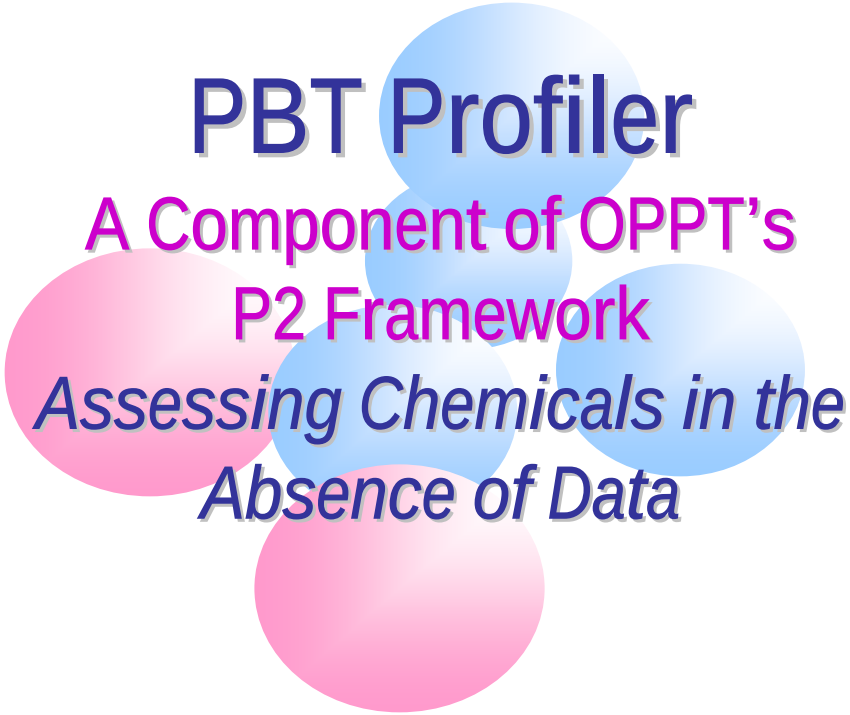
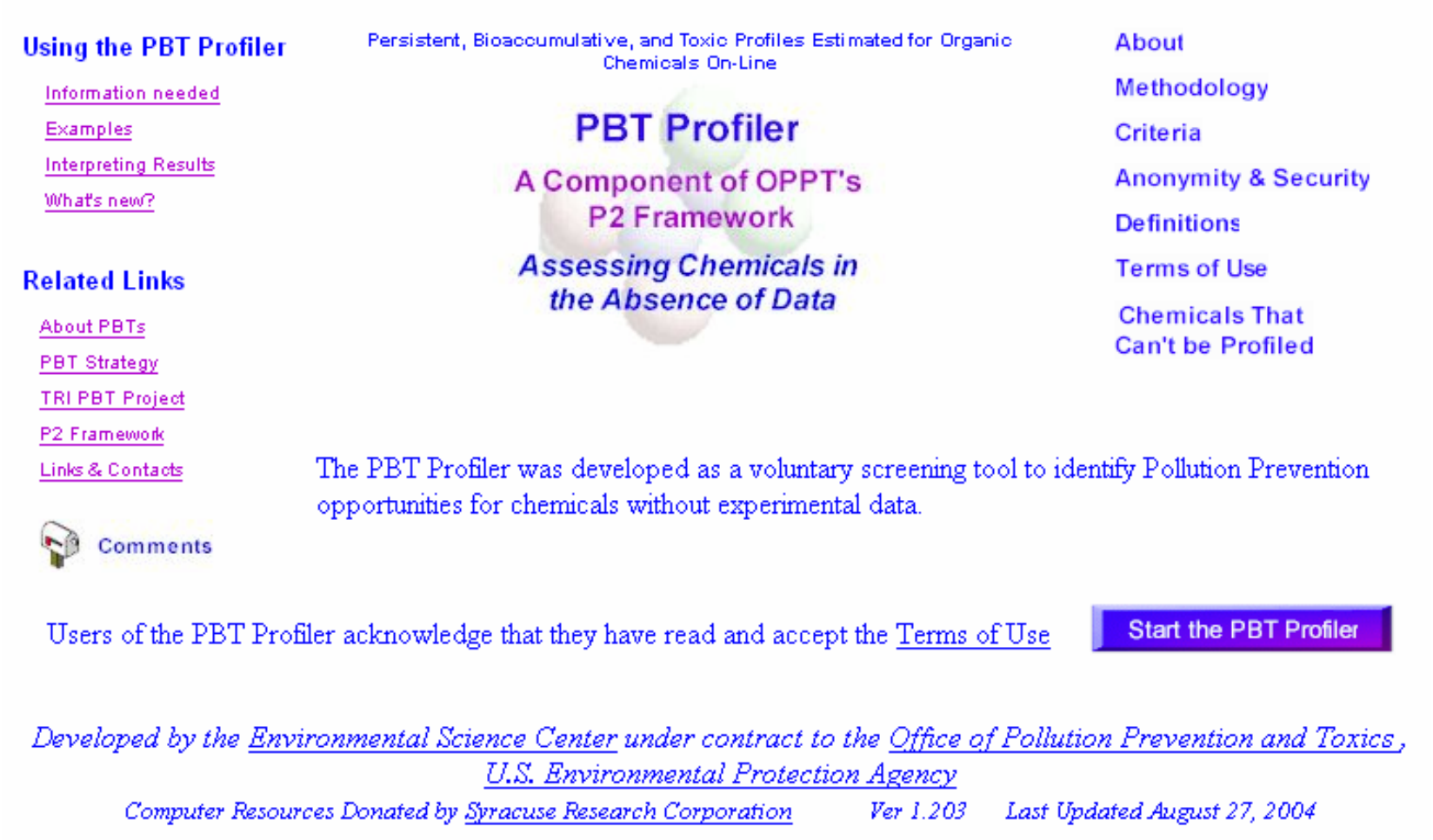
The PBT Profiler



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



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)
- Undergone 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_3 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)

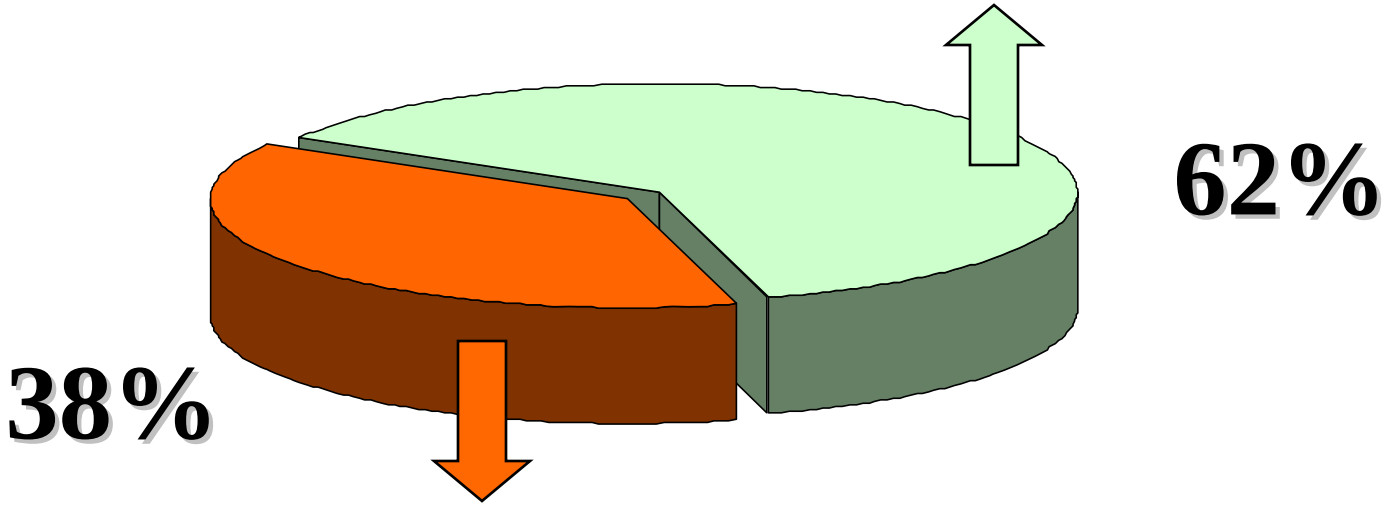
Profiler Technical Information

- 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

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]

P, B, & T Criteria

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

Bioaccumulation	Not Bioaccumulative	Bioaccumulative	
Fish BCF	< 1,000	≥ 1,000	≥ 5,000

Toxicity	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
4. EPA does not use the PBT Profiler to assess and identify new chemicals submitted as PreManufacture Notices (PMNs) under the Toxic Substances Control Act, as being in the New Chemicals Category for Persistent, Bioaccumulative, and Toxic Chemicals. Professional judgment of EPA OPPT subject matter experts is used to assign PBT concern levels to PMNs. The PBT Profiler does contain the same computer models used by EPA to screen PMNs for "P" and "B". However, for PMNs, "T" is determined by EPA OPPT human health experts using nearest analog analysis and is based on chronic oral systemic toxicity to humans, mammals, and birds.

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

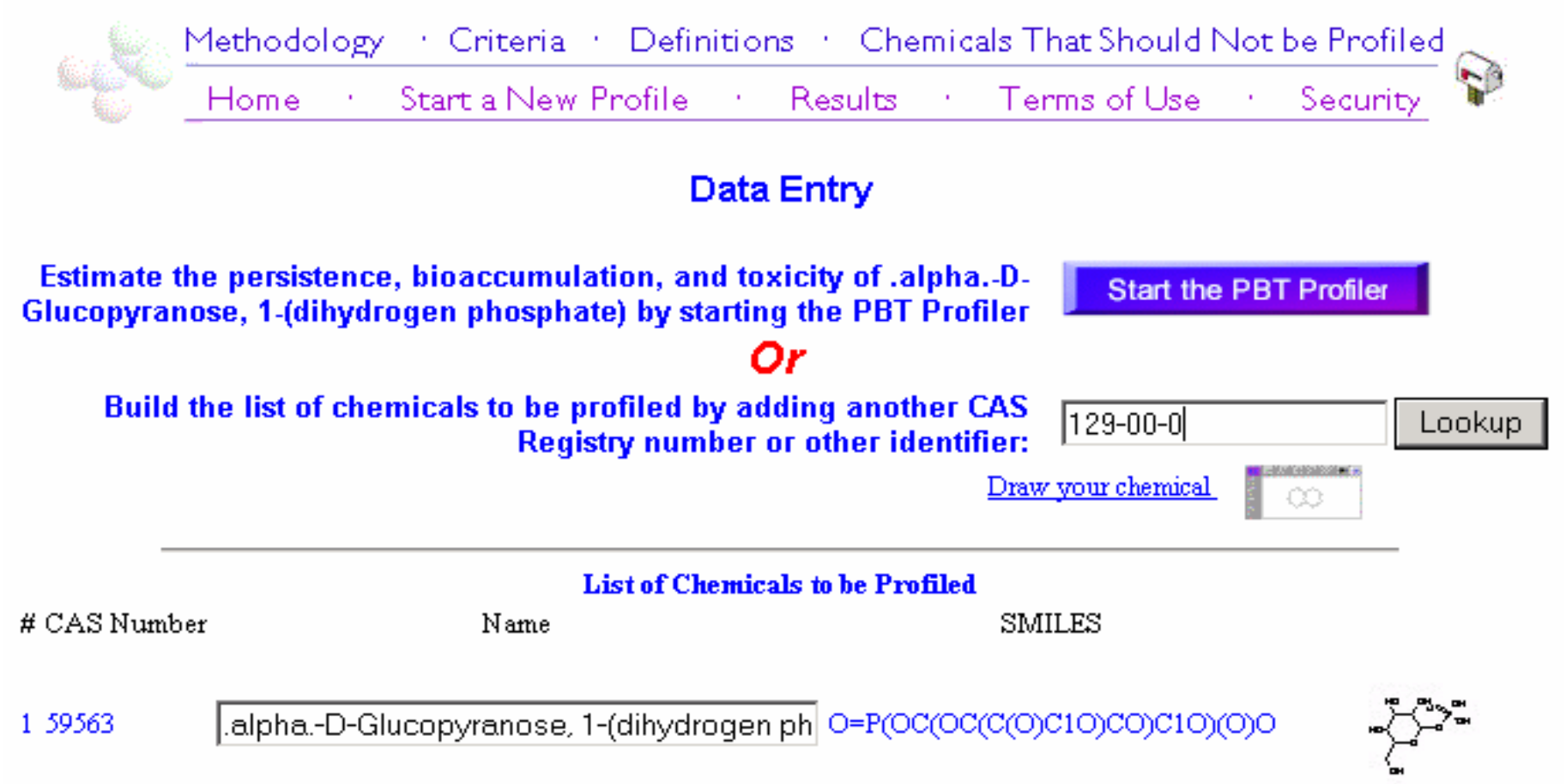
Before Using the Profiler (II)

Before running the PBT Profiler:

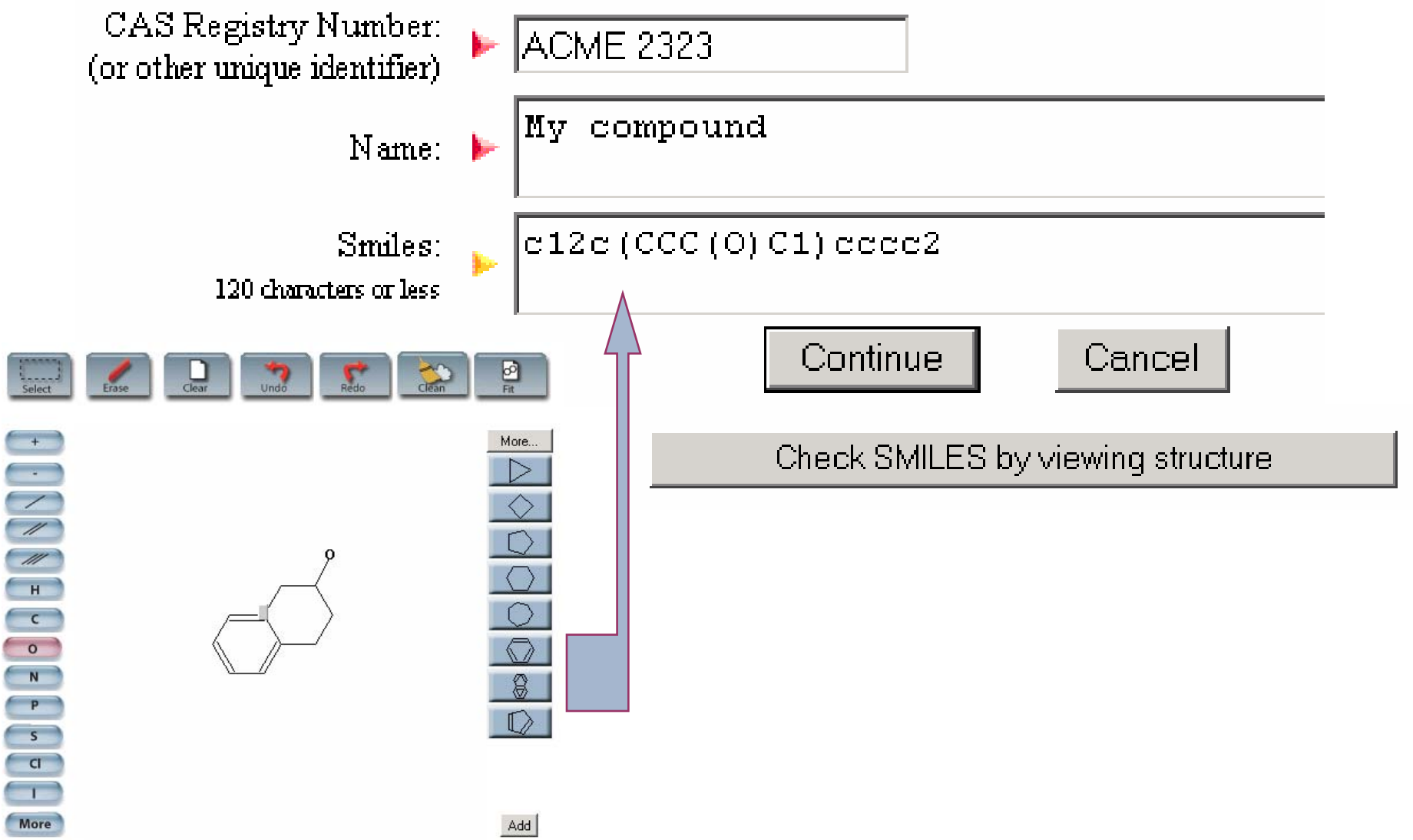
1. Determine the structure of the chemical you want to profile. Also have a chemical name and ID number (preferably a CAS Registry number) available.
2. Establish if any persistence, bioaccumulation, and toxicity data are available for your chemical. Chemicals with experimental data should not be profiled - 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



Data Entry – Structure



PBT Profiler Results

Results

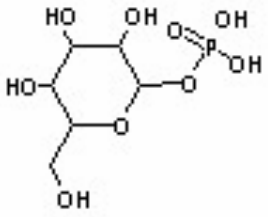
Orange or red highlights indicate that the EPA criteria have been exceeded.
Black-and-white version

Persistence			Bioaccumulation	Toxicity

59-56-3 .alpha.-D-Glucopyranose, 1-(dihydrogen phosphate)

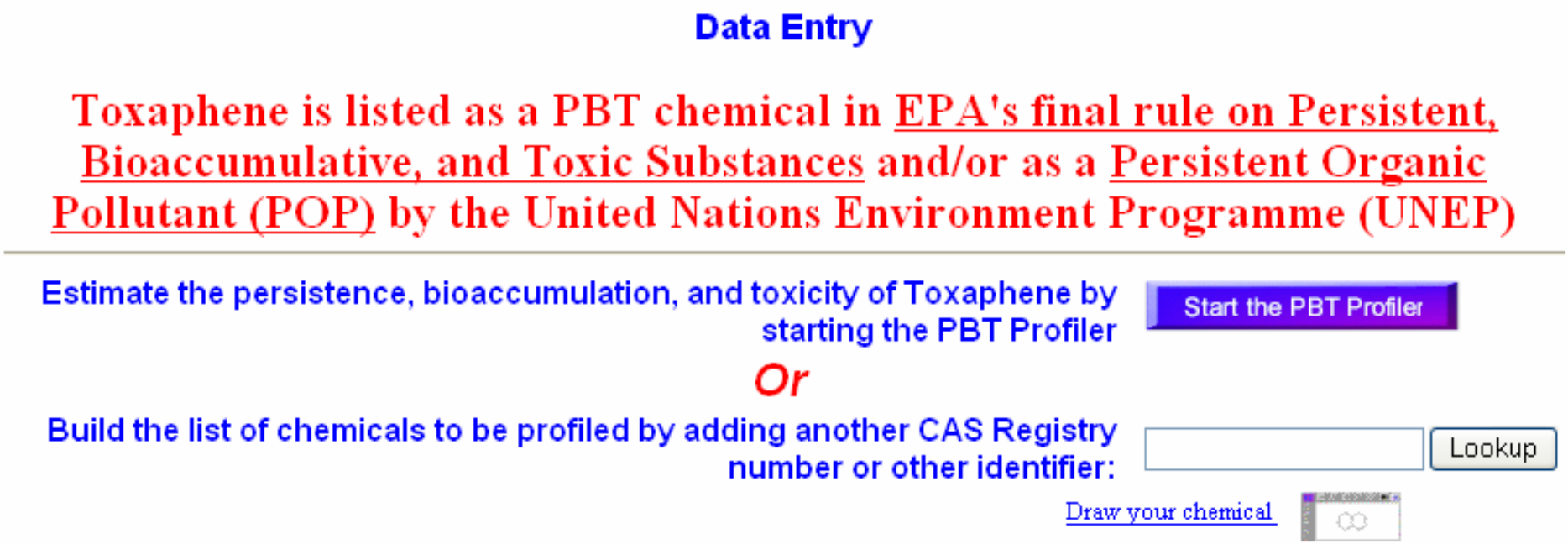
PBT Profiler Estimate = PBT

Media	Half-Life (days)	Percent in Each Medium	BCF	Fish ChV (mg/l)
Water	8.7	34%	3.2	2,700,000
Soil	17	65%		
Sediment	78	0%		
Air	0.046	0%		



P2 Considerations and more information

Data Entry – Warning Flags



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

Results – PBT Criteria Exceeded

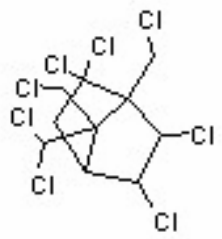
Persistence			Bioaccumulation	Toxicity

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	BCF	Fish ChV (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

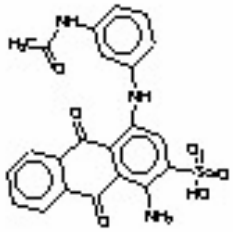
Results – Chemical Categories

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	BCF	Fish ChV (mg/l)
Water	60	38%	3.2	21
Soil	120	62%		
Sediment	540	0%		
Air	0.079	0%		



P2 Considerations and more information

- Based on its structure, this chemical may belong to the dianilines category. Members of this category may have potential human health concerns. More information and category definitions.

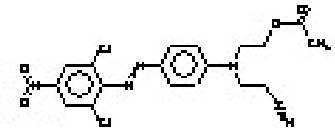
Results - No Affect at Saturation

Persistence | Bioaccumulation | Toxicity

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

PBT Profiler Estimate = PBT

Media	Half-Life (days)	Percent in Each Medium	BCF	Fish ChV (mg/l)
Water	180	2%	10	0.032 *
Soil	360	70%		
Sediment	1,600	28%		
Air	0.22	0%		



P2 Considerations and more information

* The predicted water solubility, 0.0058 mg/l, is less than the estimated ChV, 0.032 mg/l. There may be no effect at saturation.

P2 Considerations Information to Manage Risk

Pollution Prevention (P2) Considerations for "Phenol, 2,4,5-trichloro-"

PBT Profiler Estimate = P B T

Persistence Summary

Partitioning The PBT Profiler has estimated that if released to the environment, 'Phenol, 2,4,5-trichloro-' is expected to be found predominately in soil. It is also expected to be found in water and sediment.

Transformation and Persistence The PBT Profiler has estimated that 'Phenol, 2,4,5-trichloro-' is expected to be found predominately in soil and its persistence estimate is based on its transformation in this medium. Its half-life in soil, 120 days, exceeds the PBT Profiler criteria of >= 2 months (and <= 6 months). Therefore, 'Phenol, 2,4,5-trichloro-' is estimated to be persistent in the environment.

Pollution Prevention Considerations The PBT Profiler has estimated that the physical and chemical properties of 'Phenol, 2,4,5-trichloro-' indicate that it may have the potential to leach through soil and enter groundwater.

Long-Range Transport distances (CTD) The PBT Profiler has estimated that 'Phenol, 2,4,5-trichloro-' has a CTD in air of 2,400 Km. Using a published set of criteria, this value is considered relatively high, and 'Phenol, 2,4,5-trichloro-' has the potential to travel long from its original point of release.

Release Scenarios The following table provides the percent estimated in each environmental media using different release scenarios. The color of the estimates indicates if the PBT Profiler criteria have been exceeded in each medium, based on the following estimated half-lives for 'Phenol, 2,4,5-trichloro-': Water 60 days, Soil 120 days, Sediment 540 days, Air 7.5 days

Release to each Medium(Kg)			Percent in each medium			
Air	Water	Soil	Air	Water	Soil	Sed
1,000	1,000	1,000	1	13	84	2
1,000	1	1,000	1	1	98	0
1,000	1	1	13	6	80	1
1,000	1,000	1	5	55	31	8
1	1,000	1,000	0	14	84	2
1	1,000	1	0	86	1	13
1	1	1,000	0	0	100	0

Bioaccumulation Summary

Bioconcentration The estimated bioconcentration factor (BCF) for 'Phenol, 2,4,5-trichloro-' , 58, does not exceed the PBT Profiler criteria.

Bioaccumulation Estimate The PBT Profiler estimates that 'Phenol, 2,4,5-trichloro-' is not expected to bioaccumulate in the food chain.

Toxicity Summary

Fish Chronic Toxicity The estimated fish chronic toxicity value (ChV) for 'Phenol, 2,4,5-trichloro-' , 0.053 mg/l, exceeds the PBT Profiler criteria (<0.1 mg/l).

Toxicity Estimate The PBT Profiler estimates that 'Phenol, 2,4,5-trichloro-' is estimated to be toxic to fish.

Validation of Profiler Methodology

- **External**
  - **Comparison of Aquatic Toxicity Experimental Data with EPA/OPPT/SAR Prediction on PPG Polymers**

    J. S. Chun, J. V. Nabholz, and M. J. Wilson. PPG Industries, Inc., Pittsburgh, PA, and US EPA, OPPTS, Washington, DC.
  - **Comparison of Environmental Fate Data from the PBT Profiler with Data Found in the Literature**

    Dr. H. Burleigh-Flayer, PPG Industries, Inc., Pittsburgh, PA.

    Both studies are available on the Sustainable Futures web site
- **Internal**
  - **Comparison of PBT Profiler results with evaluated environmental persistence values published in Mackay, D; Shiu, W.Y.; Ma, K. Physical-Chemical Properties & Environmental Fate on CD-ROM. CRC Press. ISBN/ISSN: 0849321921 (2000).**
  - **Study available at http://www.pbtprofiler.net/methodology.asp**

Security and Anonymity

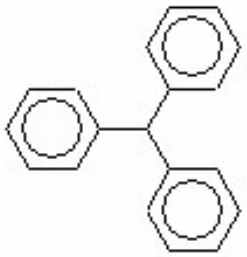
- All connections to the PBT Profiler are completely anonymous
- No user-entered or chemical information is purposefully or systematically written to a disk drive or other permanent storage device
- The only data collected are the number of home page visits (hits) and profiles run
- Computer code available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

P2 and the PBT Profiler

PBT Profiler Estimate = PBT

Screening estimates indicate this chemical may be a PBT - a P2 Assessment may allow further evaluation

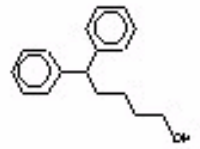
Media	Half-Life (days)	Percent in Each Medium	BCF	Fish ChV (mg/l)
Water	38	8%	2,700	0.027
Soil	75	53%		
Sediment	340	39%		
Air	1	1%		



P2 Considerations and more information

PBT Profiler Estimate = PBT

Media	Half-Life (days)	Percent in Each Medium	BCF	Fish ChV (mg/l)
Water	15	18%	170	0.12
Soil	30	73%		
Sediment	140	9%		
Air	0.75	1%		



P2 Considerations and more information

Profiler and EPI Differences (I)

- **Half-life in water, soil and sediment**
  - **Profiler multipliers = 1/2/9**
  - **Default EPI multipliers = 1/1/4**
- **Result**
  - **Half-lives in soil and sediment are longer in the Profiler estimates**
  - **Differences in the percent in each environmental compartment**
- **Reason**
  - **Design feature to obtain the persistence ranking for the Profiler Summary Output**

Profiler and EPI Differences (II)

- **Toxicity estimates**
  - **ECOSAR always uses the estimated Kow; the Profiler will use an experimental value, if available**
- **Air half-life**
  - **The Profiler uses both the hydroxyl radical and ozone reaction rates**
- **Level 3 multimedia (Fugacity) model**
  - **EPI may use a different Henry's Law constant**

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