PBT Profiler Use in Industry to Screen HPV Chemicals

SC Johnson Case Study

John Weeks

December 2006

tomorrow's legacy today
SUSTAINABILITY

SC Johnson
A FAMILY COMPANY

Priority Environmental Concern

- **There is wide agreement that chemicals of greatest concern are those that:**
  - **P**ersist (P), and
  - **B**ioaccumulate (B), and
  - present **T**oxicity (T) concerns, i.e., **PBT**s.
- **Fraction of all chemicals have been tested to determine if they are PBT.**
- **Greenlist is helping to make better choices for the future; emphasis is on the large volume RMs.**
- **PBT profiling is aimed at all raw materials, as an important check.**

Environmental Opportunities

- **PBT profiling is one aspect of SCJ's RUM (Restricted Use Materials) process.**
- **Regulatory compliance is not our objective, but PBT profiling will help us avoid regulatory problems, e.g. for vPvB chemicals under EU's REACH.**
- **61% of consumers say they would prefer PBT free (Roper, 1993).**
- **EPA and SCJ teamed up to assess our raw materials using the PBT Profiler.**

PBTs Are a Global Concern

- **U.S. HPVs, TRI, TSCA PMNs**
  - EPA PBT Profiler for PMNs, PP (voluntary)
- **EU**
  - U.K. Chemical Stakeholders Forum – List of Chemicals of Concern
  - EC: European Chemicals Bureau Tech. Guidance Doc. criteria and PBT list.
  - OSPAR
  - REACH (vPvB)
- **Canada**
  - DSL screening
- **Great Lakes Binational Toxics Strategy**
- **UNEP Stockholm Convention on Persistent Organic Pollutants**
- **LRTAP Convention**

Environmental Profiling SCJ & EPA

- EPAs program is intended to increase the no. of chemicals examined.
- SCJ – was the first Consumer Products Co. to partner w/EPA with the aim to ID and eliminate PBTs.
- Computer-based model was used to estimate PBT of each raw material in use and considered for future use by SC Johnson.
- Initial PBT screen of raw materials completed with the assistance of an EPA contractor: SRC
- Additional data collection was undertaken.
- All alleged PBTs identified were reclassified as RUMs.
- Reformulation can be necessary; but further data collection exonerated some.

PBT Profiler Background

- **Developed by EPA with help from:**
  - American Chemistry Council,
  - Chlorine Chemistry Council,
  - Synthetic Organic Chemical Manufacturers Association, and
  - contributions of Environmental Defense.
- **PBT Profiler uses a subset of methods from EPA's Pollution Prevention program and routine TSCA chemical screening.**
- **We realize limitations of the QSAR methodology.**

P-Dichlorobenzene

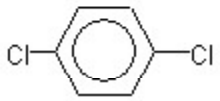
Results

Orange or **red** highlights indicate that the EPA criteria have been exceeded.
Black-and-white version

Persistence			Bioaccumulation	Toxicity
Media	Half-Life (days)	Percent in Each Medium	BCF	Fish ChV (mg/l)
Water	38	14%	89	1.1
Soil	75	74%		
Sediment	340	1%		
Air	50	11%		

106-46-7 Benzene, 1,4-dichloro- (pDCB)

PBT Profiler Estimate = PBT



P2 Considerations and more information

Start a New Profile | Add More Chemicals to Your Profile

The PBT Profiler Results are available for 20 minutes

Octachlorostyrene

Results

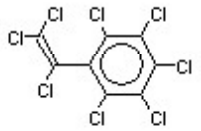
Orange or red highlights indicate that the EPA criteria have been exceeded.
Black-and-white version

Persistence	Bioaccumulation	Toxicity

29082-74-4 Octachlorostyrene

PBT Profiler Estimate = PBT !

Media	Half-Life (days)	Percent in Each Medium	BCF	Fish ChV (mg/l)
Water	180	1%	15,000	Not Estimated
Soil	360	40%		
Sediment	1,600	59%		
Air	14	0%		



P2 Considerations and more information

! Persistent and bioaccumulative chemicals may eventually reach relatively high levels in living organisms. Without clear data on toxicity, to be conservative it should be assumed that this chemical might have PBT characteristics. An independent assessment of toxicity to humans and the environment should be conducted on this chemical to determine if it might be a PBT.

Start a New Profile | Add More Chemicals to Your Profile

Data Entry

Octachlorostyrene is listed as a PBT chemical in EPA's final rule on Persistent, Bioaccumulative, and Toxic Substances and/or as a Persistent Organic Pollutant (POP) by the United Nations Environment Programme (UNEP)

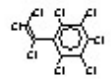
Estimate the persistence, bioaccumulation, and toxicity of Octachlorostyrene by starting the PBT Profiler Start the PBT Profiler

Or

Build the list of chemicals to be profiled by adding another CAS Registry number or other identifier: Lookup

Draw your chemical

List of Chemicals to be Profiled

#	CAS Number	Name	SMILES	
1	29082-74-4	Octachlorostyrene	Clc(c(Cl)c(Cl)c1C(Cl)=C(Cl)Cl)c(Cl)c1Cl	

Update Name

Black-and-white version

Developed by the Environmental Science Center under contract to the Office of Pollution Prevention and Toxics , U.S. Environmental Protection

EPA's PBT Criteria

Persistence			Bioaccumulation	Toxicity
Half-Life:	**(Orange) Moderate**	**(Red) High Concern**	**BCF:**	**Fish ChronicValue:**
			Moderate (Orange)	**Moderate (Orange)**
			≥ 1,000	**< 10 mg/L**
Water:	**≥ 2 months**	**> 6 months**		
Soil:	**≥ 2 months**	**> 6 months**	**High Concern (Red)**	**High Concern (Red)**
Air:	**-**	**> 2 days**	**≥ 5,000**	**< 0.1 mg/L**
Sed:	**≥ 2 months**	**> 6 months**		

Identification of Substances

- **Identification of the substances in all of our raw materials was a non-trivial task.**
- **Several thousand raw materials were examined.**
- **2,150 unique chemicals were identified in current SCJ product formulations.**
- **Fragrance materials are being handled separately (details below).**

Identification - CAS Numbers

- **SCJ's databases contained Chemical Abstracts Service numbers for many but not all of the materials.**
- **Some raw materials were actually formulations, so their composition with CAS numbers was investigated.**
- **Materials considered proprietary: Suppliers were contacted. (If no identification, they could be considered RUMs.)**

Refinement of List

- **Inorganic materials were identified and set aside (120).**
- **Chemical structures were obtained to the extent possible from the Syracuse Research Corp.'s (SRC) SMILECAS database. (1,333)**
- **Some of the structures are representative of mixtures.**
- **If the raw material is a formulation, active components that constitute > 5% were identified.**

Other Categories

- **Polymers that are likely to contain a representative, relatively low molecular weight component. (representative oligomers were examined)**
- **High molecular weight polymers.**
  - Molecules with MW > 1,000 cannot be profiled, but are generally recognized not to be PBTs.
- **Materials where a chemical structure could not be determined.**
  - We have used corn kibbles, bacteria, enzymes, and sawdust.

Breakdown of SCJ Chemicals By Category

Chemical Category	Number of Chemicals	Profiled?
Discrete organics	1,299	Yes
Mixtures with a representative component	535	Yes
Inorganics	120	No
Polymers with a representative component	69	Yes
Polymers (high molecular weight)	52	No
High molecular weight materials (e.g., sawdust) that do not require profiling	39	No
Structure not available	36	No
Total	2,150	

Profiler Results

- **1,903 chemicals were screened using an automated procedure in collaboration with the Risk Assessment Division, EPA/OPPT.**
- **Chemicals with 3 aspects of “medium” or greater were flagged.**
- **Chemicals with toxicity “not estimated” were also flagged for assessment.**
- **Total number flagged was 173 (9 %).**

PBT Profiler Screening Results Summary

P	B	T	Number of Chemicals
Medium	Medium	Not Estimated	4
Medium	Medium	Medium	23
Medium	Medium	High	66
Medium	High	Not Estimated	1
Medium	High	High	16
High	Medium	Not Estimated	9
High	Medium	High	15
High	High	High	39

Further Investigation

- **The first aspect approached was Persistence.**
- **Primary tool for finding references was BIOLOG, an SRC database of abstracted biodegradation data.**
- **Conflicting data were resolved by reference to other sources, especially the HSDB.**
- **Data indicated that 36 more materials were expected to biodegrade.**

Hydrolysis

- **Four additional chemicals were judged not to be persistent based on a knowledge of the chemistry of their functional groups.**
- **Schiff's base, ketal, and alpha-chloroethers were expected to hydrolyze.**
- **Esters were not assumed to be rapidly hydrolyzable, although many are.**
- **Hydrolysis products will be considered.**

Fragrance Components

- **The Research Institute for Fragrance Materials (RIFM) agreed to collaborate in an independent but supportive effort.**
- **RIFM identified 2,150 components of commercial fragrances, which were run through the PBT Profiler in collaboration with EPA.**
- **RIFM also provided expert analysis for some fragrance components (25) that had been identified by SCJ for further assessment.**

Structural Analogs

- **A group of structurally related musks were judged to be biodegradable based on experimental data for a few members of the class. RIFM data were consistent with BIOLOG references.**
- **Expert opinion was relied upon to examine analogs of the other remaining flagged chemicals.**
- **As a result, an additional 101 chemicals were judged to be biodegradable and not persistent.**
- **Classes included hydrocarbons, terpenes, functionalized fatty acids, and natural extracts.**

More On the Inorganic Chemicals

- **Although these 120 chemicals could not be profiled, some additional screening has been done for PBT characteristics.**
- **56 were found in the FDA's Everything Added to Foods in the United States list (EAFUS).**
- **Some other substances can clearly be recognized not to be PBTs: e.g. bone meal, cultured enzymes, sawdust, corn meal, honey.**
- **Others will require further investigation.**

What Remains of the Flagged Organic Chemicals?

- **Only 16 raw materials emerged from the screening process of the 2,150 materials used by SCJ.**
- **Of these:**
  - **6 were fragrance components, being addressed by RIFM.**
  - **10 non-fragrance chemicals failed initial PBT screening.**

Of the chemicals for follow-up:

- **Most were colorants and dyes.**
  - Including UV protectant
- **Silicone materials were also represented.**
  - Most silicones have been exonerated based on weight of evidence (PDMS).
- **An insecticidal active ingredient had been under consideration by SCJ, but now we will avoid it.**

Non-Fragrance Chemicals: Final Outcome

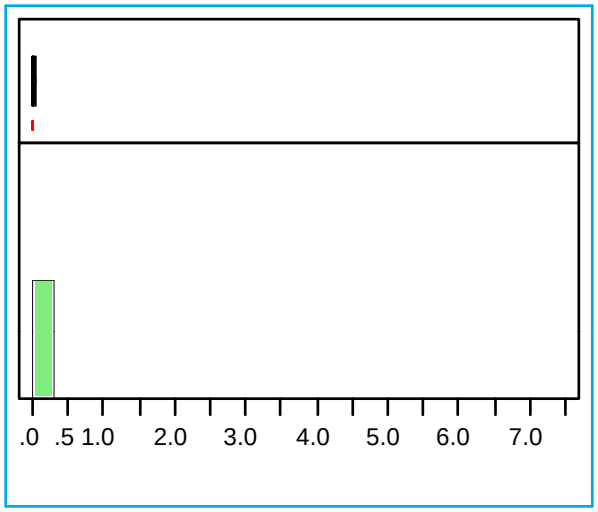
- **5/10 were exonerated based on additional data and analysis.**
- **The remaining 5/10 will no longer be purchased by SC Johnson: They are no longer needed or substitutes were found.**

Fragrance Components: Still Being Studied

- **Some measured data has been identified.**
- **Advanced QSARs are helpful.**
- **Preliminary aquatic toxicity testing indicates that these components are generally less toxic than originally predicted.**
- **Additional testing by the fragrance industry is being worked out.**
- **Full testing batteries would be very expensive.**

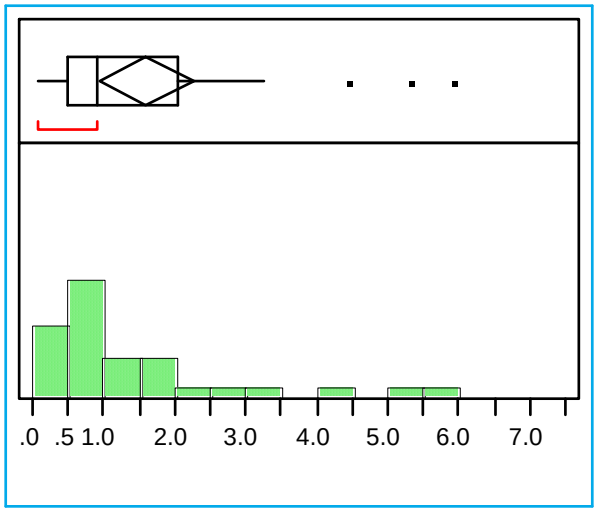
Preliminary Aquatic Toxicity Data on Fragrance Components

Estimated Fish Chronic Value



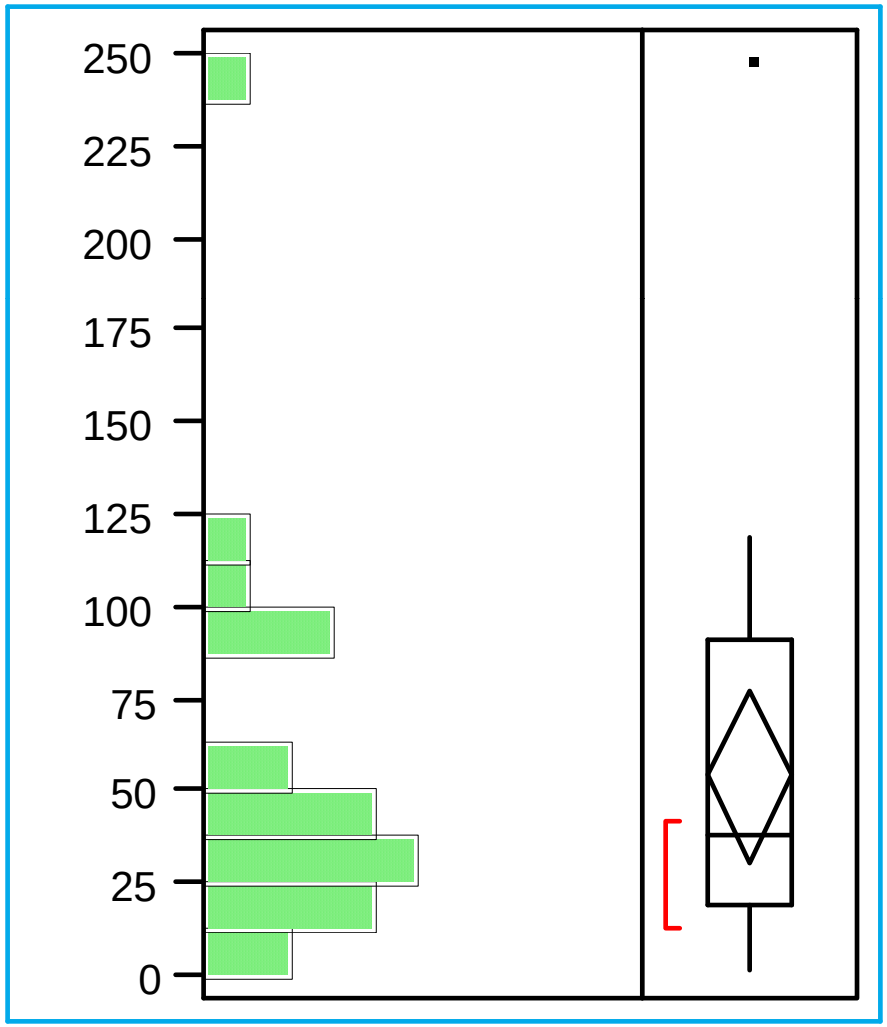
mg/liter

Measured Fish Chronic Value



mg/liter

Ratio of Measured to Estimated Fish Chronic Value: Distribution



Conclusions

- **The PBT Profiler was an important cost-effective tool to identify chemicals requiring our attention.**
- **Other sources and expert judgement were needed to refine the list.**
- **Our goal is to remove PBT chemicals from our product line.**

There Is More To Be Done!

- **Materials new to us will continue to be screened and evaluated. Testing will be undertaken only as necessary.**
- **Prioritization of the possible types of testing will depend on the preliminary results, and practicality of testing: costs, timing.**
- **Aquatic toxicity testing and routine biodegradability tests (e.g. OECD 301) are early options.**
- **RIFM and fragrance manufacturers continue work on fragrance components.**
- **Removal of suspect chemicals from our formulas will be done if necessary.**

Link for public access to the PBT Profiler:

http://www.pbtprofiler.net/