

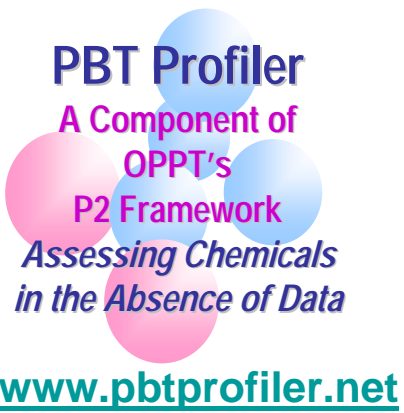



## PBT Profiler Seminar

GLC RDX Conference  
Detroit, Michigan  
October 27, 2004

Sponsors: Clean Manufacturing Technology and Safe Materials  
Institute, USEPA, and Consortium for Environmental Risk Management

## The PBT Profiler






## The PBT Profiler Estimates Persistence, Bioconcentration potential, and fish chronic Toxicity from chemical structure

Using the PBT Profiler

- [Information needed](#)
- [Database](#)
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Persistence, Bioconcentration, and Toxic Profiles Estimated for Organic Chemicals On-Line

### PBT Profiler


A Component of CPPT's P2 Framework  
Assessing Chemicals in the Absence of Data

About

- [Methodology](#)
- [Criteria](#)
- [Accuracy & Security](#)
- [Definitions](#)
- [Terms of Use](#)
- [Chemicals That Can't be Profiled](#)

The PBT Profiler was developed as a voluntary screening tool to identify Pollution Prevention opportunities for chemicals without experimental data.

Users of the PBT Profiler acknowledge that they have read and accept the [Terms of Use](#) [Start the PBT Profiler](#)



## PBT Profiler Development

- Created with input from over 100 beta test participants from industry, academia, and government
- Developed by EPA as a collaborative effort with industry (ACC, SOCMA, CCC) and NGOs (ED)
- Underwent formal EPA scientific peer review



## How Does the PBT Profiler Work?

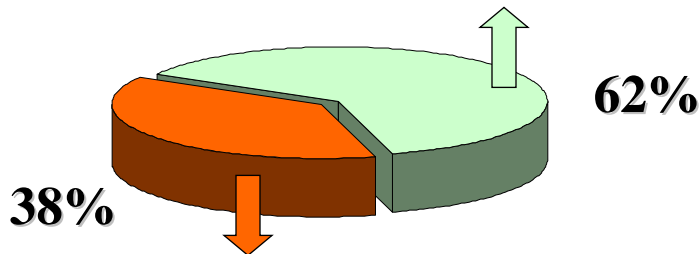
- Estimates physical/chemical and fate properties
  - Persistence: WS,  $K_{ow}$ , VP, Henry's Law constant, OH• and O<sub>3</sub> reaction rates, MP, MW, and ultimate biodegradation
  - Bioaccumulation: BCF
  - Toxicity: fish chronic value (ChV) from ECOSAR
- Uses a level 3 multi-media model to estimate distribution in water, soil, sediment, and air
- Compares P, B, and T estimates to EPA criteria and formats results in color-coded output (Level I)
- Provides quantitative results (Level II) and additional information for P2 assessments (Level III)



## Why Use the PBT Profiler?

**Of the 80,000 Chemicals on the TSCA Inventory, the PBT Profiler can profile 2/3rds or more**

**Chemicals That Can Be Profiled (62%)**



**Chemicals That Should Not Be Profiled (38%)**

[Mixtures can be profiled if a representative structure is identified]



## Profiler Technical Information

- Overall logic and page design - active server pages (ASP) - VB script and HTML
- Database queries – MS Access (ODBC)
- Estimation programs – Modified EPI libraries
- Level 3 fugacity model – active-x dll (VB)
- Chemical viewer – ISAPI dll (Delphi)
- Structure drawing program – java applet



## P, B & T Criteria

<b>Persistence</b>	Not Persistent	Persistent	
Water, soil, sediment	< 60 d	≥ 60 d	> 180 d
Air	≤ 2 d		> 2 d

<b>Bioaccumulation</b>	Not Bioaccumulative	Bioaccumulative	
Fish BCF	< 1,000	≥ 1,000	≥ 5,000

<b>Toxicity</b>	Not Toxic	Toxic	
Fish ChV (EPA New Chemical Program Criteria)	> 10 mg/L Or No Effects at Saturation	0.1-10 mg/L	< 0.1 mg/L



## Before Using the Profiler (I)

### Purpose of the PBT Profiler:

Identifying materials that may need additional technical evaluation for Persistence, Bioaccumulation and Toxicity characteristics.

1. The PBT Profiler is a predictive screening tool to be used when data are not available. [More information](#)
2. For technical reasons, there are certain chemicals (or chemical classes) that should not be profiled with the PBT Profiler. [More information](#)
3. The PBT Profiler is a screening tool, PBT estimations rendered by the PBT Profiler are not sufficient for definitive PBT determinations. The PBT Profiler is a research, not regulatory, tool to identify chemicals that may need further evaluation for potential Persistence, Bioaccumulation and Toxicity characteristics. [More information](#)

To continue using the PBT Profiler, please acknowledge that you have read and understand the issues and considerations discussed above.

I have read and understand the issues and considerations discussed above



## Before Using the Profiler (II)

### Before running the PBT Profiler:

1. Determine the structure of the chemical you want to profile. Also have a chemical name and ID number (preferably a CAS Registry number) available.
2. Establish if any persistence, bioaccumulation, and toxicity data are available for your chemical. Chemicals with experimental data should not be profiled - the PBT Profiler is a screening-level predictive tool.
3. Read and acknowledge the PBT Profiler [Terms of Use](#)

Start the PBT Profiler



## Data Entry – Lookup Database

[Methodology](#) · [Criteria](#) · [Definitions](#) · [Chemicals That Should Not be Profiled](#)  
[Home](#) · [Start a New Profile](#) · [Results](#) · [Terms of Use](#) · [Security](#)

### Data Entry

Estimate the persistence, bioaccumulation, and toxicity of  $\alpha$ -D-Glucopyranose, 1-(dihydrogen phosphate) by starting the PBT Profiler

[Start the PBT Profile](#)

Or

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

[Lookup](#)

[Enter your chemical](#)

#### List of Chemicals to be Profiled

#	CAS Number	Name	SMILES
1	12303	<input type="text" value="alpha-D-Glucopyranose, 1-(dihydrogen ph"/>	<input type="text" value="O=C1OC(O)C(O)C(O)C(O)C1O"/>



## Data Entry – Chemical Information

CAS Registry Number:   
(or other unique identifier)

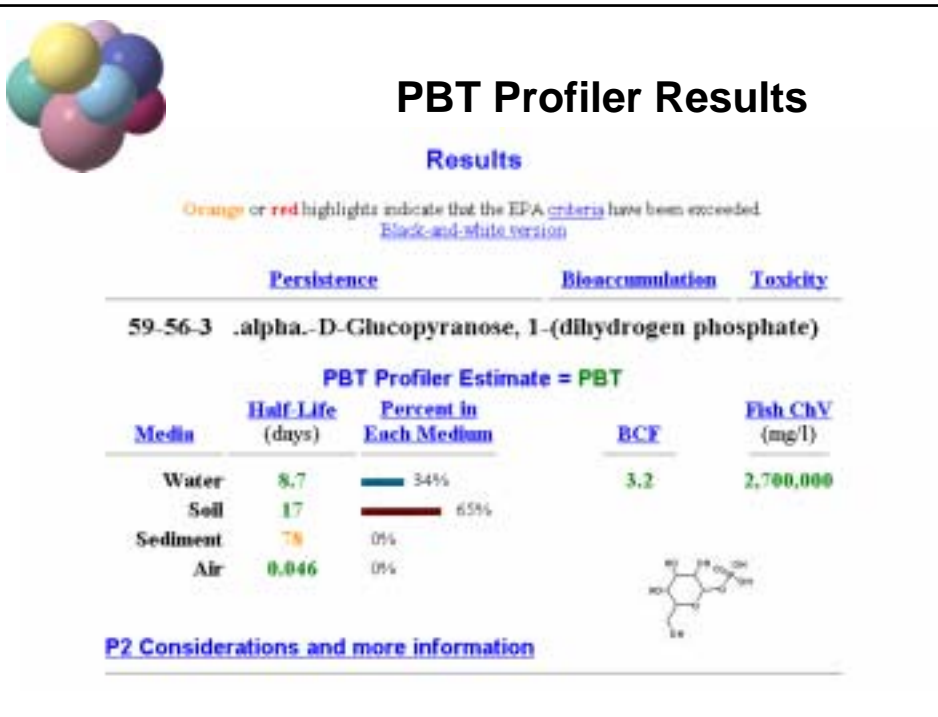
Name:

Smiles:   
120 characters or less

[Continue](#)

[Cancel](#)





**Data Entry – Warning Flags**

**Data Entry**

Tenaxphene 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)

Between the persistence, bioaccumulation, and toxicity of Tenaxphene by using 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:  [Submit](#)

[Clear search](#)

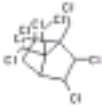
- Other flags
  - Metals
  - High molecular weight compounds (> 1,000)
  - Mixtures (representative structure provided)



## Results – PBT Criteria Exceeded

Persistence		Bioaccumulation		Toxicity
8001-35-2 Toxaphene				
PBT Profiler Estimate = PBT				
Screening estimates indicate this chemical may be a PBT - a P2 Assessment may allow further evaluation				
Media	Half-Life (days)	Percent in Each Medium	BCE	Fish CV (mg/l)
Water	180	2%	5,600	0.003
Soil	360	53%		
Sediment	1,600	45%		
Air	7.1	0%		

[P2 Considerations and more information](#)



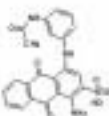

## Results –Chemical Categories

### Results

Orange or red highlights indicate that the EPA [criteria](#) have been exceeded.  
[Black and white version](#)

Persistence		Bioaccumulation		Toxicity
66736-54-7 2-Anthracenesulfonic acid, 4-[[3-(acetylamino)phenyl]amino]-1-amino-9,10-dihydro-9,10-dioxo-				
PBT Profiler Estimate = PBT				
Media	Half-Life (days)	Percent in Each Medium	BCE	Fish CV (mg/l)
Water	68	38%	3.2	21
Soil	129	67%		
Sediment	548	0%		
Air	0.079	0%		

[P2 Considerations and more information](#)



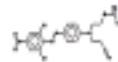
Based on its structure, this chemical may belong to the disinlines category. Members of this category may have potential human health concerns. [More information and category definitions.](#)



## Results - No Effect at Saturation

5261-31-4 Propanenitrile, 3-[2-(acetyloxy)ethyl]-4-(2,6-dichloro-4-nitrophenyl)azo-phenyl amino -

Media	Half-life (days)	PBT Profiler Estimate - PBT Percent in Each Medium	BCE	EqA CAV (mg/l)
Water	180	1.2%	18	0.032 *
Soil	360	70%		
Sediment	1,680	28%		
Air	0.22	0%		



### P2 Considerations and more information

\* The predicted water solubility, 0.032 mg/l, is less than the estimated BCE, 18 mg/l. There may be no effect at saturation.



## Chemicals That Can Not be Profiled

- Chemicals With Experimental Data
- Inorganic Chemicals
- Reactive Chemicals
- Salts (Organic Salts)
  - Sodium (Na), Potassium (K), and ammonium (NH<sub>4</sub><sup>+</sup>) salts can be Profiled
- High Molecular Weight Compounds (MW > 1000)
- Chemicals with Unknown or Variable Composition
- Mixtures
- Surfactants
- Highly Fluorinated Compounds



## Security and Anonymity

- All connections to the PBT Profiler are completely anonymous
- No user-entered or chemical information is purposefully or systematically written to a disk drive or other permanent storage device
- The only data collected are the number of home page visits (hits) and profiles run
- Computer code available on request



## P2 and the PBT Profiler





## Sample Chemicals to Show PBT Profiler Capabilities

PBT Profiler Capability	CAS Registry #
Flag for Metals	54-64-8
Flag for chemicals on EPA's PBT list and UNEP's POPs list	35822-46-9
Flag for Mixtures	1319-73-9
Results are All Green - no criteria exceeded	59-56-3
Results are All Red - all three criteria exceeded	8001-35-2
Persistent and bioaccumulative chemical with toxicity not estimated flag on results page	29082-74-4
Link to EPA's Chemical Categories for human health concerns	66736-54-7
Molecular weight > 1,000 flag	71216-03-0
Aquatic toxicity is NES - No Effects at Saturation	5261-31-4