

The HPV Information System as a Source of Surfactant Listings for CleanGredients™

Lauren Heine
Topher Buck
Teresa McGrath
GreenBlue

Overview

- Project Goals
- Background: CleanGredients™
- Project Methodology
- Findings and Recommendations
 - HPVIS Features and Functionality
 - Data and Data Quality

GreenBlue is a nonprofit institute that stimulates the creative redesign of industry by focusing the expertise of professional communities to create practical solutions, resources, and opportunities for implementing sustainability.

Purpose of this HPVIS project

The purpose of this project was to investigate the utility and practical application of HPVIS (and the HPV data in general) as a source of data for CleanGredients™.

To this end, we sought to answer several questions:

- How can HPV data be used to advance green chemistry in 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)?
- How many of the chemicals (surfactants) listed in HPVIS are eligible for listing in CleanGredients™?

What is CleanGredients™?

A database of Industrial & Institutional (I&I) cleaning product ingredients and their characteristics* to:

- help **formulators** identify ingredients that may be useful for green product formulation
- provide opportunity for **raw material suppliers** to showcase their ingredients with especially positive environmental and/or human health and safety attributes

* By **characteristics** we mean functional properties such as critical micelle concentration, physical properties such as biodegradability, and associated human and environmental health toxicological information.

EPA's Design for the Environment (DfE)

www.epa.gov/dfe

DfE is one of EPA's premier partnership programs, working with industry sectors to compare and improve the human health and environmental risks, as well as the performance and cost, of existing and alternative products, processes, and practices.

DfE programs include:

- Formulator Program
- Safer Detergent Stewardship Initiative (SDSI)
- Partnership projects to evaluate options (flame retardants, lead solder, dry cleaning, etc.)

#1 Formulator Question

Is there a list of safer chemicals we can use in making our ingredient choices?

General Product Information

Company Information

- Company Name
- Web Address
- Contact and Sales Information

Ingredient Information

- Product Name
- Product Description and Suggested Applications
- Charge Class
- Chemical Classification
- Material Safety Data Sheets, Technical Fact Sheets, Handling and Storage Directions
- Compliance with EU Detergent Directive

Physical-Chemical Properties

- Physical Form
- % Active Surfactant
- Hydrophile-Lipophile Balance (HLB)
- Density/Specific Gravity
- Cloud Point
- Flash Point
- Critical Micelle Concentration
- Surface Tension

Environmental & Human Health Information

Tier I Surfactant Attributes

- Acute Aquatic Toxicity (Fish, Daphnia, Algae)
- Biodegradability (including degradation products)

Tier II Surfactant Attributes

- Sensitization
- Irritancy
- Acute Mammalian Toxicity (Oral, Dermal)
- VOC Content
- Presence of APEs

Tier III Surfactant Attributes

- Life Cycle Assessments
- Risk Assessments
- Endocrine Disruption test data
- Additional Aquatic Toxicity (Microtox, Chronic)
- Other Product Features
- Origin of Feedstock

Search by Performance/Physical Properties

Logged in as Test User from TestCorp. Log out
[Search](#) | [Your Account](#) | [Help](#)



[Hide Advanced Options](#)

Charge Class ⓘ	Application ⓘ	Supplier ⓘ	Text ⓘ
<input type="text" value="All"/>	<input type="checkbox"/> Hard Surface Cleaner <input type="checkbox"/> Hand Dish Soap <input type="checkbox"/> Carpet <input type="checkbox"/> Laundry	<input type="text" value="All"/>	<input type="text"/>
Chemical Class ⓘ	CAS # ⓘ	Biodegradability ⓘ	Aquatic Toxicity ⓘ
<input type="text" value="All"/>	<input type="text" value="All"/>	<input type="text" value="All"/>	<input type="text" value="All"/>
HLB ⓘ	Physical Form ⓘ	Flash Point ⓘ	CMC ⓘ
Min: <input type="text"/> Max: <input type="text"/>	<input type="text" value="All"/>	Min: <input type="text"/> Max: <input type="text"/> °C <input type="text"/>	Min: <input type="text"/> Max: <input type="text"/>
% Active Surfactant ⓘ	Sp. Gr. ⓘ or Density ⓘ	Cloud Point ⓘ	pH ⓘ
Min: <input type="text"/> Max: <input type="text"/>	Min: <input type="text"/> Max: <input type="text"/> Sp Gr <input type="text"/>	Min: <input type="text"/> Max: <input type="text"/> °C <input type="text"/>	Min: <input type="text"/> Max: <input type="text"/>
<input type="button" value="Search"/> <input type="button" value="Reset"/>			



Initial Search Results

 <p>AG 6202</p>	<p>Nonionic</p> <p>Alkyl Polyglucosides</p> <table border="1"> <tr> <td>22</td> <td>Liquid</td> <td>25°C</td> <td>16</td> </tr> <tr> <td>65%</td> <td>1.15</td> <td>>100°C</td> <td>7</td> </tr> </table>	22	Liquid	25°C	16	65%	1.15	>100°C	7	Ready	>100	Meets DfE Screen
22	Liquid	25°C	16									
65%	1.15	>100°C	7									
 <p>Monatropo 1620</p>	<p>Nonionic</p> <p>Alkyl Polysaccharide</p> <table border="1"> <tr> <td>-</td> <td>Liquid</td> <td>149°C</td> <td>-</td> </tr> <tr> <td>70%</td> <td>0.98</td> <td>-</td> <td>7</td> </tr> </table>	-	Liquid	149°C	-	70%	0.98	-	7	Ready	>10 and ≤ 100	Meets DfE Screen
-	Liquid	149°C	-									
70%	0.98	-	7									
 <p>Videt EGM</p>	<p>Blend</p> <p>Surfactant- concentrate</p> <table border="1"> <tr> <td>-</td> <td>Liquid</td> <td>-</td> <td>-</td> </tr> <tr> <td>-</td> <td>1.16</td> <td>-</td> <td>-</td> </tr> </table>	-	Liquid	-	-	-	1.16	-	-	Ready	>10 and ≤ 100	Meets DfE Screen
-	Liquid	-	-									
-	1.16	-	-									
 <p>Coconut oil fatty acids 61788-47-4 (CAS #)</p>	<p>Anionic</p> <p>Fatty Esters (Other than Glycol, Glycerol, etc.)</p> <table border="1"> <tr> <td>-</td> <td>-</td> <td>-</td> <td>-</td> </tr> </table>	-	-	-	-	Ready	>10 and ≤ 100	Meets DfE Screen				
-	-	-	-									

Click on product name

Deep Dive into Product Information



Search

| [Your Account](#)

| [Help](#)

General Ingredient Information

Company	 Vitech International Inc. Website
Technical Sales Name	Sharon Lishman
Technical Sales Phone	1-800-796-1896
Technical Sales Email	sharonl@winchemicals.com
Product Name	Videt EGM
Status	new
Charge Class	Blend
Chemical Class	Surfactant- concentrate
Product Description	Surfactant concentrate
Applications	-
Suggested Uses	Used for RTU and concentrated VOC free glass cleaners and All Purpose Cleaners.
MSDS File	 Videt EGM2 MSDS.pdf - 46.69 KB
Technical Data File	 Videt EGM tech data sheet.pdf - 63.51 KB

Ingredient-Level Environmental Summary

DfE Screen Yes

Tier I

Tier I Ingredient Attributes require the submission of test data and third party review. [More Info](#).

Acute Aquatic Toxicity [Show Details](#)

Reviewed Category	>10 and ≤100 mg/L
Fish LC₅₀	>100 mg/L
Daphnia EC₅₀	10-100 mg/L
Algae IC₅₀	10-100 mg/L

Biodegradability [Show Details](#)

Reviewed Category	Readily Biodegradable
Percent Degraded	≥60%
Duration	28 days
	Meets 10-day window
Toxic / Persistent Degradation Products	No

Requirements to List Surfactants on CleanGredients™

1. **Full ingredient formulation disclosure**
2. **Data** derived from GLP test data and/or literature sources for:
 1. **Biodegradability**
 2. **Acute Aquatic Toxicity**
3. **Ingredient biodegradability:** All surfactant components and preparations must be ultimately biodegradable without degradation products of concern*.

*Compounds classified by GHS as Acute Category 1 or 2 for aquatic toxicity and that are not ultimately biodegradable.

DfE Screen for Surfactants

An ingredient that meets the DfE Screen is an ideal candidate for use in an institutional and industrial (I&I) cleaning product recognized by the EPA Design for the Environment (DfE) Formulator Program.

<u>Aquatic Toxicity Level</u> (L/E/IC50 Value)	Ideal DfE Candidate
≤1 ppm	May be acceptable if ultimate biodegradation occurs within a 10-day window with out products of concern*
>1 ppm and ≤10 ppm	Ultimate biodegradation occurs within a 10-day window without product of concern
>10 ppm	Ultimate biodegradation occurs within 28 days without products of concern

* Products of concern are compounds classified by GHS as Acute Category 1 or 2 for aquatic toxicity and that are not ultimately biodegradable. (GHS Acute Category 1 or 2 refers to L/E/IC₅₀ ≤ 10ppm. Ultimately biodegradable refers to >60% mineralization in 28days.)

HPVIS as a Source of Data for the CleanGredients™ Surfactants Module

- **Identify HPV surfactants**
130 HPV surfactants identified via chemical class test plans and the HPV Tracker
www.environmentaldefense.org/documents/2724_HPVTraacker.xls
- **Identify surfactants that meet the three requirements for listing on CleanGredients™ :**
 1. Surfactant must have test data on biodegradability
 2. Surfactant must have test data or modeled data on at least one species for acute aquatic toxicity.
 3. Surfactant must be at least ultimately biodegradable (>60% mineralization in 28d).

Screen Surfactants for Biodegradation Data

130	Surfactants were identified in HPVIS.
79	Chemicals were eliminated due to an absence of biodegradation data. Note: the data set for each surfactant was evaluated for biodegradation data, but modeled data and data based on analog chemicals in the same chemical class (“read across” data) were not considered acceptable to fulfill this data requirement.
13	Chemicals were eliminated due to insufficient or conflicting data.
21	Chemicals were eliminated because they demonstrated less than 60% mineralization in 28 days.
17	HPV surfactants qualified for listing 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™, a surfactant 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.
- Results
 - Of the 17 surfactants with sufficient biodegradation data, four were eliminated due to a lack of aquatic toxicity data.
 - One surfactant without aquatic toxicity data in HPVIS was nevertheless deemed eligible for listing in CleanGredients™ after supplementing the HPVIS data with aquatic toxicity values that the U.S. EPA Design for the Environment Formulator Program had predicted for this chemical as part of their (earlier) review of this surfactant.

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 (68526-83-0) was nonspecific with respect to linear vs. branched structure.
- Results: four surfactants were excluded due to uncertainty with respect to the degree of branching in the tested chemical.

Final Results

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

Table 2 of Report: Chemicals Qualifying for 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

Functionality Comments

- It would be helpful to be able to search by “use” (e.g., solvent, surfactant). This information was often included in the test plan.
- Browse tool tab views and matrix views are useful for scanning all chemicals in a category. This function was adequate for our purposes.
- Special reports generated with the query tool were not user-friendly (i.e., search for amine or nitrogen did not return any results).
- There were a number of broken links in the browse tool (e.g., “Back to detailed query results” did not always work).
- Overall, the navigation links added efficiency.

Data Quality Comments (1 of 2)

- Completeness. HPVIS is not a complete set of HPV-sponsored chemicals. Currently, to find a test plan or robust summary, one must search both HPVIS and HPV robust summaries and test plan data.
Recommendation: allow user to search HPVIS and to see chemicals that have robust summary or test plans which have not yet been entered into the database.
- Consistency. Data in the HPV Robust Summaries do not always match what is in HPVIS. For example, fatty nitrogen amines was split into two categories (amines and ether amines) in 2004, but this was not yet reflected in HPVIS.
- Test summaries do not 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 > 1000mg/L, when the actual measure was "no effect at saturation" (e.g., CAS No. 1338-46-30)

Data Quality Comments (2 of 2)

- Metadata definitions are not available for all categories.
 - “Read across” is not defined
 - “Biodegradability indicator” is not defined, so the precise meaning of readily biodegradable is not clear.
- *Recommendation: distinguish between sponsored and supporting chemicals so that users do not have to open the test plans to distinguish between them.* Chemicals included in the “Sponsored Chemical” section often are not HPV chemicals but have been included in the submission as supporting chemicals.
- Data adopted from HPVIS for use in CleanGredients™ require expert review and validation.
- Useful. Overall, we will almost certainly use HPVIS again in the future to identify candidate chemicals for additional CleanGredients™ modules (solvents, chelating agents, builders, etc.).

END