



Lessons Learned: Differentiating Chemicals in Alternatives Assessments and Identifying the Availability of Safer Alternatives for Policy Purposes

June 9th, 2010

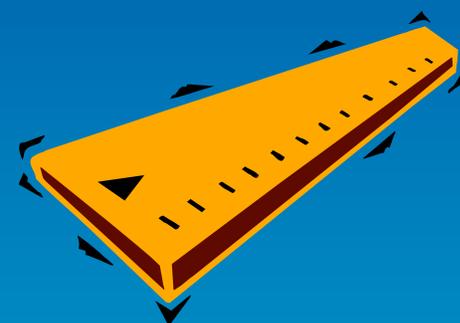
Libby Sommer, Environmental Scientist

How do I
measure
safer
chemistry?



Measuring stick must be:

- Transparent
- Science-based
- Green Chemistry-driven





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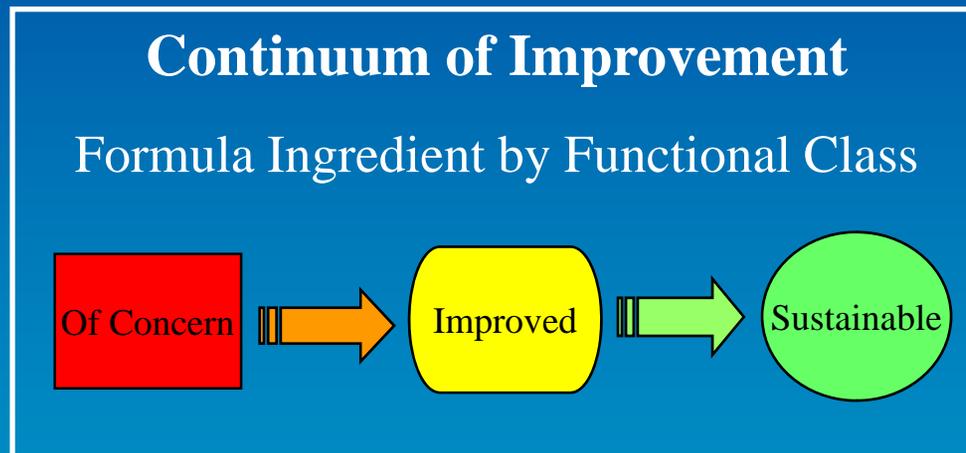
- EPA DfE Criteria for Safer Ingredients
- Why did DfE Develop the Criteria?
- Application for Alternatives Assessments
- Application for Safer Product Labeling Program
- CleanGredients®

EPA DfE Measures of Safer Chemistry



Criteria for Safer Ingredients

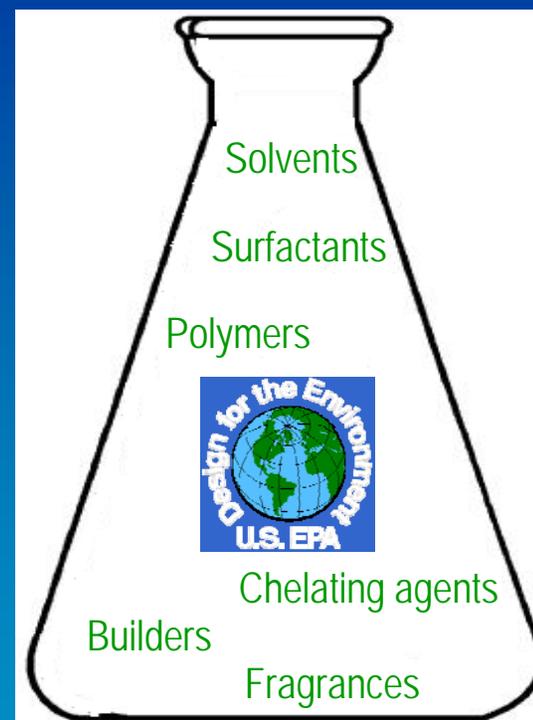
- Functional ingredient classes
 - Solvents
 - Surfactants
 - Fragrances
 - Chelating agents
- Master Criteria
 - Generally low hazard



Why did DfE Develop Safer Chemicals Criteria?



- Treatment of New Chemicals under TSCA
- Leverage EPA toxicological tools and expertise
- Transparency
- Product formulators asked for a list of safer chemicals for product development





DfE Criteria for Safer Ingredients

Authoritative Lists

- International Agency for Research on Cancer (IARC)
- National Toxicology Program (NTP)
- EPA Carcinogens List
- EU CMR List
- EU Risk Phrases

Evaluation of Experimental Data

- Globally Harmonized System (GHS)
- EPA New Chemicals Program
- EPA TSCA 8(e) reporting



DfE Criteria for Safer Ingredients

Human Health Toxicity

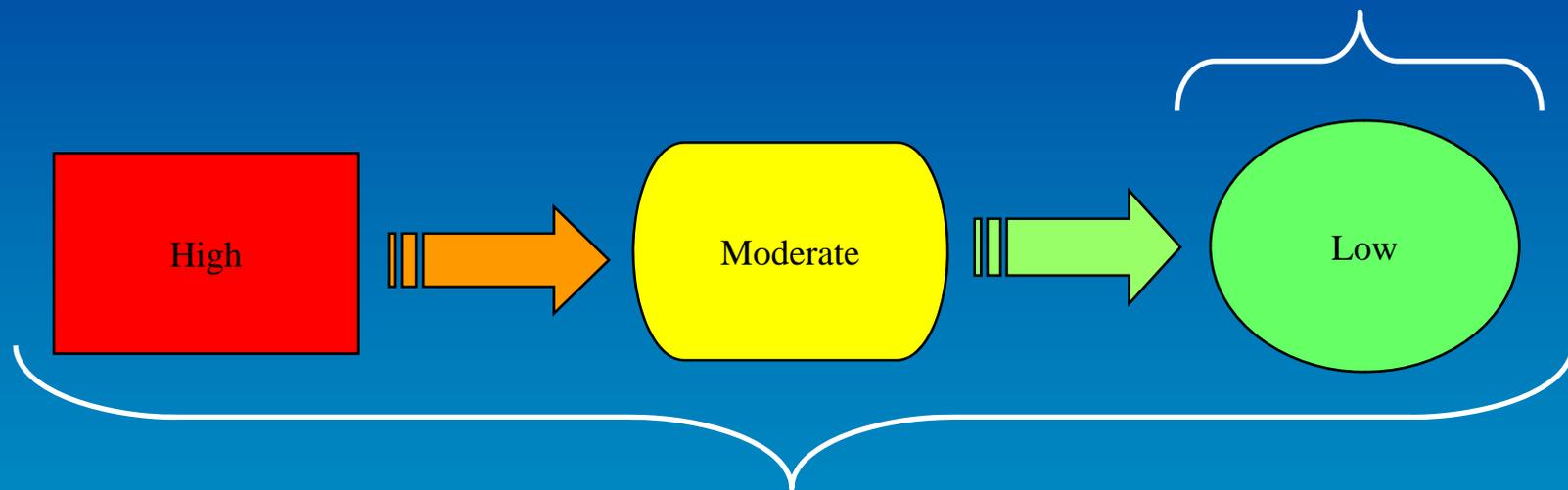
- Acute mammalian toxicity
- Carcinogenicity
- Genetic toxicity
- Neurotoxicity
- Repeated dose toxicity
- Reproductive and developmental toxicity
- Respiratory sensitization
- Skin sensitization

Environmental Fate & Effects

- Aquatic toxicity
- Bioaccumulation potential
- Biodegradation
- Eutrophication

Application to Alternatives Assessment

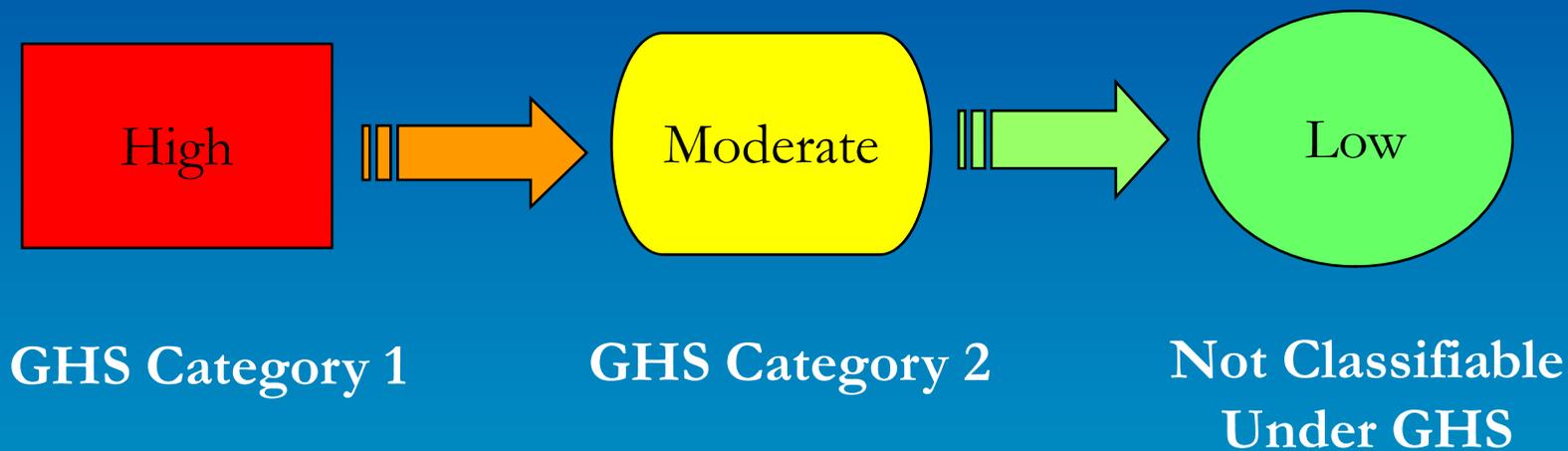
Master Criteria – used in Safer Product Labeling



Expanded Master
Criteria – to be used in
Alternatives Assessment

Example of Expanded Criteria – *Draft*

Repeated Dose/Systemic Toxicity



Example of Expanded Criteria – *Draft*

Reproductive & Developmental Toxicity



Dose effect level
 < 50 (oral) under
 GHS Cat 1 or 2
 (derived from
 TSCA 8(e)
 criteria)

Dose effect level
 50 - 250 (oral)
 under GHS Cat
 1 or 2 (derived
 from TSCA 8(e)
 criteria)

Not Classifiable
 Under GHS; or
 Dose effect level
 >250 (oral) under
 GHS Cat 1 or 2
 (derived from
 TSCA 8(e) criteria)

Data Preferences

High Weight of
Evidence

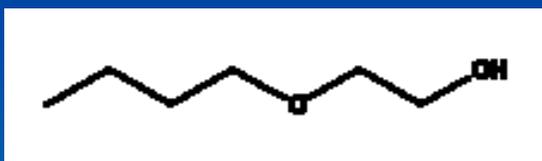


Low Weight of
Evidence

- Experimental data
- Analogs
- Models

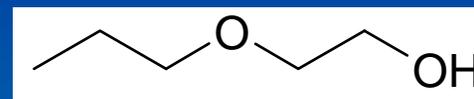
Structure-Activity Relationships (SARs)

Identifying Chemicals of Concern



2-Butoxyethanol

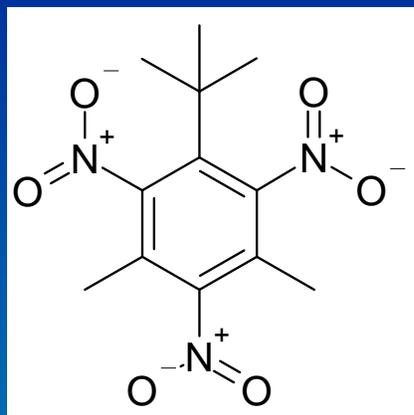
- Solvent used widely in cleaning products
- Human health concerns include hemolysis leading to toxicity in kidney, spleen and liver.
- GHS Category 2 for Repeated Dose Toxicity (oral and inhalation studies in rats)



n-Propoxyethanol

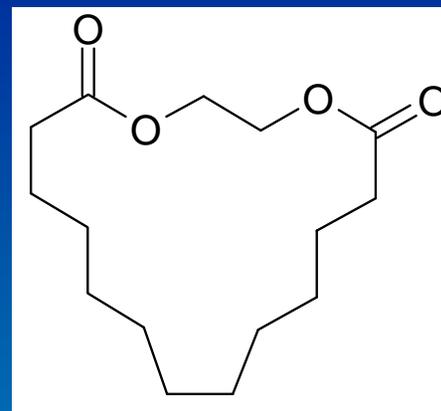
- Also can be used as a solvent in cleaning products
- Similar structure and belongs to the same chemical class as 2-butoxyethanol.
- GHS Category 2 for Repeated Dose Toxicity (oral and inhalation studies in rats)

Suggesting Safer Substitutes (Fragrances)



Musk xylol

- Appears designed for maximum environmental persistence—nitro and t-butyl groups
- May bioaccumulate
- Potentially toxic to aquatic organisms
- May be an indirect toxicant, inhibiting the ability of cells to excrete harmful chemicals



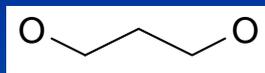
Ethylene brassylate

- Faster biodegradation—ester linkages
- Fragrance houses have worked with EPA's Design for the Environment Formulator Program to replace musk xylol with ethylene brassylate

DfE Criteria for Solvents

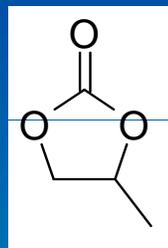
- Alcohols

- e.g. 1,3 propanediol



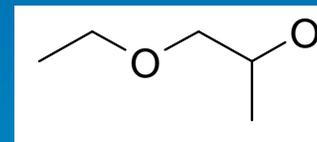
- Esters

- e.g. propylene carbonate



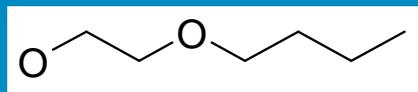
- Propylene glycol ethers

- e.g. propylene glycol ethyl ether



- Ethylene glycol ethers

- 2-butoxyethanol





DfE Criteria for Solvents

- Key Hazard Attributes of Concern
 - Acute Mammalian Toxicity
 - Carcinogenicity
 - Neurotoxicity
 - Repeated Dose Toxicity
 - Reproductive & Developmental Toxicity
 - Environmental Fate and Toxicity
 - Aquatic Toxicity
 - Biodegradability
 - Bioaccumulation Potential



Example: Solvents Criteria

Name	1,3-Propanediol
Acute Mammalian Toxicity	Not classifiable under GHS; low toxicity
Carcinogenicity	Not classified by authoritative bodies; based on modeling and expert judgment, low concern
Neurotoxicity	Not classified under GHS; dose effect levels exceed GHS thresholds
Repeated Dose	Not classified under GHS; effect level > 1000 mg/kg
Repro/Devel Toxicity	Not classified under GHS; NOAEL of 800 mg/kg exceeds TSCA 8(e) dose effect level
Environmental Fate & Toxicity	Meets New Chemicals Program criteria for low aquatic toxicity, rapid biodegradation, and low bioaccumulation potential

Status

Passes DfE Criteria for Solvents

CleanGredients® - Marketplace for Green Chemistry Ingredients



- Leverages EPA green chemistry expertise and tools
- CleanGredients is a marketplace...
 - for suppliers to showcase safer chemical ingredients for cleaning products, and
 - for formulators to find those ingredients.
- Identifies ingredients that meet DfE Criteria for Safer Ingredients

CleanGredients®

Search by Performance/P-Chem/Tox Properties



https://db.cleangredients.org - CleanGredients™ » Surfactant Search - Mozilla Firefox

Logged in as **Topher Buck** from **TestCorp.**
[Log out](#)

search your account

Charge Class ⁱ	Application ⁱ	Supplier ⁱ	Text ⁱ
<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 ⁱ	CAS # ⁱ	Biodegradability ⁱ	Aquatic Toxicity ⁱ
<input type="text" value="All"/>	<input type="text" value="All"/>	<input type="text" value="All"/>	<input type="text" value="All"/>
HLB ⁱ	Physical Form ⁱ	Flash Point ⁱ	CMC ⁱ
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 ⁱ	Sp. Gr. ⁱ or Density ⁱ	Cloud Point ⁱ	pH ⁱ
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"/>

Disclaimer: Only data on acute aquatic toxicity, biodegradability, and degradation products are reviewed by a designated third party for purposes of listing in the CleanGredients(tm) database. All other data and product information are provided by ingredient suppliers who are individually responsible for the accuracy of the information. All TestCorp and GreenBlue Ingredients are fictional and are provided for demonstration purposes only.

If you experience technical difficulties or have any suggestions or comments, please let us know at info@cleangredients.org

CleanGredients® Search Results



https://db.cleangredients.org - CleanGredients™ » Surfactant Search - Mozilla Firefox

Supplier	Product Name ID	Charge Class				Biodeg- radability ⓘ	Acute Aquatic Toxicity ⓘ L/EC50 ⓘ [mg/L]	DfE Screen† ⓘ
		Chemical Class						
		HLB	Form	Flash	CMC			
%Act	Sp. Gr.	Cloud	pH					
Uniqema	Monatropo 1620	Nonionic Alkyl Polysaccharide				Ready	>10 and ≤100	Meets DfE Screen
Air Products & Chemicals (Tomah Products)	Tomadol 400	-				Ready	≤1	Meets DfE Screen
Cognis Corporation	Glucopon 625 UP	Nonionic Alkyl glucosides				Ready	>1 and ≤10	Meets DfE Screen
	Magnesium lauryl sulfate 3097-08-3 (CAS #)	Anionic Linear alkyl sulfate				Ready	>10 and ≤100	Meets DfE Screen
Stepan Company	BIO-SOFT® N1-5 PF696	Nonionic Alcohol Ethoxylates				Ready	>1 and ≤10	Meets DfE Screen
CLER	LAS CLER Standard	Anionic Linear alkylbenzene sulfonate, sodium salt				Ready	>1 and ≤10	Meets DfE Screen



Summary

- EPA DfE develops green chemistry criteria to define safer chemicals
- Criteria have applications in alternatives assessment and product labeling
- Criteria could serve as the basis for alternatives assessment by other programs



Thank you!

For more information:

Libby Sommer

sommer.elizabeth@epa.gov

202-564-1065

<http://www.epa.gov/dfe>