I. ABSTRACT

This project was undertaken to investigate the utility and practical application of the HPV data set and HPVIS as a component of or data source for CleanGredients™, an online database of cleaning product ingredients. We assessed HPVIS as a tool to generate data for the CleanGredients™ surfactants module. As a first step, we screened the HPV data set for surfactant-type chemicals. The list of 1387 chemicals was downloaded from HPV Tracker, and each chemical was given a "use class" designation (solvent, surfactant, intermediate, etc.). The data for each of the 130 surfactants identified was evaluated for biodegradation data. Due to an absence of data, insufficient or conflicting data, and data indicating less than 60% mineralization in 28 days, only 17 surfactants listed on HPV qualified for listing on CleanGredients™ based on biodegradation data requirements. Of the 17 surfactants with sufficient biodegradation data, four were eliminated due to a lack of aquatic toxicity data, and four others were excluded due to uncertainty with respect to the degree of branching in the tested chemical (as identified by CAS number). In the end, we identified nine surfactants in HPVIS that are eligible for listing on CleanGredients™. In general, we found the browse tool to be the most useful means of searching HPVIS. We also concluded that HPV Tracker is a simpler means of downloading the entire list of HPV chemicals than extracting this data from HPVIS. Unfortunately, a combination of data gaps and usability shortcomings compromise the utility of the system in several respects. HPVIS still has some way to go before it is likely to be widely regarded as particularly useful and user-friendly.

II. BACKGROUND

Chemicals found in formulated products, particularly cleaning products, have a wide spectrum of negative impacts on the environment and human health. Each year, tons of toxic chemicals found in cleaning products pollute the air, water, and soil through their release either during or after use.[1] These chemicals compromise environmental systems at a range of scales, from individual organisms to regional biota. Negative impacts on people are equally severe. For example, workers in the cleaning services industry experience relatively high rates of injury, many of which are due to the toxicity of the chemicals found in cleaning products—particularly floor and carpet-maintenance products, disinfectants, and specialty cleaners. These chemicals can cause headaches, asthma, burns, permanent eye damage, major organ damage, and even cancer.[2] Occupants of buildings cleaned with such products may also be at risk.

As awareness and demand grow for improved cleaning products, formulators are increasingly seeking sources of ingredients to enable their products to succeed in the marketplace, meet government regulations, and qualify for eco-label certification. Currently, however, reliable and scientifically credible information on the human and environmental health attributes of appropriate chemical alternatives is difficult, costly, and time-consuming to locate. For many formulators, even knowing what information is relevant (let alone collecting it) presents a significant hurdle.

III. WHAT IS CLEANGREDIENTS™?

CleanGredients™ is an online database of institutional and industrial (I&I) cleaning product ingredients that is intended to bridge this information gap. It is designed to help formulators

[1] http://www.wrppn.org/Janitorial/jp4.cfm
[2] Lehman, D. Mar 2000. Health Facilities Mgt Magazine: 'Implementing Environmentally Friendly Cleaning Practices'

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identify ingredients that have potential environmental and/or human health and safety benefits and to help manufacturers and producers of cleaning product ingredients showcase their ingredients with potential environmental and/or human health and safety benefits. CleanGredients™ presents reliable, technical, ingredient-specific information on standard physical and chemical properties plus relevant environmental and human health attributes, thereby aligning broad environmental and human health goals with the cleaning product industry's business objectives. CleanGredients™ supports formulation of high-quality cleaning products, whether to meet internal corporate objectives, regulations, voluntary product recognition programs, or national and international eco-labels.

The mission of CleanGredients™ is to:

- provide suppliers a showcase for their innovate chemical ingredients;
- facilitate formulators' selection of ingredients for environmentally preferable product formulation;
- align environmental, human health, and business goals;
- support voluntary and regulatory compliance initiatives;
- make chemical ingredient information broadly available; and
- support the movement of green chemistry into commerce.

CleanGredients™ is organized by ingredient class (surfactants, solvents,…), allows users to search by chemical/physical properties (charge class, pH,…) or CAS number, and offers accurate scientific information facilitating smart design decisions. At present, only the surfactants module has been completed; modules for solvents and chelators/builders are being developed, with more to follow. CleanGredients™ contains human and environmental health, safety, and sustainability-related information on both proprietary ingredient formulations and commodity chemicals, all of which are useful to formulators.

The attributes for each ingredient class are selected by an expert stakeholder committee through a consensus process, in order to provide a rational and science-based framework to promote the understanding and application of proactive and precautionary design principles. The committee prioritizes attributes using a tier structure: For each chemical entered into the database, the key human health and environmental attribute data (Tier 1 data) must be reviewed by an independent, qualified third party. In the case of surfactants, this includes full product formulation (component) information and data for acute aquatic toxicity and biodegradability. All surfactants and components of surfactant preparations listed in CleanGredients™ must be ultimately biodegradable (i.e., pass the threshold level of 60% mineralization in the prescribed test in 28 days) without degradation products of concern.

CleanGredients™ is a project of the Green Blue Institute (GreenBlue), a non-profit, 501(c)(3) tax-exempt organization. Our mission is to stimulate the creative redesign of industry by focusing the expertise of professional communities to create practical solutions, resources, and opportunities for implementing sustainability.

IV. PURPOSE/SCOPE OF THIS HPVIS PROJECT

The purpose of this project was to investigate the utility and practical application of the HPV data set and HPVIS as a component of or data source for CleanGredients™. In carrying out this project, this purpose was addressed by seeking to answer several questions:

- How can HPV data be incorporated into tools, like CleanGredients™, designed to facilitate decision-making processes to advance green chemistry as a component of product design?
- How accessible is the data in HPVIS, and how easy is it to find and extract specific subsets of the data?
- How many of the chemicals listed in HPVIS are relevant to the formulation of industrial and institutional cleaning products (e.g., surfactants)?

III. PROJECT METHODOLOGY

In this project HPVIS was assessed as a tool to generate data for the CleanGredients™ surfactants database. In order for a surfactant to be listed on CleanGredients™, the chemical must meet three requirements:

1. It must have test data on ultimate biodegradability
2. It must have test data or modeled data on at least one species for acute aquatic toxicity.
3. It must be at least ultimately biodegradable (>60% mineralization in 28d).

Screen HPVIS for Surfactants

We began by screening the HPVIS database for surfactant-type chemicals. The entire list of chemicals was downloaded from HPV Tracker (found at www.environmentaldefense.org/documents/2724_HPVTracker.xls), as this is not a convenient function directly from HPVIS (i.e., as far as we could determine, HPVIS does not possess the functionality needed to pull a complete list of HPV chemicals from HPVIS at once, and, in any case, HPVIS comprises only a subset of the HPV chemicals). The 1387 chemicals were each given a "use class" designation (solvent, surfactant, intermediate, etc.), based on the descriptions in the HPV test plans submitted by each sponsor company. This was a labor-intensive process in which we opened each test plan and read until we found the described use and could assign each chemical to a unique use class. Making these use class designations consequently involved some amount of interpretation and was not simply a matter of querying HPVIS. In cases of chemicals that span two or more use classes, we selected the most common use, as described in the test plan, or, if this was not clear, the use most relevant to CleanGredients™ (e.g., if a chemical was listed as both an intermediate and a solvent, we assigned it to the solvent use class). In many cases we were unable to assign use classes to chemicals because their test plans have not yet been added to HPVIS or to HPV (*http://cfpub.epa.gov/hpv-s/*). The results of this screen are presented in Table 1 below. The resulting 130 surfactants were then singled out for further review.

Table 1: Relevant HPV use categories for CleanGredients™

Use class	Number of chemicals
Antioxidant	14
Bleach Activator	1
Chelator	1
Coalescent	3
Dye	12
Emulsifier	7
Flavor additive	14
Fragrance	71
Optical brightener	7
Oxygen scavenger	1

Use class	Number of chemicals
Pesticide/pesticide additive	4
pH Adjustor	6
Plasticizer	32
Preservative	7
Propellant	2
Solvent	126
Surfactant	**130**
UV absorber	4
Wax	8
Other *	937
Total	**1387**

* Includes categories not relevant to CleanGredients™ and chemicals not yet listed in HPVIS.

Screen Surfactants for Biodegradation Data

The data set for each surfactant was evaluated for biodegradation data. As stated above, in order to be eligible for listing in CleanGredients™, surfactants must have relevant ultimate biodegradation test data and have data demonstrating that the chemical is at least 60% degraded in 28 days. Modeled data and data based on analog chemicals in the same chemical class ("read across" data) were not acceptable to fulfill this data requirement. Due to an absence of data (79 chemicals), insufficient data or conflicting data (13 chemicals), and data indicating less than 60% mineralization in 28 days (21 chemicals), only 17 surfactants listed on HPV would qualify to be listed on CleanGredients™ based on biodegradation data requirements.

Screen Surfactants for Aquatic Toxicity Data

The list of eligible surfactants was further pared down due to lack of aquatic toxicity data. To meet the data requirements of CleanGredients™, the chemical must have at least one data point for acute aquatic toxicity. Unlike biodegradability data, modeled test data for aquatic toxicity is acceptable to fulfill this requirement. Data on analogs ("read across" data) were not accepted to fulfill the data requirement. Of the 17 surfactants with sufficient biodegradation data, four were eliminated due to a lack of aquatic toxicity data. One surfactant chemical without aquatic toxicity data in HPVIS was nevertheless deemed eligible for listing in CleanGredients™ by supplementing the HPVIS data with aquatic toxicity data that was modeled for this chemical in a previous project.

Additional Screening

Finally, the list of eligible surfactants was screened further to exclude those characterized by a lack of clarity with respect to its chemical structure. For example, in one case the CAS number was nonspecific with respect to linear vs. branched structure (68526-83-0). Four surfactants were excluded due to uncertainty with respect to the degree of branching in the tested chemical.

Final Results

After all considerations, nine chemicals were found to be eligible for listing on CleanGredients™ with confidence. These surfactants are listed in Table 2. Other chemicals may be added after further research is done to support the data found in HPVIS.

Table 2: HPV Chemicals Listed in CleanGredients™.

CAS No.	Chemical Name	Biodeg Status	Aq Tox: Fish	Aq Tox: Daphnia	Aq Tox: Algae	Pass DfE Screen	Meets Clean-Gredients listing reqmts
1338392	Sorbitan, monolaurate	Ultimate (>60% in 28d)	75mg/L	No data	No data	Yes	Yes
1338438	Sorbitan, monooleate	Ultimate (>60% in 28d)	>1000mg/L	No data	No data	Yes	Yes
112696	Hexadecylamine, N,N-dimethyl-	At least ultimate (>60% in 28d)	0.1mg/L	Not toxic at saturation (est.)	Not toxic at saturation (est.)	Yes	Yes
124221	1-Dodecanamine	Ready (>60% in 28d) *	0.42mg/L	0.09mg/L (est.)	0.45mg/L (est.)	Yes	Yes
61788918	Amines, dimethylsoya alkyl	Ultimate (>60% in 28d)	0.1mg/L	No data	No data	No	Yes
61791319	Ethanol, 2,2'-iminobis-, N-coco alkyl derivs.	Ultimate (>60% in 28d)	0.47mg/L	0.38mg/L	No data	No	Yes
120401	Dodecanamide, N,N-bis(2-hydroxyethyl)-	Ready (>60% in 10d)*	No data** 6.2mg/L (SAR)	No data** 1.2mg/L (SAR)	No data** 1.2mg/L (SAR)	Yes	Yes
68603429	Amides, coco, N,N-bis(hydroxyethyl)	Ready (>60% in 14d, 84% in 28d)	6.7mg/L	2.15mg/L	No data	Yes	Yes
68584225	Benzenesulfonic acid, C10-16-alkyl derivs.	At least ultimately (>60% in 28d)	5.6 mg/L	2.9mg/L	14mg/L	No	Yes

* Data supported by data from the literature.
** This chemical was included because the aquatic toxicity data (missing from HPVIS) was generated using structure-activity relationship (SAR) modeling as part of an earlier project.

V. OBSERVATIONS AND RECOMMENDATIONS: USER INTERFACE

We found the HPVIS database to be very useful for viewing the biodegradation or aquatic toxicity test results for an entire chemical category at once. Both the browse tool's tab view (Figure 1) and the matrix report view (Figure 2) were useful in scanning all chemicals in a category. In contrast, we found that special reports generated with the query tool are not user-friendly. For example, neither the search term "amine" nor "nitrogen" for the submission name returned any results (Figure 3). The endpoint results report tool was not used in this project.

Figure 1: Tabular view of biodegradation studies for Fatty Nitrogen Derived Amines category.

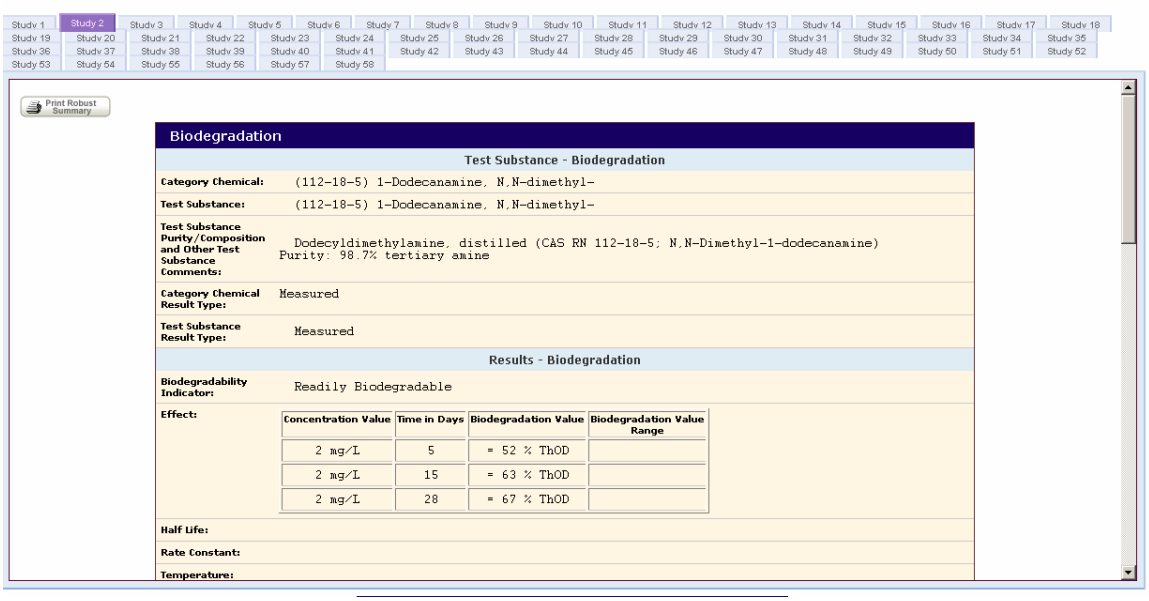


Figure 2: Matrix view of aquatic toxicity studies for linear alkyl benzene sulfonic acids category.

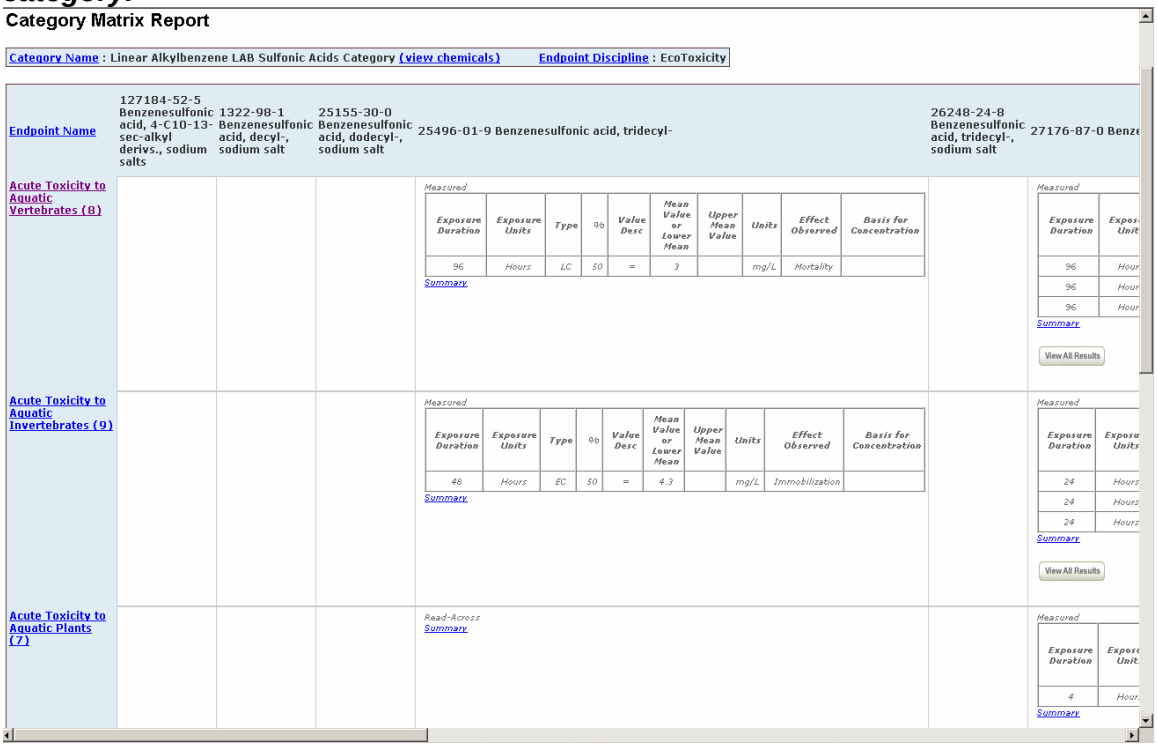
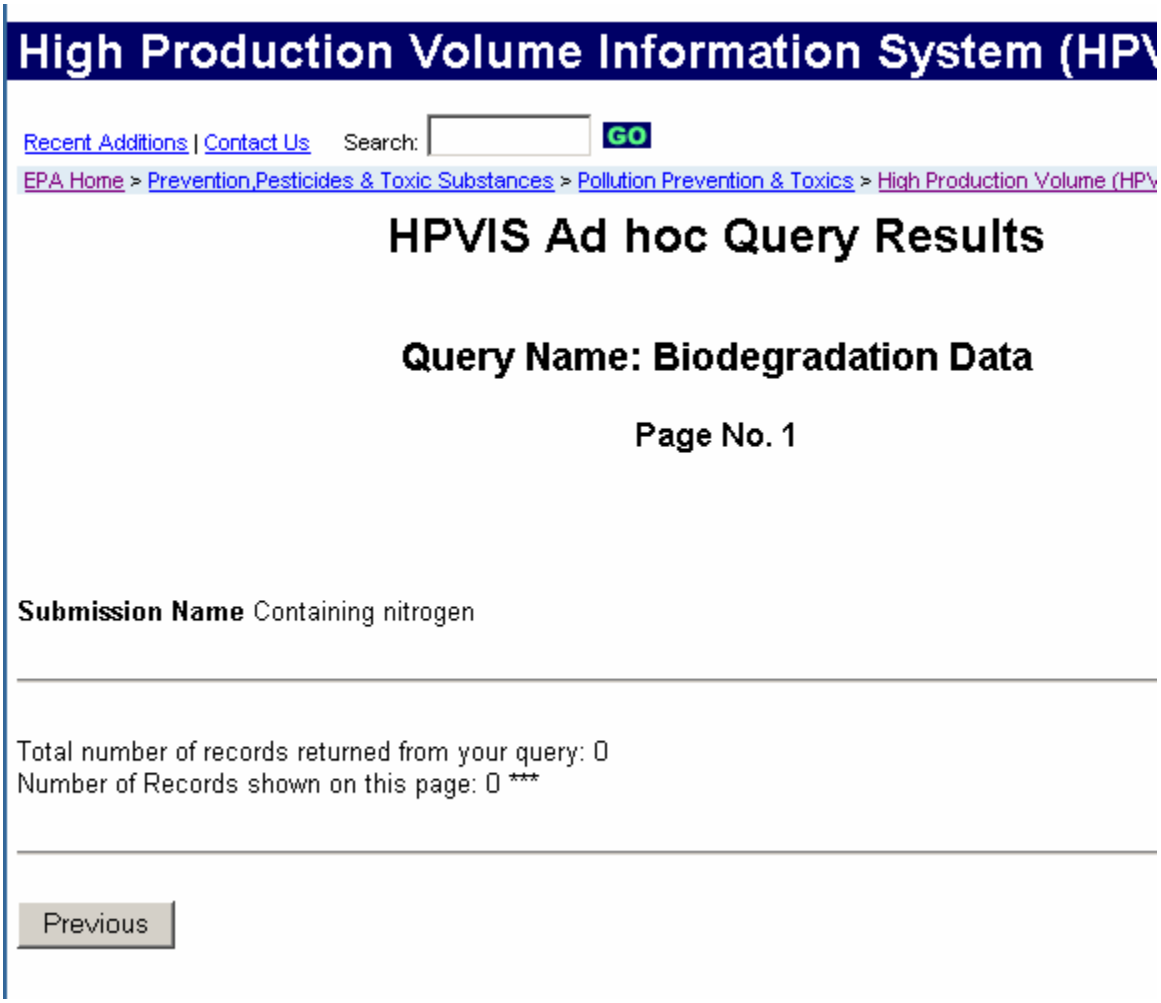


Figure 3: Screen shot from attempted search for "Fatty Nitrogen Derived Amines" submission



In general, because our project was focused on a small number of specific chemical categories, relatively simple database queries were sufficient for our purposes, and we found the browse tool to be the most useful means of searching HPVIS.

During our research, we discovered a few broken links in the browse tool. For example, the "back to detailed query results" buttons did not always work. Overall, however, the navigation links added efficiency to the HPVIS user interface.

The ability to search by "use" (e.g., solvent, surfactant, acid, dye) would be helpful, though this information is not always available in the test plans.

VI. OBSERVATIONS AND RECOMMENDATIONS: DATA

The fact that the HPVIS is not a complete set of HPV-sponsored chemicals is noted in the introductory text to the database. Currently, if a user is looking for a test plan or robust summary for a chemical, s/he must search both HPVIS and the HPV robust summaries and test plan data. The utility of the database would be augmented if a user could search HPVIS and

see chemicals that have robust summaries or test plans but that have not yet been entered into the database.

The data found in the HPV robust summaries and test plan search does not always match what is in HPVIS. For example, “Fatty Nitrogen Derived Amines” was split into two categories (“amines” and “ether amines”) in 2004. This split has yet to be reflected in HPVIS.

Test summaries don’t always include the sponsor’s interpretation of the study or whether they used it as a key study or not. In some cases, aquatic toxicity is reported as >1000 when the actual measure is “no effect at saturation” (e.g., CAS No. 1338-46-3).

Metadata definitions are not available for all categories. For example, “Biodegradability indicator” is not defined, so the precise meaning of “readily biodegradable” is not entirely clear. For another example, “read across” is not defined.

We observed that chemicals included in the “Sponsored Chemical” section often are not HPV chemicals but have been included in the submission as supporting chemicals. Unfortunately, no such distinction is made in HPVIS; users must open the test plans to distinguish between sponsored and supporting chemicals.

VII. SUMMARY AND CONCLUSIONS

As a general rule, we had reasonably few difficulties searching HPVIS, though it must be acknowledged that our approach necessitated relatively little use of HPVIS’s search capabilities and that we ended up using HPV Tracker—instead of HPVIS—as a means of downloading the entire list of chemicals that is far simpler than extracting this data set from HPVIS. It must also be remembered that our subsequent screening steps were taken outside HPVIS (using a spreadsheet) rather than by specifying a series of increasingly restrictive queries in HPVIS. A combination of data gaps and usability shortcomings (e.g., broken links and limitations in query tool special reports) do compromise the utility of HPVIS in several respects. The system still has some way to go before it is likely to be widely regarded as particularly useful and user-friendly. In any case, we would almost certainly explore the use of HPVIS again in the future to identify candidate chemicals like solvents, chelators, pH adjustors, and so forth for listing in additional CleanGredients™ modules as we develop them.

APPENDIX: COMPARISON OF CLEANGREDIENTS™ SURFACTANT ATTRIBUTES AND HPVIS ENDPOINTS.

CleanGredients™ Surfactant Attributes	HPVIS Endpoints
Company Information	
Company Name	
Web Address (URL)	
Contact Information	
Technical Sales Information	
Salesperson	
Title	
Contact Information	
General Information	
Product Name	
Supplier Product Number	
Charge Class	
Chemical Classification	
CAS Number	
Product Description	
Suggested Applications	
Material Safety Data Sheets (MSDS)	
Technical Fact Sheets	
Handling and Storage	
Compliance with EU Detergent Directive	
Chemical-Physical Properties	***Chemical-Physical Properties***
Physical Form	Melting Point
Percent Active Surfactant	Boiling Point
pH	Vapor Pressure
Hydrophile/Lipophile Balance (HLB)	Partition Coefficient
Density/Specific Gravity	Water Solubility
Cloud Point	Density/Specific Gravity
Flash Point	Viscosity
Critical Micelle Concentration	Surface Tension
	Dissociation Constant
	Non-Saturated pH

CleanGredients™ Surfactant Attributes	HPVIS Endpoints
	Solubility in Different Media
	Granulometry
	Flash Point
	Flammability
	AutoFlammability
	Explosivity
	Chemical Reactivity
	Oxidation Properties
	Oxidation Reduction Potential
Human and Ecological Health Attributes	***Environmental Fate and Pathways***
Acute Aquatic Toxicity (Fish, Daphnia, Algae)	Photodegradation
Additional Aquatic Toxicity (Microtox, Chronic)	Stability in Water
Acute Mammalian Toxicity (Oral, Dermal)	Transport Between Environmental Compartments Fugacity/Dist Endpoint
Neurotoxicity	Biodegradation
Carcinogens, Mutagens, and Reproductive Toxins (CMR)	Stability in Soil
Irritancy	Adsorption/Desorption to Soil
Sensitization	Bioaccumulation
Biodegradability	Mode of Degradation in Actual Use
Degradation Products	BOD5, COD, or BOD5/COD Ratio
Bioaccumulation potential	Monitoring Data
VOC Content	Field Studies Data
Presence of alkylphenol ethoxylates (APEs)	***Ecotoxicity***
Endocrine Disruption Potential	Acute Toxicity to Aquatic Vertebrates
Life Cycle Assessment Results	Acute Toxicity to Aquatic Invertebrates
Risk Assessment Results	Acute Toxicity to Aquatic Plants
Origin of Feedstock	Chronic Aquatic Vertebrate Toxicity
Bioderived	Chronic Aquatic Invertebrate Toxicity
Performance Properties	Toxicity to Terrestrial Plants
Other Product Features	Toxicity to Soil Dwelling Organisms
	Toxicity to Non-Mammalian Terrestrial Species
	Bioeffects
	Biotransformation

CleanGredients™ Surfactant Attributes	HPVIS Endpoints
	Mammalian Health Effects
	Acute Toxicity
	Repeated-Dose Toxicity
	Genetic Toxicity in vivo
	Genetic Toxicity in vitro
	Reproductive Toxicity
	Developmental Toxicity/Teratogenicity
	Mammalian Health Effects Other
	Pharmacokinetics and Metabolism
	Skin Irritation
	Eye Irritation
	Skin Sensitization
	Carcinogenicity
	Immunotoxicity
	Neurotoxicity
	Acute Toxicity