human								Ecotox		Fate		Physical	
	C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
							Single	Repeated*	Single	Repeated*										
Data from Scientific Sources or MSDS		Multiple negative results (ToxNet)		No dev toxicity obs in rat/mice (oral) up to 4,500 mg/kg on d 7-13 gestation (ExPub: Shephards)		LD_{50} (rat, mice, oral) >10,400 mg/kg; LD_{50} (rabbit, oral) >5000 mg/kg (ChemID Plus)						H334 A and Rs classification (AOEC)						Not explosive, NFPA rating =0	HMIS and NFPA =0
Data from ToxServices Assessment								HERA, 13 week study results									HERA, based on common features			
Data from REACH Dossier §		Not clastogenic in the *in vitro* test using cultured human lymphocytes and not mutagenic in the Ames assay in both the presence and absence of metabolic activation.	There was no effect of treatment with the test material on fertility and general reproductive performance	Dose levels of 10% and 5% lipase in the diet caused slight growth retardation of fetuses; slight reductions in maternal body weight gain and food consumption occurred at the 10% lipase dose level only. No teratogenic potential of lipase was demonstrated at any of the dose levels used.		LD_{50} (oral, rat) > 2,700 mg TOS/L		NOAEL (rat, oral) ≤ 1,080.2 mg TOS/kg bw/d		No neuro-toxic behavior observed during 96 day STOT testing (NOAEL (rat, oral) ≤ 1,080.2 mg TOS/kg bw/d)	The enzyme Lipase is classified as a dermal non-sensitiser. (SI≤ 1.4 at all concentrations tested)		Erythema and edema scores = 0; Lipase is classified as Non Dermal Irritant	No ocular effects observed; Lipase should be classified as Non Irritant	LC_{50} (fish, 96h)>402 mg TOS/L (68.3 mg aep /L); EC_{50} (*daphnia*, 48 hr) >235 mg TOS/L (37.4 mg aep/L); EC_{50} (algae 72h) = 97 mg TOS/L (17.6 mg aep/L)		The enzyme substance is readily biodegradable and has no bioaccumulation potential, thus cellulase has no PBT or vPvB properties.			
Hazard Level	DG	L	L	L	DG	L	DG	L	DG	L	L	H	L	L	M	DG	L	L	L	L

§ REACH Dossier information available at: http://apps.echa.europa.eu/registered/data/dossiers/DISS-dffb4072-e4a3-47ae-e044-00144f67d031/DISS-dffb4072-e4a3-47ae-e044-00144f67d031_DISS-dffb4072-e4a3-47ae-e044-00144f67d031.html

Benchmark = BM 2f [27]

[27] This benchmark level is based on the High hazard score for respiratory sensitization. This is a non-verified GreenScreen™ assessment and may not be used to make public promotional or product claims.

Mannanase, endo-1,4-beta CAS# 37288-54-3

	Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
	C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
							Single	Repeated*	Single	Repeated*										
Data from Scientific Sources or MSDS	Short term tests and a consideration of structure have shown that it is not likely to be a carcinogenic hazard to man											H334	May cause eye or skin irritation						Not explosive	
Data from REACH dossier §		Mannanase is negative for the induction of structural and numerical chromosome aberrations in both the presence and absence of metabolic activation, with no genotoxicity or cytotoxicity observed in the Ames test				LD_{50} (oral, rat) >5,000 mg test material as is/kg, LC_{50} (rat, inh) > 4.95 mg test material as is/kg		In the absence of any toxicologically significant findings in the 13 week treatment, NOAEL in this study was considered to be the highest dose administered, > 83 mg TOS/kg; >75 mg total protein/kg bw/day		No neurobehaviors observed at NOAEL			Max. erythema and edemo scores = 0	Conjunctivae score = 0.3 (fully rev), chemosis score = 0, respectively	LC_{50} (trout) ≥ 100 mg TOS/L , 55.5 mg aep/L; EC_{50} (*daphnia*) ≥ 100 mg TOS/L , 55.5 mg aep/L; EC_{50} (algae) ≥ 100 mg TOS/L , 55.5 mg aep/L		Readily biodegradable; not classified as PBT or vPvB	log Kow ≤ 4.5; "no bioaccumulation potential"		
Hazard Level	L	L	DG	DG	DG	L	DG	L	DG	L	DG	H/M[28]	L	L	L	DG	L	L	L	DG

§ REACH dossier information available at: http://apps.echa.europa.eu/registered/data/dossiers/DISS-dffb4072-e391-47ae-e044-00144f67d031/AGGR-a2386156-641e-451d-b6cb-8107be3cb345_DISS-dffb4072-e391-47ae-e044-00144f67d031.html#AGGR-a2386156-641e-451d-b6cb-8107be3cb345

Benchmark = BM U

Ignoring Data Gaps, Benchmark = BM 3c [29]

[28] Without additional support for a high score, e.g., classification by AOEC as A or Rs (unlike with the other enzymes) the score was assumed to be Moderate.

[29] This benchmark level is based on the Moderate hazard score for respiratory sensitization. This is a non-verified GreenScreen™ assessment and may not be used to make public promotional or product claims.

Protease (Subtilisin), CAS# 9014-01-1

	Group I Human						Group II and II* Human								Ecotox		Fate		Physical	
	C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
							Single	Repeated *	Single	Repeated *										
Data from Scientific Sources or MSDS			N			H302,RZZ LD_{50}=3,700 mg/kg bw; Oral rat LD_{50}=2,000 mg/kg bw	H335					H334; Asthma indicated (HazMap)	H315	H318 H319					Not explosive, NFPA rating = 0	HMIS and NFPA = 0
Data from ToxServices Assessment			HERA 2007, no toxicity observed	HERA 2007, no toxicity observed											H400 LC_{50}>100 mg/L		Henkel 1990, Swisher 1969, expected to meet 10 and 28 biodegradation windows			
Data from REACH Dossier §		no clastogenic or mutagenic effects observed, w or w/o metabolic activation				H302, GHS Cat IV LD_{50}=1,800 mg test matl/L	H335 (inh, lungs)	NOAEL (rat, oral) = 360-891 mg TOS/kg bw/d				H334	H315; fully rev mean erythema and edema scores = 0.43 and 0.8, respectively	H318, H319; fully rev mean Conjunctivae and Chemosis scores = 0.8 and 0.3, respectively	HERA 2007, EC_{50} = 0.1 @ t=13 mg/L	H411; EC_{50}(minnow, 32d)=0.21 mg aep/L; NOEC (minnow) = 0.042 mg aep/L; Cat Chronic 2	Readily biodegradable (in water)	No bioaccumulation potential; Log Kow ≤ 4.5		
Hazard Level	DG	L	L	L	DG	M	M	L	DG	DG	DG	M	M	M[30]	vH	H	L	L	L	L

§ REACH Dossier information available at: http://apps.echa.europa.eu/registered/data/dossiers/DISS-9e9eedca-d1f2-3356-e044-00144f67d031/DISS-9e9eedca-d1f2-3356-e044-00144f67d031_DISS-9e9eedca-d1f2-3356-e044-00144f67d031.html

Benchmark = BM U

Ignoring Data Gaps, Benchmark = BM 2f [31]

[30] GHS classifications indicate H or vH hazard scores, but reliable data show that effects are fully reversible and moderate.

[31] This benchmark level is based on the very High hazard score for acute aquatic toxicity. This is a non-verified GreenScreen™ assessment and may not be used to make public promotional or product claims.

Calcium chloride, anhydrous CAS# 10043-52-4

	Group I Human					Group II and II* Human								Ecotox		Fate		Physical	
	C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
							Single	Repeated*	Single	Repeated *										
Data from Scientific Sources or MSDS		Mutagenic for mammalial somatic cells, bacteria and/or yeast				Oral, rat, LD_{50} = 1,000 mg/kg bw							Skin irritant (burns)	Eye irritant, H319, R36	LC_{50} (fish) = 100 mg/L; LC_{50} = 10,650 mg/L; EC_{50} = 2,400 mg/L *Daphnia*				NFPA = 0	NFPA = 0; Not flammable
Data from REACH Dossier §		Negative in 2 rabbit studies		NOAEL (oral,rabbit) = 169 mg/kg bw/d; NOAEL (oral, mse) > 189 mg/kg bw/d; NOAEL (oral, rat) > 176 mg/kg bw/d		LD_{50} (oral, rabbit) = 500-1,000 mg/kg bw; LD_{50} (dermal) > 5,000 mg/kg bw							Rabbit study data indicates non irritating to moderate irritating (Draize)	Data indicates moderatelv to hiehlv irritatine: Eye Irrit. 2; H319	LC_{50} (fish, 96 h) ≥ 4,630 mg/L; EC_{50} (*daphnia*, 48 h) = 2,400 mg/L	EC_{50} (*daphnia*, 21 d) = 610 mg/L				
Data from ToxServices Assessment		OECD SIDS: negative for genotoxicity in several *in vitro* assays in bacterial and mammalian cells	UNEP 2002: no adverse effects seen at all dose levels			OECD 2002: LD_{50}= 1,940-2,045 mg/kg for mice; LD_{50} = 3,798-4,179 mg/kg for rats; LD_{50} = 507-1,000 mg/kg for rabbits		UNEP 2002: A limited oral repeated dose toxicity study shows no adverse effect of calcium chloride on rats fed 1,000-2,000 mg/kg bw/day for 12 months			UNEP 2002: not sensitizing in guinea pigs				L/EC_{50} (*daphnia*, 96 hr) = 649 mg/L			UNEP 2002: does not bioaccumulate		
Hazard Level	DG	M	L	L	DG	M	DG	L	DG	DG	L	DG	M	H	L	DG	DG	L	L	L

§ REACH dossier data available at: http://apps.echa.europa.eu/registered/data/dossiers/DISS-e7627168-f7ad-63fd-e044-00144f67d031/DISS-e7627168-f7ad-63fd-e044-00144f67d031_DISS-e7627168-f7ad-63fd-e044-00144f67d031.html and http://apps.echa.europa.eu/registered/data/dossiers/DISS-9eb43f6f-23a1-5205-e044-00144f67d031/AGGR-186c7377-893b-4af9-bbbe-4f44af2a27a0_DISS-9eb43f6f-23a1-5205-e044-00144f67d031.html#AGGR-186c7377-893b-4af9-bbbe-4f44af2a27a0

Benchmark = BM U
Ignoring Data Gaps, Benchmark = BM 2e [32]

[32] This benchmark level is based on the Moderate hazard score for mutagenicity. This is a non-verified GreenScreen™ assessment and may not be used to make public promotional or product claims.

Ethoxylated fatty alcohol, C_{11}-C_{15}, (Softanol 90), CAS# 68131-40-8

	Group I Human					Group II and II* Human								Ecotox		Fate		Physical	
	C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
							Single	Repeated*	Single	Repeated*										
Data from Scientific Sources or MSDS						LD50 (Oral rat) 1,800 mg/kg (MSDS) Oral rat 2,380 mg/kg [CIDP]					H317 R43		H315	H318 H319 R41	LC_{50}= 0.1 mg/L (trout); LC_{50}= 4.1 mg/L (*daphnia*); R51/53; H400	ChV = 0.021 mg/L H413 H411	$T_{1/2}$ (water) = 8.7d ; $T_{1/2}$ (soil) = 17d	BCF = 71	Liquid polymer not expected to be explosive or otherwise highly reactive; NFPA = 0	FP=193°C; NFPA =1
Data from REACH Dossier[33]		3 negative studies for mutagenicity opr chromosomal aberrations				LD_{50} (oral, rat) ≥ 2,000 mg/kg bw; LD_{50} (dermal, rat) > 2,000 mg/kg					Sens Cat 1B, H317; Stimulation index = 1.6, 1.7 & 5.1 at 5, 10 and 25%, respectively		Mean viability score = 64.7 (episkin); non irritating. Confirmed w read across for Softanol 50 data	Conjunctivae mean score = 0.22 (fully rev)	LC_{50} (trout) = 1.53 mg/L; EC_{50} (*daphnia*) = 5.66 mg/L; EC_{50} (algae) = 1.03 mg/L	Chronic Cat 2; H411	Readily biodegradable in water	Log Kow ≥ 4.5; log Pow = 5.9-6.2; bioaccumulative		
Hazard Level	DG	L	DG	DG	DG	M	DG	DG	DG	DG	M	DG	M[34]	M[35]	H	vH[36]	L[37]	M[38]	L	M

Benchmark = BM 2f [39]

[33] REACH data for Softanol 30 was used as an appropriate analog: http://apps.echa.europa.eu/registered/data/dossiers/DISS-9ffc01cf-c195-2bc9-e044-00144f67d031/DISS-9ffc01cf-c195-2bc9-e044-00144f67d031_DISS-9ffc01cf-c195-2bc9-e044-00144f67d031.html

[34] Despite the REACH dossier assessment of non-irritating, presence of analog data indicating potential effect, and GHS classification indicating high hazard results in assigning a Moderate hazard score.

[35] Data indicates fully reversible impact, and GHS classification indicates potential for greater concern.

[36] vH hazard score based on modeled value for ecotoxicity for Softanol 90.

[37] Persistence data for water and soil used, as these media represent over 90% of the partition of chemical upon entering the environment.

[38] LogKow for Softanol 30 indicates moderate bioaccumulation potential, although modeled BCF value for Softanol 90 suggests low bioaccumulative potential.

[39] This benchmark level is based on the very High hazard score chronic aquatic toxicity. This is a non-verified GreenScreen™ assessment and may not be used to make public promotional or product claims.

Phenoxyethanol, CAS# 122-99-6

	Group I Human					Group II and II* Human								Ecotox		Fate		Physical	
	C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
							Single	Repeated*	Single	Repeated*										
Data from Scientific Sources or MSDS			may cause reproductive effects [HazMap]			LD_{50} (Oral rat) 1,260-1,840 mg/kg bw; LD_{50} (oral, mse) = 933 mg/kg bw; Acute tox Cat 4, H302 [MSDS]	Eye & skin effects observed, Kidney, repro effects observed		CNS effects observed; solvent syndrome [HazMap]				mild skin irritant (rabbit, 24h) [MSDS]: Cat 2 irritant [HSDB]	Can cause corneal damage [HazMap]; [MSDS] Eye irritant Cat 2A; H319; one rabbit study indicates moderate eye irritant	LC_{50} (*fathead minnow*, 96 hr)=344 mg/L	ChV = 65 mg/L	t ½ (d) = 15 (water); 30(soil)[40]	BCF = 1.5	Not explosive; NFPA = 0	119°C; NFPA = 0
Data from REACH Dossier §		multiple negative studies w and w/o metabolic activation	NOAEL (P) = 1,875-3,700 mg/kg, (F1) = 1,875 mg/kg, (F2) = 375 mg/kg; caused red body wt in neonate (red postnatal survival in F1); maternal toxicity at 300-600 mg/kg	Study indicates no effect to development, but impact on maternal toxicity		LD_{50} (oral, rat) = 1,850 mg/kg bw; LC_{50} (inh, rat) >1,000 mg/m3; LD_{50} (dermal, rat) = 14,391 mg/kg bw;(dermal, rabbit) =≥2,214 mg/kg	NOAEL (oral, rat) = 80-2,500 mg/kg; NOAEL (inh, rat) = 48.2 mg/m3; NOAEL (dermal, rabbit) = 500-2,000 mg/kg		CNS depression noted in one study		Not sensitizing in 3 studies		mean irritation scores for erythema from 0.3 – 2, fully reversible	H319; multiple studies indicate fully reversible (1 exception) effects to cornea, iris, conjunctivae and chemosis; Cat 2 irritant	LC_{50} (*f minnow*, 96 hr) = 344-4,778 mg/l; LC_{50} (*danio*, 96 hr) = 154 – 312.1 mg/l; EC_{50}(algae, 72 hr) > 500 mg/l	NOEC (*fathead minnow*, 34 d) = 23-105.5 mg/L; NOEC (*daphnia*, 21d) = 9.43 – 22.5 mg/l	readily biodegradable	BCF = 0.3493; log Kow = 1.16		
Hazard Level	DG	L	M	L	DG	M	M	DG	M	DG	L	DG	M	M[41]	L	M	M	vL	L	M

§ REACH Dossier information available at: http://apps.echa.europa.eu/registered/data/dossiers/DISS-9d9ec9aa-68cf-6ad9-e044-00144f67d249/DISS-9d9ec9aa-68cf-6ad9-e044-00144f67d249_DISS-9d9ec9aa-68cf-6ad9-e044-00144f67d249.html

Benchmark = BM U

Ignoring Data Gaps, Benchmark = BM 3b,c,d [42]

[40] Based on PBT Profiler model, this chemical will preferentially partition into water or soil. Sediment and air values are not relevant and not considered in the hazard score.

[41] Data indicates moderate hazard (which trumps GHS hazard statement, which indicates high hazard).

[42] This benchmark level is based on the Moderate hazard scores for Reproductive toxicity, multiple Group II Hazards (AT, ST, N, IrS and IrE), chronic aquatic toxicity and Flammability. This is a non-verified GreenScreen™ assessment and may not be used to make public promotional or product claims.

Propylene Glycol, CAS# 57-55-6

	Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
	C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
							Single	Repeated*	Single	Repeated*										
Data from Scientific Sources or MSDS						Oral LD_{50} = 20,000 mg/kg bw	CNS effects observed LC_{50} (aer, rabbit, 2 hr) = 317.042 mg/l		CNS effects observed LC_{50} (aer, rabbit, 2 hr) = 317.042 mg/l		Skin sensitizer			Eye irritant	LC_{50} = 40,613 mg/L LC_{50} = 18,340 mg/L EC_{50} = 19,000 mg/L	ChV = 1,400 mg/L	Water: 8.7 d; Soil:17 d (sed & air not relevant media)	BCF = 3.2	NFPA = 0	NFPA = 1; FP: 104 °C
Data from REACH Dossier [§]						LD_{50} (oral, rat) ≥ 19,700 mg/kg bw; LC_{50} (inh, rabbit) > 300,000 mg/m3; LD_{50} (dermal, rabbit) > 2,000 mg/kg		NOAEL (blood) = 443 mg/kg (oral, cat, 94 d); NOAEC (body wt) = 1,000 mg/m3 (inh, rat, 90 d); dermal, rat = no tumor increases			multiple guinea pig studies indicate no sensitizing effects		not irritating (rabbit study)	not irritating (rabbit study)	LC_{50} (fish, 96h) > 10,000 mg/L; LC_{50} (*daphnia*, 96h) = 18,800 mg/L; EC_{50} (algae, 96h) = 19,000 mg/L	ChV (30 d) = 2,500 mg/L	readily biodegradable	BCF = 1.4		
Data from ToxServices assessment	UNEP 2001: Non-GLP compliant animal studies indicate no effect	UNEP 2001: Reported as negative for genotoxity	UNEP 2001: No evidence of reproductive toxicity in two generation animal study	UNEP 2001: No evidence of effect in four non-GLP compliant animal studies		UNEP 2001: Oral rat LD_{50} = 22,000 mg/kg; Oral mice LD_{50} = 24,900; Oral guinea pig LD_{50} = 19,700 mg/kg bw		UNEP 2001: No clear effects within the 10-100 mg/kg guidance values were identified in multiple tests.			UNEP 2001: Two non-GLP compliant human studies reported no sensitizing effects		UNEP 2001: Acute dermal irritation/corrosion animal study indicated not classifiable as skin irritant (GHS definition)	UNEP 2001: Acute eye irritation/corrosion animal study indicated not classifiable as eye irritant	UNEP 2001: LC_{50} values for multiple species range from 18,340 – 51,600 mg/L	UNEP 2001: Assumed to be low based on rapid biodegradability and BCF<500	UNEP 2001: While no studies following modern guidelines have been reported, the weight of evidence supports that this chemical is readily biodegradable	UNEP 2001: BCF = 1.4 (based on log Kow=-0.78)	UN 2011: Not expected to contain high energy bonds or oxidizing species which may cause reactivity	UNEP 2001: Classified as a GHS flammable liquid
Hazard Level	L	L	L	L	DG	L	M	L	M	DG	L	DG	L	L	L	L	M	vL	L	L

[§] REACH dossier data available at: http://apps.echa.europa.eu/registered/data/dossiers/DISS-9d9b1d87-f99a-6f9b-e044-00144f67d249/DISS-9d9b1d87-f99a-6f9b-e044-00144f67d249_DISS-9d9b1d87-f99a-6f9b-e044-00144f67d249.html

Benchmark = BM 3a,c [43]

[43] This benchmark level is based on the Moderate hazard score for persistence and Group II endpoints. This is a non-verified GreenScreen™ assessment and may not be used to make public promotional or product claims.

Proxel, CAS# 2634-33-5 (Ingredient 1: ≥10-20% 1,2-benzisothiazolin-3-one)

	Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
	C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
							Single	Repeated*	Single	Repeated*										
Data from Scientific Sources or MSDS						Oral (rat) LD_{50} = 1,020 mg/kg; Oral (mse) LD_{50} = 1,150 mg/kg bw; H302, Cat 4 Acute Toxic					at conc > 0.05%, Cat 1 Skin Sens, H317	occupational asthmagen observed in chemical worker [HazMap]	H315	H318	LC_{50} (trout, 96 h) = 2.18 mg/L; EC_{50} (*daphnia*, 48 h) = 2.94 mg/L; H400	ChV = 0.1 mg/L H410	t 1/2 D =15 (water); 30 (soil)	BCF = 3.2	NFPA = 0; Not explosive	NFPA = 0; FP > 100°C
Data from ToxServices Assessment		EC 2012, not mutagenic based on multiple studies	EC 2012, not likely to induce reproductive toxicity	EC 2012, EPA 2005, classified as GHS Category 2				EC 2012, multiple studies with LOAEL between 10 - 100		EC 2012, EPA 2005, multiple studies with no effects	EC 2012, studies used to classify as GHS Category 1A		EC 2012, rabbit study with skin irritation	EC 2012, rabbit study with severe irritation			EPA 2012, modeled data with half-life of 30 days			
Hazard Level	DG	L	L	L	DG	M	DG	M	DG	L	H	M	H	vH	vH	vH	H	vL	L	L

Benchmark = BM U

Ignoring Data Gaps, Benchmark = BM 2c,f [44]

[44] This benchmark level is based on the High hazard score for persistence + Moderate and High Group II and II* effects; and for very High acute and chronic ecotoxicity, and eye irritation. This is a non-verified GreenScreen™ assessment and may not be used to make public promotional or product claims.

Proxel, CAS# 1310-73-2 (Ingredient 2: ≥5-10% sodium hydroxide)

	Group I Human					Group II and II* Human								Ecotox		Fate		Phys.	
	C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
							Single	Repeated*	Single	Repeated*										
Data from Scientific Sources or MSDS													R35; H314	GHS Cat 1	LC_{50} (daphnia) = 40.38 mg/l 48 hr					
Data from REACH Dossier §	Long-term (41 yr) study indicates esophageal carcinoma after ingestion; one study indicates potential renal cancer risk with exposure to fumes						occ exposure (inh) caused irrev lung damage				Not sensitizing (human study)		Skin Corr 1A (≥2 - <5%); H314; erythema score = 4 (not rev)	Eye Damage 1; H318; conj score >2.5, cornea score >2 (not fully rev)	EC_{50} (fish) = 99 mg/l 48 hr; EC_{50} (*daphnia*) = 40.4 mg/L					
Data from ToxServices Assessment		OECD 2002: negative data in *in vitro* and *in vivo* mutagenicity/genotoxicity tests	OECD 2002: not expected to be systematically available in the body under normal use and handling conditions. Therefore, it will not reach the reproductive organs	OECD 2002: not expected to be systematically available in the body under normal use and handling conditions. Therefore, it will not reach the fetus		Oral rabbit LD_{50} = 325 mg/kg			Listed in Boyes as neurotoxicant. However NaOH is not expected to be systematically available in the body under normal use and handling conditions. Therefore, it will not reach the brain		OECD 2002: Due to the wide and historical use of NaOH with no known human cases of dermal sensitization being reported, NaOH is not considered to be a dermal sensitizer.		OECD 2002: *in vivo* and *in vitro* experiments demonstrate that NaOH is corrosive to skin	OECD 2002: Data from *in vivo* studies with concentrations up to 3.0% indicate that low levels of NaOH is irritating to eyes, and higher concentrations are likely severely irritating or corrosive to eyes.	EC 2000: LC_{50}s for various species range from 45.4 mg/L to 189 mg/L			EC 2000: Based on its high water solubility, NaOH is not expected to bioconcentrate in organisms.	GHS Category 1 chemical corrosive to metals	EC 2000: not flammable
Hazard Level	M[45]	L	L	L	DG	M	H	DG	L	DG	L	DG	vH	vH	M	DG	DG	L	M	L

§ REACH dossier information available at: http://apps.echa.europa.eu/registered/data/dossiers/DISS-9ea1ebb9-dbf1-0959-e044-00144f67d031/DISS-9ea1ebb9-dbf1-0959-e044-00144f67d031_DISS-9ea1ebb9-dbf1-0959-e044-00144f67d031.html

Benchmark = BM U

Ignoring Data Gaps, Benchmark = BM 2e,f [46]

[45] Low confidence in occupational exposure reports lowers hazard score from H to M.

[46] This benchmark level is based on the Moderate hazard score for carcinogenicity, High single exposure Systemic toxicity and very High hazard scores for skin and eye irritation. This is a non-verified GreenScreen™ assessment and may not be used to make public promotional or product claims.

Sorbitol (crystalline), CAS# 50-70-4 (70% mixture with water)

	Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
	C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
							Single	Repeated*	Single	Repeated*										
Data from Scientific Sources or MSDS		Numerous negative results (GeneTox, CCRIS)	Not on Prop 65 list			Oral LD50 15,900 mg/kg bw; Oral LD50 (mse) 17,800 mg/kg bw (MSDS)										ChV = 270,000 mg/L	Water = 2.3 Soil = 4.7[47]	BCF = 3.2	NFPA = 0; stable	NFPA = 0
Additional Scientific Sources			DART: 3 generation study indicates no reproductive effect	no adverse effects observed [HazMap]											Determined to not be toxic based on predicted EC_{50} (fish, *daphnia*, algae) ≥ 2,000 mg/L					
Hazard Level	DG	L	L	L	DG	L	DG	DG	DG	DG	DG	DG	DG	DG	L	L	L	vL	L	L

Benchmark = BM U

Ignoring Data Gaps, Benchmark = BM 4 [48]

[47] Based on PBT Profiler model, only water and soil persistence are relevant for this chemical.

[48] This benchmark level is based on the Low hazard score for endpoints with adequate data. This is a non-verified GreenScreen™ assessment and may not be used to make public promotional or product claims.

Base Detergent Compounds

Alcohols, C_{12-15}, ethoxylated, CAS# 68131-39-5

	Group I Human					Group II and II* Human								Ecotox		Fate		Physical	
	C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
							Single	Repeated*	Single	Repeated*										
Data from Scientific Sources or MSDS		Negative results for chromosomal and gene tests				Oral, rat, LD_{50} = 2,000 mg/kg							Mild skin irritant	H318	EC_{50} (*water flea*) = 0.37 – 0.43 mg/l; LC50 (*r. trout*) = 0.775-1.3 mg/l; H400	ChV = 0.007 mg/L	Water = 15; Soil = 30[49]	170	Not explosive	Flashpoint > 201°F
Data from REACH Dossier §		Ames study = negative; CHO aberration tests = negative	2 generation test (rat, dermal) NOAEL ≥ 250 mg/kg bw/d – no effects observed	2 generation test (rat, dermal) NOAEL ≥ 250 mg/kg bw/d – sporadic impact on maternal weight observed		LD_{50} (rat, oral) > 5,000 mg/kg bw; LC_{50} (rat,inh) >100 mg/m3; LD_{50} (rat, dermal) 2,000 mg/kg		NOAEL (rat, oral) ≥ 150 mg/kg bw/d			Guinea pig study indicates non-sensitizing		rabbit studies indicate non-irritating (max erythema and edema scores = 2.2 and 1.7, respectively)	rabbit study indicates max irr score (conjunctivae) = 0.7; H318	LC_{50} (fish, 96 hr) = 1.7 - 3.1 mg/L; EC_{50} (*daphnia*, 48 h) = 0.14 mg/L; EC_{50} (algae, 72 hr) = 0.75 mg/L	NOEC (fish, 30d) ≥ 0.28 mg/L; NOEC (*daphnia*, 21d) = 0.77 mg/L		readily biodegradable, but failing 10-day window		
Hazard Level	DG	L	L	M	DG	M	DG	L	DG	DG	L	DG	M	M[50]	vH	H[51]	L	L	L	L

§ REACH Dossier information available at: http://apps.echa.europa.eu/registered/data/dossiers/DISS-9ff36fdd-4412-2450-e044-00144f67d031/AGGR-babf4325-2d30-4ae3-b5db-533a2a571cca_DISS-9ff36fdd-4412-2450-e044-00144f67d031.html#L-20812ecf-0b85-4dd6-b00b-3e582363ab5a

Benchmark = BM U

Ignoring Data Gaps, Benchmark = BM 2e,f [52]

[49] This information is estimated based on a grouping of similar compounds. Sediment and air determined to be irrelevant media for assessment.

[50] With only one study available, and with hazard statement H318, assume at least a moderate hazard of eye irritation.

[51] Hazard score based on data rather than modeled estimates.

[52] This benchmark level is based on the Moderate developmental toxicity and very High acute aquatic toxicity scores. This is a non-verified GreenScreen™ assessment and may not be used to make public promotional or product claims.

Sodium laureth sulfate, CAS# 9004-82-4

	Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
	C	M	R	D	E	AT	ST Single	ST Repeated*	N Single	N Repeated*	SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
Data from Scientific Sources or MSDS	Long-term carcinogenicity studies did not indicate any potential of AES to induce tumours. [HERA 2003]	In all the *in vitro* and *in vivo* assays there was no indication of genetic toxicity of AES. [HERA 2003]	Substantial information is available on teratogenicity, embryotoxicity and toxicity to reproduction of AES. Taken all together, it can be concluded that AES is not cumulatively toxic to pregnant rats and did not reveal teratogenic, developmental or reproductive effects at the highest tested dose levels of >300 mg/kg body weight per day.[HERA 2003]			(Oral, rat) LD_{50}= 1,600 mg/kg; low acute dermal toxicity to rats. [HERA 2003]		NOEL (oral, rat) = 75 mg/kg bw/d (2 yr study) [HERA 2003]			AES are not considered to be skin sensitizers [HERA 2003]		H315; At concentrations between 10 and 30%, the AES solutions exhibit mild to moderate irritancy under the conditions of an occluded patch test. AES concentrations below 1% are virtually non-irritating under the conditions of the acute skin irritation testing protocol [HERA 2003]	Eye irritant, H318	Water flea, EC_{50} = 2.43-4.01 mg/L; The 24-96 h LC_{50} values for seven different fish species range between 0.39 mg/L to 450 mg/L; For *Daphnia magna*, the acute EC_{50} values range between 1 and 50 mg/L were reported for AES; For algae, typical EC_{50} values range from 4 to 65 mg/L.	ChV= 0.28 mg/L	Water=38d, Soil= 75d[53]	BCF = 71	Not explosive	Flashpoint: 25.6°C; H226
Data from REACH Dossier §														H319						
Hazard Level	L	L	L	L	DG	M	DG	M	DG	DG	L	DG	H	vH	H	H	H	vL	L	M

§ REACH Dossier information available at: http://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/cl-inventory/view-notification-summary/55818

Benchmark = U

Ignoring Data Gaps, Benchmark = BM 2c,f [54]

[53] These values estimated using PBT Profiler model for sodium lauryl ether sulfate. Air and Sediment determined to not be relevant media for this chemical.

[54] This benchmark level is based on the High hazard score for persistence, Moderate hazard score for acute toxicity and systemic toxicity, High hazard score for skin irritation and ecotoxicity, and very High hazard score for eye irritation. This is a non-verified GreenScreen™ assessment and may not be used to make public promotional or product claims.

Calcium Chloride, dihydrate, CAS# 10035-04-8

	Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
	C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
							Single	Repeated*	Single	Repeated*										
Data from Scientific Sources or MSDS		Mutagenic and tumerogenic effects in animals				LD_{50}= 20,500 mg/kg bw				CNS effects observed									Not explosive	Not flammable
Hazard Scores from ToxServices Assessment	DG	H	DG	DG	DG	DG	DG	DG	DG	DG	DG	DG	DG	DG	DG	DG	DG	DG	L	L
Hazard Level	DG	H	DG	DG	DG	L	DG	DG	DG	M	DG	DG	DG	DG	DG	DG	DG	DG	L	L

Benchmark = BM 1e [55]

[55] This benchmark level is based on the High hazard score for mutagenicity. This is a non-verified GreenScreen™ assessment and may not be used to make public promotional or product claims.

Sodium Citrate, anhydrous, CAS# 68-04-2

	Group I Human					Group II and II* Human								Ecotox		Fate		Physical	
	C	M	R	D	E	AT	ST Single	ST Repeated*	N Single	N Repeated*	SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
Data from Scientific Sources or MSDS						See footnote[56]: IV, LD_{50} = 170 IP, LD_{50} = 1,548 IP, LD_{50} = 1,364							Skin irritant	Eye irritant					Not explosive; NFPA = 0	Combustible; NFPA = 0
Data from REACH Dossier §		Neg Ames test; Neg chromosome aberration test (oral, rat)		Multiple animal studies (oral) for teratogenicity indicate no discernible effects		LD_{50} (oral, mse) = 5,400 mg/kg bw; LD_{50} (dermal, rat) > 2,000 mg/kg bw		NOAEL (oral, rat, 10 d) > 8,000 mg/kg bw/d			Guinea pig study, no sensitizing effects		Rabbit study, overall irritation score = 0.11, fully reversible	Rabbit study, conjunctivae score = 0.5, chemosis score = 0.7, both fully reversible	LC_{50} (fish, 24h) > 10 mg/L; EC_{50} (mussels, 48 hr) > 50 mg/L; EC_{50} (*daphnia*, 24 hr) = 1,525 mg/L		readily biodegradable (citric acid)	BCF = 3.2		
Data from ToxServices assessment	UNEP 2001 (citric acid[57]): no difference between control and experimental groups	CCRIS 2011: negative Ames test results	UNEP 2001: no effects observed (citric acid)			ESIS 2000: Oral rat LD_{50} = 6,500 - 12,100 mg/kg, Oral mouse LD_{50} = 5,000 – 7,100 mg/kg					ESIS 2000: not sensitizing to guinea pigs				ESIS 2000: L/EC_{50} > 5,600 mg/L (*daphnia*)		ESIS 2000: readily biodegradable (98% within 48 hr)			
Hazard Level	L	L	L	L	DG	L	DG	L	DG	DG	L	DG	L	L	M	DG	L	vL	L	M

§ REACH Dossier information available at: http://apps.echa.europa.eu/registered/data/dossiers/DISS-9d83210a-6ed4-5a31-e044-00144f67d249/DISS-9d83210a-6ed4-5a31-e044-00144f67d249_DISS-9d83210a-6ed4-5a31-e044-00144f67d249.html

Benchmark = BM U

Ignoring Data Gaps, Benchmark = BM 3b,d [58]

[56] These test data refer to non-oral routes of exposure: IV = intravenous, IP = intraparenteral. Neither of these experimental routes of exposure is used to determine hazard score for GreenScreen™ or for GHS.

[57] Citric acid (CAS # 77-92-9) is a transformation product of sodium citrate.

[58] This benchmark level is based on the Moderate hazard score for acute aquatic toxicity and flammability. This is a non-verified GreenScreen™ assessment and may not be used to make public promotional or product claims.

Water, CAS# 7732-18-5

	Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
	C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
							Single	Repeated*	Single	Repeated*										
Data from Scientific Sources or MSDS	Negative results	Negative results	Negative results			LD_{50} (oral rat) = 89,800 mg/kg											Naturally occurring inorganic compound		Stable inorganic compound	Non-flammable
Data from non-verified GreenScreen conducted by SciVera**	used as a negative control in many experimental studies	negative results in experimental studies	negative results in an experimental study	negative results in an experimental study	Experimental judgment (see footnote 59)	LD_{50} (oral, rat) = 89,800 mg/kg	Experimental judgment	Experimental judgment (see footnote 59)	Experimental judgment (see footnote 59)	Experimental judgment (see footnote 59)	Experimental judgment (see footnote 59)	Experimental judgment (see footnote 59)	Experimental judgment (see footnote 59)	Experimental judgment (see footnote 59)	Experimental judgment (see footnote 59)	Experimental judgment (see footnote 59)	Naturally occurring inorganic compound	Experimental judgment (see footnote 59)	Experimental judgment based on stability and lack of reactivity with most materials	Non-flammable
Hazard Level	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L	H	L	L	L

** Accessed at http://theic2.org/hazard-assessment

Ignoring Data Gaps, Benchmark = BM 4 [60]

[59] Low potential for effect based on physical properties and general evidence as an essential chemical for normal biological and physiological function.

[60] Because this is an inorganic compound, and because all other hazard endpoints are low, its persistent nature does not affect the overall benchmark score. This is a non-verified GreenScreen™ assessment and may not be used to make public promotional or product claims.

Appendix D Data Resources and References

Data Resources:

Common Chemical Name: MSDS

CAS No.: MSDS

Individual Chemical Listed on TURA: MA Toxics Use Reduction Act Chemical List for Reporting Year 2012 http://www.mass.gov/eea/docs/dep/toxics/approvals/chemlist.pdf

Chemical Name (Synonyms): MSDS; U.S. National Library of Medicine, ChemIDplus Advanced [ChemIDplus] or [CIDP], http://chem.sis.nlm.nih.gov/chemidplus/

Molecular Weight: U.S. National Library of Medicine, ChemIDplus Advanced [ChemIDplus] or [CIDP], http://chem.sis.nlm.nih.gov/chemidplus/

Viscosity: U.S. National Library of Medicine, Hazardous Substances Data Bank (HSDB), http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB; MSDS

Physical State at Room Temperature: MSDS

Vapor Pressure in mmHg at ~ 20°C: U.S. National Library of Medicine, Hazardous Substances Data Bank (HSDB), http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB; U.S. National Library of Medicine, HAZMAP, http://hazmap.nlm.nih.gov/index.php; MSDS

Persistence, Bioaccumulation, & Toxicity Data (PBT): U.S. Environmental Protection Agency's PBT Profiler**,** http://www.pbtprofiler.net/

International Agency for Research on Cancer (IARC): http://www.iarc.fr/

Neurotoxicity: REACH Registration database: http://echa.europa.eu/information-on-chemicals/registered-substances; U.S. National Library of Medicine, HAZMAP, http://hazmap.nlm.nih.gov/index.php

Other recognized health effects: Asthma – Association of Occupational and Environmental Clinics Database, http://www.aoecdata.org/ExpCodeLookup.aspx; The Endocrine Disruption Exchange (TEDX) List of Potential Endocrine Disruptors, http://endocrinedisruption.org/endocrine-disruption/tedx-list-of-potential-endocrine-disruptors/chemicalsearch; International Chemical Safety Cards [ICSC], www.expub.com ; U.S. National Library of Medicine, Hazardous Substances Data Bank (HSDB), http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB; Chemical Hazard and Alternatives Toolbox [ChemHAT], http://www.chemhat.org/; Registry of Toxic Effects of Chemical Substances [RTECS], www.expub.com; MSDS

Reproductive/Developmental Toxicity: CA Prop 65 List, http://www.oehha.ca.gov/prop65/prop65_list/files/041913P65list.pdf; Registry of Toxic Effects of

Chemical Substances [RTECS], www.expub.com; U.S. National Library of Medicine, HAZMAP, http://hazmap.nlm.nih.gov/index.php; Healthy Building Network [Pharos], http://www.pharosproject.net/; MSDS

Target Organs (CNS, Liver, Other): U.S. National Library of Medicine, HAZMAP, http://hazmap.nlm.nih.gov/index.php; National Institute for Occupational Safety and Health [NIOSH] Pocket Guide, http://www.cdc.gov/niosh/npg/

Acute Toxicity (LD_{50}, LC_{50}): U.S. National Library of Medicine, ChemIDplus Advanced [ChemIDplus] or [CIDP], http://chem.sis.nlm.nih.gov/chemidplus/; Registry of Toxic Effects of Chemical Substances [RTECS], www.expub.com; U.S. National Library of Medicine, Hazardous Substances Data Bank (HSDB), http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB; REACH Registration database: http://echa.europa.eu/information-on-chemicals/registered-substances; MSDS

Flash Point: U.S. National Library of Medicine, Hazardous Substances Data Bank (HSDB), http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB; MSDS

Reactivity: U.S. National Library of Medicine, Hazardous Substances Data Bank (HSDB), http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB; International Chemical Safety Cards [ICSC], www.expub.com; MSDS

Aquatic Toxicity: Chemical Hazard and Alternatives Toolbox [ChemHAT], http://www.chemhat.org/; ECOTOX, www.expub.com; U.S. National Library of Medicine, Hazardous Substances Data Bank (HSDB), http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB; MSDS

R-phrases and H-Statements: REACH Registration database: http://echa.europa.eu/information-on-chemicals/registered-substances; MSDS

H-Statements: EU Harmonized substance search: http://echa.europa.eu/web/guest/information-on-chemicals/cl-inventory-database; MSDS

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Appendix E: GreenScreen Hazard Scoring Criteria

	Information Type	Information Source	List Type		High (H)	Moderate (M)	Low (L)	
Carcinogenicity (C)	Data	GHS Criteria & Guidance			GHS Category 1A (Known) or 1B (Presumed) for any route of exposure	GHS Category 2 (Suspected) for any route of exposure or limited or marginal evidence of carcinogenicity in animals (See Guidance)	Adequate data available, and negative studies, no structural alerts, and GHS not classified.	
	A Lists	EPA-C (1986)	Authoritative		Group A, B1 or B2	Group C	Group E	
		EPA-C (1996, 1999, 2005)	Authoritative		Known or Likely		Not Likely	
		EU CMR (1)	Authoritative		Category 1 or 2	Category 3		
		EU CMR (2)	Authoritative		Carc 1A or 1B	Carc 2		
		EU H-statements	Authoritative		H350 or H350i	H351		
		EU R-phrases	Authoritative		R45 or R49	R40		
		EU SVHC	Authoritative		Reason for inclusion: Carcinogenic			
		GHS-[COUNTRY]* Lists (*Korea, Japan, Indonesia, Australia, Europe, New Zealand, and Taiwan)	Screening		Category 1A or 1B	Category 2	Not Classified	
		IARC	Authoritative		Group 1 or 2A	Group 2B	Group 4	
		MAK	Authoritative		Carcinogenic Group 1 or 2	Carcinogenic Group 3, 4, or 5		
		NIOSH-C	Authoritative		Occupational Cancer			
		NTP-RoC	Authoritative		Known or Reasonably Anticipated			
		Prop 65	Authoritative		Known to the state to cause cancer			
	B Lists	EPA-C(1986)	Authoritative		Group D			
		EPA-C (1999)	Authoritative		Suggestive Evidence, but not sufficient to assess human carcinogenic potential			
		EPA-C (2005)	Authoritative		Suggestive evidence of carcinogenic potential			
		IARC	Authoritative		Group 3			
Mutagenicity/Genotoxicity (M)	Information Type	Information Source	List Type		High (H)	Moderate (M)	Low (L)	
	Data	GHS Criteria & Guidance			GHS Category 1A (Known) or 1B (Presumed) for any route of exposure	GHS Category 2 (Suspected) for any route of exposure or limited or marginal evidence of mutagenicity in animals (See Guidance)	Adequate data available, and negative studies for both chromosomal aberrations and gene mutations, no structural alerts, and GHS not classified.	
	A Lists	EU CMR (1)	Authoritative		Category 1 or 2	Category 3		
		EU CMR (2)	Authoritative		Muta 1A or 1B	Muta 2		
		EU H-statements	Authoritative		H340	H341		
		EU R-phrases	Authoritative		R46	R68		
		EU SVHC	Authoritative		Reason for inclusion: Mutagenic			
		GHS-[COUNTRY]* Lists (*Korea, Japan, Indonesia, Australia, Europe, New Zealand, and Taiwan)	Screening		Category 1A or 1B	Category 2	Not Classified	
	B Lists	MAK	Authoritative		Germ Cell Mutagen 1, 2, or 3a			
		MAK	Authoritative		Germ Cell Mutagen 3b or 5			

	Information Type	Information Source	List Type		High (H)	Moderate (M)	Low (L)	
Reproductive Toxicity (R)	Data	GHS Criteria & Guidance *Note: GHS Reproductive Toxicity includes both reproductive and developmental effects, while the Green Screen separates them into two distinct hazard endpoints. This classification must be based on reproductive effects alone.*			GHS Category 1A (Known) or 1B (Presumed) for any route of exposure	GHS Category 2 (Suspected) for any route of exposure or limited or marginal evidence of reproductive toxicity in animals (See Guidance)	Adequate data available, and negative, no structural alerts, and GHS not classified.	
	A Lists	EU H-statements	Authoritative		H360F, H360FD, H360Fd	H360Df, H361f, H361fd		
		EU R-phrases	Authoritative		R60	R62		
		GHS-[COUNTRY]* Lists (*Korea, Japan, Indonesia, Australia, Europe, New Zealand, and Taiwan)	Screening		Category 1A (Known); Category 1B (Presumed)	Category 2 (Suspected)	Not Classified (i.e. positively determined to be negative)	
		NTP-OHAaT	Authoritative		Clear Evidence of Adverse Effects - Reproductive		Clear Evidence of No Adverse Effects - Reproductive	
		Prop 65	Authoritative		Known to the state to cause reproductive effects-Male or Female			
	B Lists	NTP-OHAaT	Authoritative		Limited Evidence of Adverse Effects - Reproductive or Some Evidence of Adverse Effects - Reproductive			
						Limited Evidence of No Adverse Effects - Reproductive or Some Evidence of No Adverse Effects - Reproductive		
					Insufficient Evidence for a Conclusion - Reproductive Toxicity			
	Information Type	Information Source	List Type		High (H)	Moderate (M)	Low (L)	
Developmental Toxicity (D)	Data	GHS Criteria & Guidance *Note: GHS Reproductive Toxicity includes both reproductive and developmental effects, while the Green Screen separates them into two distinct hazard endpoints. This classification must be based on developmental effects alone.*			GHS Category 1A (Known) or 1B (Presumed) for any route of exposure	GHS Category 2 (Suspected) for any route of exposure or limited or marginal evidence of developmental toxicity in animals (See Guidance)	Adequate data available, and negative, no structural alerts, and GHS not classified.	
	A Lists	EU H-statements	Authoritative		H360FD, H360D, H360Df, or H362	H360Fd, H361d, H361fd		
		EU R-phrases	Authoritative		R61 or R64	R63		
		GHS-[COUNTRY]* Lists (*Korea, Japan, Indonesia, Australia, Europe, New Zealand, and Taiwan)	Screening		Category 1A or 1B	Category 2	Not Classified	
		NTP-OHAaT	Authoritative		Clear Evidence of Adverse Effects - Developmental		Clear Evidence of No Adverse Effects - Developmental	
		Prop 65	Authoritative		Known to the state to cause developmental effects			
	B Lists	G&L	Screening		Developmental Neurotoxicant			
		Boyes-N	Screening		Developmental Neurotoxicity Effects			
		MAK	Authoritative		Pregnancy Risk Group A or B			
						Pregnancy Risk Group C		
					Pregnancy Risk Group D			
		NTP-OHAaT	Authoritative		Limited Evidence of Adverse Effects - Developmental or Some Evidence of Adverse Effects - Developmental			
						Limited Evidence of No Adverse Effects - Reproductive or Some Evidence of No Adverse Effects - Developmental		
					Insufficient Evidence for a Conclusion - Developmental Toxicity			
	Information Type	Information Source	List Type		High (H)	Moderate (M)	Low (L)	
Endocrine Activity (E)	Data	All Available Data			Evidence of endocrine activity and related human health effect.	Evidence of endocrine activity.	Adequate data available, and negative studies, and no structural alerts.	
	A Lists	EU ED	Screening				Category 3a	
		EU SVHC	Authoritative		Reason for Inclusion: Endocrine Activity			
	B Lists	EU ED	Screening		Category 1 or 2			
					Category 3b			
		OSPAR	Screening		Endocrine Disruptor			
		SIN	Screening		Reason for Inclusion: Endocrine Disruptor			
		TEDX	Screening		Listed on the TEDX List of Potential Endocrine Disruptors			

Acute Mammalian Toxicity (AT)

Information Type	Information Source	List Type	Very High (vH)	High (H)	Moderate (M)	Low (L)
Data	GHS Criteria & Guidance		GHS Category 1 or 2 for any route of exposure	GHS Category 3 for any route of exposure	GHS Category 4 for any route of exposure	GHS Category 5 or adequate data available, and negative studies, no structural alerts, and GHS not classified.
Guidance Values for Animal Data (see GHS for further information)	Oral LD_{50} (mg/kg)		≤50	>50-300	>300 - 2000	>2000
	Dermal LD_{50} (mg/kg)		≤200	>200-1000	>1000 - 2000	>2000
	Inhalation-Gas or Vapor LC_{50}(mg/L)		≤2	>2-10	>10 - 20	>20
	Inhalation-Dust/Mist/Fumes LC_{50} (mg/L)		≤0.5	>0.5-1.0	>1 - 5	>5
A Lists	DOT	Authoritative	Class 2.3 Group A, or Class 6.1 Group 1 or Group 2	Class 6.1 Group 3		
	EU H-statements	Authoritative	H300, H310, or H330	H301, H311, or H331	H302, H312, or H332	
	EU R-phrases	Authoritative	R26, R27 or R28			
	GHS-[COUNTRY]* Lists (*Korea, Japan, Indonesia, Australia, Europe, New Zealand, and Taiwan)	Screening	Category 1 and 2	Category 3	Category 4	Category 5 and "Not Classified"
B Lists	DOT	Authoritative	Class 2.3 Group B			
				Class 2.3 Group C		
						Class 2.3 Group D
	EPA-AMT	Authoritative	Extremely Hazardous Substance			
	EU R-phrases	Authoritative		R20, R21, or R22		
			R23, R24, or R25			
	WHMIS	Screening	D1A Toxic			
			D1B Toxic			

Systemic Toxicity/Organ Effects (ST)

Single Exposure

Information Type	Information Source	List Type	Very High (vH)	High (H)	Moderate (M)	Low (L)
Data	GHS Criteria & Guidance		GHS Category 1 Single Exposure for any route of exposure	GHS Category 2 Single Exposure for any route of exposure	GHS Category 3 Single Exposure for any route of exposure	Adequate data available, and negative studies, no structural alerts, and GHS not classified
GHS Guidance Values for Animal Data (see GHS for further information)	Oral (mg/kg-bw)		≤300	>300-2000		
	Dermal (mg/kg-bw)		≤1000	>1000-2000		
	Inhalation-Gas or Vapor (mg/L/4h)		≤10	>10-20		
	Inhalation-Dust/Mist/Fumes (mg/L/4h)		≤1.0	>1.0-5.0		
A Lists	EU H-statements	Authoritative	H370	H371	H335	
	EU R-phrases	Authoritative	R39, R39/23, R39/24, or R39/25, R39/26, R39/27, R39/28	R68/20, R68/21, or R68/22,	R37	
	GHS-[COUNTRY]* Lists (*Korea, Japan, Indonesia, Australia, Europe, New Zealand, and Taiwan)	Screening	Category 1	Category 2	Category 3	"Not Classified"

Repeated* Exposure

Information Type	Information Source	List Type	Very High (vH)	High (H)	Moderate (M)	Low (L)
Data	GHS Criteria & Guidance			GHS Category 1 Repeated Exposure for any route of exposure	GHS Category 2 Repeated Exposure for any route of exposure	Adequate data available, and negative studies, no structural alerts, and GHS not classified
GHS Guidance Values for Animal Data (see GHS for further information)	Oral (mg/kg-bw/day)			≤10	>10-100	>100
	Dermal (mg/kg-bw/day)			≤20	>20-200	>200
	Inhalation-Gas or Vapor (mg/L/6h/day)			≤0.2	>0.2-1.0	>1.0
	Inhalation-Dust/Mist/Fumes (mg/L/6h/day)			≤0.02	>0.02-0.2	>0.2
A Lists	EU H-statements	Authoritative		H372	H373	
	EU R-phrases	Authoritative		R48/23, R48/24, R48/25	R48/20, R48/21, R48/22	
	GHS-[COUNTRY]* Lists (*Korea, Japan, Indonesia, Australia, Europe, New Zealand, and Taiwan)	Screening		Category 1	Category 2	"Not Classified"
B Lists	EU R-phrases	Authoritative		R48 "Danger of serious damage to health by prolonged exposure"		

		Information Type	Information Source	List Type	Very High (vH)	High (H)	Moderate (M)	Low (L)
Neurotoxicity (N)	Single Exposure	Data	GHS Criteria Systemic Toxicity/Organ Effects using USEPA Risk Assessment Guidance to define applicable neurotoxic effects.		GHS Category 1 Single Exposure for any route of exposure	GHS Category 2 Single Exposure for any route of exposure	GHS Category 3 Single Exposure for any route of exposure	Adequate data available, and negative studies, no structural alerts, and GHS not classified
		A-Lists	GHS-[COUNTRY]* Lists (*Korea, Japan, Indonesia, Australia, Europe, New Zealand, and Taiwan)	Screening	Category 1	Category 2	Category 3	"Not Classified"
	Repeated*	Data	GHS Criteria Systemic Toxicity/Organ Effects using USEPA Risk Assessment Guidance to define applicable neurotoxic effects.			GHS Category 1 Repeated Exposure for any route of exposure	GHS Category 2 Repeated Exposure for any route of exposure	Adequate data available, and negative studies, no structural alerts, and GHS not classified
		A Lists	GHS-[COUNTRY]* Lists (*Korea, Japan, Indonesia, Australia, Europe, New Zealand, and Taiwan)	Screening		Category 1	Category 2	"Not Classified"
	Both	B Lists	EU H-statements	Authoritative			H336	
			EU R-phrases	Authoritative			R67	
			Boyes-N	Screening	Listed for Neurotoxic Effects			
			G&L	Screening	Neurotoxicant			
Skin Sensitization		Data	GHS Criteria & Guidance			GHS Category 1A (high frequency of occurrence)	GHS Category 1B (low to moderate frequency of occurrence)	Adequate data available, and negative studies, no structural alerts, and GHS not classified.
		A Lists	GHS-[COUNTRY]* Lists (*Korea, Japan, Indonesia, Australia, Europe, New Zealand, and Taiwan)	Screening		Category 1A	Category 1B	"Not Classified"
			MAK	Authoritative		Sensitizing Substances Sh (Skin) or Sah (Respiratory and Skin)		
		B Lists	EU H-statements	Authoritative		H317		
			EU R-phrases	Authoritative		R43		
Respiratory Sensitization (SnR*)		Information Type	Information Source			High (H)	Moderate (M)	Low (L)
		Data	GHS Criteria & Guidance			GHS Category 1A (high frequency of occurrence)	GHS Category 1B (low to moderate frequency of occurrence)	Adequate data available, and negative studies, no structural alerts, and GHS not classified.
		A Lists	GHS-[COUNTRY]* Lists (*Korea, Japan, Indonesia, Australia, Europe, New Zealand, and Taiwan)	Screening		Category 1A	Category 1B	"Not Classified"
			MAK	Authoritative		Sensitizing Substances Sa (Respiratory) or Sah (Respiratory and Skin)		
		B Lists	AOEC	Authoritative		Asthmagen (G)		
						Asthmagen (Rr) and/ or (Rs) and/or (Rrs)		
			EU H-statements	Authoritative		H334		
			EU R-phrases	Authoritative		R42		
Skin Irritation (IrS)		Information Type	Information Source		Very High (vH)	High (H)	Moderate (M)	Low (L)
		Data	GHS Criteria & Guidance		GHS Category 1 (Corrosive)	GHS Category 2 (Irritant)	GHS Category 3 (Mild irritant)	Adequate data available, and negative studies, no structural alerts, and GHS not classified.
		A Lists	DOT	Authoritative		Class 8		
			EU H-statements	Authoritative	H314	H315		
			EU R-phrases	Authoritative	R34 or R35	R38		
			GHS-[COUNTRY]* Lists (*Korea, Japan, Indonesia, Australia, Europe, New Zealand, and Taiwan)	Screening	Category 1	Category 2	Category 3	"Not Classified"
Eye Irritation (IrE)		Information Type	Information Source		Very High (vH)	High (H)	Moderate (M)	Low (L)
		Data	GHS Criteria & Guidance		GHS Category 1 (Irreversible)	GHS Category 2A (Irritating)	GHS Category 2B (Mildly irritating)	Adequate data available, and negative studies, no structural alerts, and GHS not classified.
		A Lists	EU H-statements	Authoritative	H318	H319	H320	
			EU R-phrases	Authoritative	R41			
			GHS-[COUNTRY]* Lists (*Korea, Japan, Indonesia, Australia, Europe, New Zealand, and Taiwan)	Screening	Category 1	Category 2A	Category 2B	"Not Classified"
		B Lists	EU R-phrases	Authoritative		R36		

	Information Type	Measurement		Very High (vH)	High (H)	Moderate (M)	Low (L)	
Acute Aquatic Toxicity (AA)	Data	GHS Criteria & Guidance		GHS Category 1	GHS Category 2	GHS Category 3	Sufficient data available and not classified	
	Guidance Values (see GHS for further information)	LC_{50} or EC_{50} (mg/L)		≤1	>1 to 10	> 10 to 100	>100	
	A Lists	DSL	Screening	*iT non-human* *Note: Could be based on acute or chronic aquatic toxicity. Only assess here if the classification is based on acute aquatic toxicity.*				
		EU H-statements	Authoritative	H400				
		EU R-phrases	Authoritative	R50	R51/53	R52/53		
		GHS-[COUNTRY]* Lists (*Korea, Japan, Indonesia, Australia, Europe, New Zealand, and Taiwan)	Screening	Category 1	Category 2	Category 3	"Not Classified"	
	B Lists	EU R-phrases	Authoritative		R51 or R52			
	Information Type	**Measurement**		**Very High (vH)**	**High (H)**	**Moderate (M)**	**Low (L)**	
Chronic Aquatic Toxicity (CA)	Data	GHS Criteria & Guidance				GHS Category 4		
		Guidance Value (mg/L)		≤0.1	>0.1 to 1.0	> 1.0 to 10	>10	
	A Lists	DSL	Screening	*iT non-human* *Note: Could be based on acute or chronic aquatic toxicity. Only assess here if the classification is based on chronic aquatic toxicity.*				
		EU H-statements	Authoritative			H413		
		EU R-phrases	Authoritative			R53		
		GHS-[COUNTRY]* Lists (*Korea, Japan, Indonesia, Australia, Europe, New Zealand, and Taiwan)	Screening			Category 4		
	B Lists	DSL	Screening	iT non-human *Note: Could be based on acute or chronic aquatic toxicity. Only assess here if the classification is based on chronic aquatic toxicity.*				
	Information Type	**Media & Measurement**	**List Type**	**Very High (vH)**	**High (H)**	**Moderate (M)**	**Low (L)**	**Very Low (vL)**
Persistence (P)	Data	**Soil or Sediment**		>180 or recalcitrant	>60 to 180	16 to 60	< 16 OR GHS "Rapid degradability"	Meets 10-day window in "Ready Biodegradation Test"
		(1/2 life in days OR Result)						
		Water		> 60 or recalcitrant	> 40 to 60	16 to 40	< 16 OR GHS "Rapid degradability"	Meets 10-day window in "Ready Biodegradation Test"
		(1/2 life in days OR Result)						
		Air		> 5 or recalcitrant	>2 to 5		< 2	
		(1/2 life in days OR Result)						
		Long-Range Environmental Transport			Evidence	Suggestive Evidence		
	B Lists	DSL	Screening	Persistent (P)				
	Information Type	**Measurement**		**Very High (vH)**	**High (H)**	**Moderate (M)**	**Low (L)**	**Very Low (vL)**
Bioaccumulation Potential (B)	Data	**BAF** (Bioaccumulation Factor)		> 5000	> 1000 to 5000	> 500 to 1000	> 100 to 500	≤ 100
		BCF (Bioconcentration Factor)		> 5000	> 1000 to 5000	> 500 to 1000	> 100 to 500	≤ 100
		Log Kow *(Log octanol-water partition coefficient)*		> 5.0	> 4.5 to 5.0	> 4.0 to 4.5		≤ 4
		Monitoring Data *(Presence in humans or wildlife)*			Evidence	Suggestive Evidence		
	A Lists	DSL	Screening	*Bioaccumulative (B)*				

	Information Type	Measurement	List Type	Very High (vH)	High (H)	Moderate (M)	Low (L)	
Reactivity (Rx)	Data - GHS Criteria & Guidance	Explosives		GHS Unstable	GHS Division 1.1, 1.2, or 1.3	GHS Division 1.4 or 1.5	Division 1.6 or Adequate data available and GHS not Classified	
		Self-reactive Substances		GHS Type A or B	GHS Type C or D	GHS Type E or F	Type G or Adequate data available and GHS not Classified	
		Substances which on contact with water emit flammable gases		GHS Category 1	GHS Category 2	GHS Category 3	Adequate data available and GHS not Classified	
		Oxidizing Gases			GHS Category 1		Adequate data available and GHS not Classified	
		Oxidizing Liquids and Solids		GHS Category 1	GHS Category 2	GHS Category 3	Adequate data available and GHS not Classified	
		Organic Peroxides		GHS Type A or B	GHS Type C or D	GHS Type E or F	Type G or Adequate data available and GHS not Classified	
		Self-heating Substances			GHS Category 1	GHS Category 2	Adequate data available and GHS not Classified	
		Substances Corrosive to Metal				GHS Category 1	Adequate data available and GHS not Classified	
	A Lists	DOT	Authoritative		Class 1 Group 1.1, 1.2, or 1.3	Class 1 Group 1.4, 1.5, or 1.6		
					Class 4.2 Group 2	Class 4.2 Group 3		
				Class 4.3 Group 1	Class 4.3 Group 2	Class 4.3 Group 3		
				Class 5.1 Group 1	Class 5.1 Group 2	Class 5.1 Group 3		
				Class 5.2 Type B	Class 5.2 Type C or D	Class 5.2 Type E or F	Class 5.2 Type G	
		EU H-statements	Authoritative	H200, H240, H241, H260, H271	H201, H202, H203, H251, H270	H204, H205, H252, H290		
		EU R-phrases	*Authoritative*	R09				
	B Lists	DOT	Authoritative	Class 4.1, Class 5.2 Type A				
		EU H-statements	Authoritative		H261, H272			
				H242				
		EU R-phrases	Authoritative	R01, R06, R07, R15				
				R02, R04, R05, R08, R14, R16, R19, R44				
		WHMIS	Screening	B6, C, or F				
	Information Type	Measurement		Very High (vH)	High (H)	Moderate (M)	Low (L)	
Flammability (F)	Data - GHS Criteria & Guidance	Flammable Liquid		GHS Category 1	GHS Category 2	GHS Category 3 or 4	Adequate data available and GHS not Classified	
		Flammable Gases (including chemically unstable gases)			GHS Category 1	GHS Category 2 or GHS Category A	GHS Category B or Adequate data available and GHS not Classified	
		Flammable Solids			GHS Category 1	GHS Category 2	Adequate data available and GHS not Classified	
		Aerosols			GHS Category 1	GHS Category 2	GHS Category 3 or Adequate data available and GHS not Classified	
		Pyrophoric Liquids			GHS Category 1		Adequate data available and GHS not Classified	
		Pyrophoric Solids			GHS Category 1		Adequate data available and GHS not Classified	
	A Lists	DOT	Authoritative	Class 3 Group 1	Class 3 Group 2 or Class 4.2 Group 1	Class 3 Group 3		
		EU H-statements	Authoritative	H224	H220, H222, H225, H250	H221, H223, H226, H227, H230		
		EU R-phrases	Authoritative		R17			
		WHMIS	Screening		B1	B3		
	B Lists	DOT	Authoritative		Class 2.1			
		EU H-statements	Authoritative		H228			
		EU R-phrases	Authoritative	R10 (Gas or Solid), R11 (Solid)				
				R10 (Liquid only)				
				R11 (Liquid only)				
					R12 (Gas only)			
		WHMIS	Authoritative		B4 or B5			
				B2				