EPA’s PBT Profiler

PBT Profiler Helps Identify Persistent, Bioconcentrating and Toxic Chemicals

Workshop on PBT Reduction Activities and Opportunities, NEWMOA Web Conference
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What is the PBT Profiler?

✓ Estimate Persistence, Bioconcentration Potential, and Fish Chronic Toxicity of a Chemical From the Structure
✓ Compares predictions to EPA regulatory criteria for PBT-related action under TRI and TSCA New Chemical Program (PMNs), and to international criteria
✓ Provides PBT-related data previously unavailable
  – Measured data retrieved if available
  – Predictions when data are lacking
✓ Useful when data are lacking about the chemical

R&D Process - Status Quo

Performance
Available
Cost

Chemicals Meeting All the Desired Criteria Will Be Evaluated Based on Additional Criteria:

Market Research
Final Product Development

Chemicals in Commerce

Industrial Chemicals
~80,000 on TSCA Inventory
~2,000 new chemicals/year
Relatively little Hazard data are available
Stakeholders make chemical choices among competing products/processes
Stakeholders are often forced to choose among chemicals without information on PBT tradeoffs.

Which chemicals are PBTs?

Pesticides
~2000
Drugs, Cosmetics, Food Additives
~2,000

Chemicals Are Considered PBTs If They Meet EPA and/or International PBT Criteria For

✓ Environmental Persistence AND
✓ Bioconcentration Potential AND
✓ Toxicity

Agenda

Chemicals and PBTs
PBT Profiler
PBT Profiler Demo
Next steps
EPA’s PBT Profiler

Persistence (P) Criteria and Color scheme in PBT Profiler

<table>
<thead>
<tr>
<th>Environmental Compartment</th>
<th>Not Persistent</th>
<th>Persistent</th>
<th>Highly Persistent</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water (EPA NCP Program)</td>
<td>&lt; 2 months</td>
<td>≥ 2 months</td>
<td>&gt; 6 months</td>
</tr>
<tr>
<td>Soil</td>
<td>&lt; 2 months</td>
<td>≥ 2 months</td>
<td>&gt; 6 months</td>
</tr>
<tr>
<td>Air (TRI)</td>
<td>&lt; 2 days</td>
<td></td>
<td>≥ 2 days</td>
</tr>
<tr>
<td>Sediment</td>
<td>&lt; 2 months</td>
<td>≥ 2 months</td>
<td>&gt; 6 months</td>
</tr>
</tbody>
</table>

Bioconcentration (B) Criteria and Color scheme in PBT Profiler

<table>
<thead>
<tr>
<th>Bioconcentration Factor, Fish BCF</th>
</tr>
</thead>
<tbody>
<tr>
<td>Low</td>
</tr>
<tr>
<td>Moderate</td>
</tr>
<tr>
<td>High</td>
</tr>
</tbody>
</table>

Fish Chronic Toxicity (T) Criteria and Color scheme in PBT Profiler

<table>
<thead>
<tr>
<th>Toxicity Concern: Fish ChV (mg/l)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Low</td>
</tr>
<tr>
<td>Moderate</td>
</tr>
<tr>
<td>High</td>
</tr>
</tbody>
</table>

| Low                              |
| Moderate                         |
| High                             |

<table>
<thead>
<tr>
<th>Toxicity Concern: Fish ChV (mg/l)</th>
</tr>
</thead>
<tbody>
<tr>
<td>&gt; 10 mg/l or no effects at saturation</td>
</tr>
<tr>
<td>&lt; 10 mg/l</td>
</tr>
<tr>
<td>&lt; 0.1 mg/l</td>
</tr>
</tbody>
</table>

Which Chemical is a PBT?

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
</tr>
</thead>
<tbody>
<tr>
<td>PBT</td>
<td>PBT</td>
<td>PBT</td>
<td>PBT</td>
</tr>
</tbody>
</table>

Low | Green
Moderate | Orange
High | Red

Status of the PBT Profiler

- Created by EPA to address the PBT Initiative
- Developed as a collaborative effort with industry (ACC, SOCMA, CCC) and NGOs (ED)
- Beta tested by more than 100 participants from industry, academia, and government
- Peer Reviewed following EPA’s Peer Review Guidelines and Peer Review is posted on EPA’s E-Docket
- http://cascade.epa.gov/RightSite/dk_public_home.htm, “quick search” for “PBT Profiler”
- Released to the public in Sept 2002 and available at no cost at www.pbtprofiler.net

Why EPA Is Making The PBT Profiler Available to Industry?

- Help Industry Pre-Screen Chemical Alternatives
- Understand Potential PBT Characteristics Of Product Alternatives Under Consideration at R&D
- Understand Potential PBT Trade-offs of Alternatives Under Consideration
- Reduce Product Development Costs
- Stimulate the Development of Environmentally Preferable Products and Processes
EPA’s PBT Profiler

Hazard-related Information from PBT Profiler
✓ Once released, will chemical go to air, water, soil, sediment?
✓ How long will chemical stay in media?
✓ Will chemical present a hazard?

www.pbtprofiler.net

PBT Profiler Environmental Media Compartments

Air

Water

Soil

Sediment

PBT Profiler

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 a new profile

Terms of Use

Need help?
Register registry item(s)
SMILES String
Query the database
Chemical structure:
## EPA’s PBT Profiler

### PBT Profiler (Output o-Xylene, CAS 95-47-6)

#### Results

<table>
<thead>
<tr>
<th>Persistence</th>
<th>Bioaccumulation</th>
<th>Toxicity</th>
</tr>
</thead>
<tbody>
<tr>
<td>95-47-6 o-Xylene</td>
<td>PBT</td>
<td></td>
</tr>
</tbody>
</table>

#### PBT Profiler Estimate = PBT

<table>
<thead>
<tr>
<th>Media</th>
<th>Half Life (days)</th>
<th>Percent in Each Medium</th>
<th>BCF</th>
<th>Fish CHL (mg/l)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>15</td>
<td>32%</td>
<td>50</td>
<td>1.1</td>
</tr>
<tr>
<td>Sediment</td>
<td>149</td>
<td>1%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Air</td>
<td>1.2</td>
<td>10%</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

#### P2 Considerations

- Water: 15 days, 32% 50, 1.1
- Sediment: 149 days, 1%
- Air: 1.2 days, 10%

### Pollution Prevention (P2) Considerations for o-xylene

#### PBT Profiler Estimate = PBT

- Return to PBT Profiler Results

#### PBT Profiler Physical/Chemical Property Estimates

- Molecular Weight: 110
- Melting Point: -46 degrees C
- Vapor Pressure: 4.3 mm Hg at 25 degrees C
- Log Kow: 3.1 at 25 degrees
- Water Solubility: 240 mg/L at 25 degrees C
- Henry’s Law Constant: 0.0066
- Hydroxyl Radical Reaction Rate Constant: 0.000000000013 cm²/molecule-s at 25 degrees C

### Overall Persistence

The overall persistence is calculated from the chemical's physical and chemical properties to estimate its persistence in the environment. The persistence is calculated using various equations and models to estimate the rate at which the chemical will degrade or persist in the environment. The overall persistence is determined by considering the chemical's half-life, bioaccumulation potential, and other factors that affect its persistence. The overall persistence is expressed as a persistence index (pI), which ranges from 0 (no persistence) to 100 (high persistence). The pI is calculated using the following equation:

\[ pI = \frac{\text{Half Life} \times \text{Bioaccumulation} \times \text{Toxicity}}{100} \]

### Reference Formulas

- The PBT Profiler estimate persistence is based on a chemical's reaction kinetic constant in soil, water, and air. It uses a log Kow equation which calculates the persistence of the chemical in the environment. The log Kow is calculated using the following equation:

\[ \log Kow = \frac{\text{Octanol-Water Partition Coefficient}}{5} \]

- The PBT Profiler estimate persistence is also based on the chemical's reaction kinetic constant in soil, water, and air. It uses a log Kow equation which calculates the persistence of the chemical in the environment. The log Kow is calculated using the following equation:

\[ \log Kow = \frac{\text{Octanol-Water Partition Coefficient}}{5} \]

### Long Range Transport (LRT)

- The Chemical Transport Model (CTM) is an expression of a chemical's potential for Long Range Transport (LRT). It provides an estimate of the long-range transport potential of a chemical. The CTM is calculated using the following equation:

\[ \text{LRT} = \frac{\text{Half Life} \times \text{Bioaccumulation}}{100} \]

The PBT Profiler estimate persistence is based on the chemical's reaction kinetic constant in soil, water, and air. It uses a log Kow equation which calculates the persistence of the chemical in the environment. The log Kow is calculated using the following equation:

\[ \log Kow = \frac{\text{Octanol-Water Partition Coefficient}}{5} \]
EPA’s PBT Profiler

Benz(a)anthracene (CAS 56-55-3)

Chemicals That Should Not be Profiled Using the PBT Profiler
- Chemicals With Experimental Data - Don’t use predicted data when measured data exist!
- Inorganic Chemicals
- Chemicals that Rapidly Hydrolyze - Acid Halides; Isocyanates; Sulfonfluryid Chlorides; Siloxanes; alpha-Chloro ethers. Note: hydrolysis products can be evaluated.
- Cationic salts of Group I, Group II, Transition metals, Actinide, and Lanthanide
- Organo Metallic Compounds
- Highly Reactive Compounds
- High MW Compounds, polymers, chems w MW > 1,000
- Mixtures – Each substance in mixture can be evaluated
- Chemicals with Unknown or Variable Composition

Benz(a)anthracene (CAS 56-55-3)

Limitations of the PBT Profiler
- Chemicals That Cannot Be Profiled (62%)
  - Discrete organics
  - Mixtures with representative component

Flag for Chemicals on PBT Lists

Mixed Xylenes (CAS 1330-20-7)

Example of Flag for Mixtures

Start a New Profile

Note: The CAS Registry Number, 1330-20-7 [Xylene mixed], corresponds to a mixture of one or more substances. The PBT Profiler selected a representative structure for this mixture. This representative structure may, or may not, correspond to the mixture you are profiling. Therefore, the Persistence, Bioaccumulation, and Toxicity of this mixture may not be accurately represented by the PBT Profiler.

As with all mixtures, the results of the PBT Profiler should be carefully scrutinized and used with caution. More information on the use of mixtures in the PBT Profiler is available on the Chemicals That Should Not Be Profiled page.

Add this Representative Structure to the Profile

Cancel
EPA’s PBT Profiler

CAS 7439-97-6

Start a New Profile

This Chemical Can Not Be Profiled.
The chemical, MERCURY, is either an inorganic compound or it contains a metallic element that the estimation methods used in the PBT Profiler were not designed for. More Information on chemicals that can not be profiled using the PBT Profiler is available on this web site.

OK

PBT Profiler 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 PBT Profiles run

PBT Profiler User Quotes

“The PBT profiler is an excellent tool to add to my risk assessment of existing and new chemicals”

“I will encourage my chemists to use it in their research projects in addition to the regulatory/tox assessment that I am responsible for.”

“We think this is a useful tool... for new raw’s we will surely check it.”

“This fits in well with our internal policy on lifecycle analysis and product stewardship.”

“The PBT Profiler is an excellent instrument for a first screening of the potential impacts of substances”

P2 & PBT screening in the absence of data

PBT Comparison of Solvent A and Potential new Alternatives (B,C)  All solvents have no data

The key to managing PBTs is Pollution Prevention

✓ The EPA PBT Profiler is an excellent tool for Chemical Choosers and Chemical Formulators

PBT Profiler: Next Steps

✓ UNH Provides technology transfer and technical assistance in PBT Profiler
✓ Identify industry partners interested in using the PBT Profiler in case studies/success stories.
✓ Identify Small Business partners interested in using the PBT profiler in the decision making process.
EPA’s PBT Profiler

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Acknowledgment

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Thank you for your time.