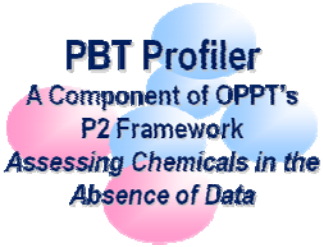
7 Estimating Persistence, Bioaccumulation, and Toxicity using the PBT Profiler



7.1 What are PBTs?

PBTs are chemicals that are toxic, persist in the environment and bioaccumulate in food chains and, as a result, pose risks to human health and ecosystems. The biggest concerns about PBTs are that they may transfer among air, water, and land, and span boundaries of programs, geography, and generations. EPA has information on some of the best known PBTs including DDT, PCBs, dioxins and furans, toxaphene, and mercury at http://www.epa.gov/opptintr/pbt/pubs/cheminfo.htm. Additional information on PBTs can be found at this EPA's New Chemical web site http://www.epa.gov/opptintr/pbt/.

7.2 What Does the PBT Profiler Do?

The PBT Profiler, available at http://www.pbtprofiler.net/, is an online hazard-screening tool that predicts a chemical's potential to persist in the environment, bio-concentrate in food chains, and be toxic, properties which cause concern for human health and the environment.

The PBT Profiler estimates Persistence, Bioconcentration potential, and fish chronic Toxicity from chemical structure and determines if the P, B, and T properties of the chemical are expected to exceed the PBT criteria established under EPA's New Chemicals Program and Toxic Release Inventory (TRI). The PBT Profiler also uses a Level III multi-media model to estimate distribution in water, soil, sediment, and air; and tells the user if the chemical belongs to a category that is known to present human health or ecological concerns as described in EPA's Chemicals Category Report.

Development

The PBT Profiler was developed by EPA through a collaborative effort with the American Chemistry Council (ACC), the Society of Chemical Manufacturers and Affiliates (SOCMA), the Chlorine Chemistry Council (CCC), and Environmental Defense. It was developed to be a voluntary screening tool to identify pollution prevention opportunities for chemicals without experimental data.

Information Needed to Use the PBT Profiler

Before you attempt to use the PBT Profiler you should review the online guidelines describing the information users should have before running the model, which is available at http://www.pbtprofiler.net/information.asp. This necessary information includes:

1. Chemical Identity: chemical name, ID Number such as CAS RN, however any other ID is acceptable;
2. Chemical Structure: discrete or representative structures must be entered using SMILES (see Appendix F of this manual for help on SMILES), CAS RN, or drawn using the applet available;
3. Nature of the Chemical: do not profile chemicals that are reactive, hydrolyze, have high molecular weight (>1,000), are of unknown or variable composition, or contain any metallic elements;
4. Chemical Composition: chemicals with variable composition cannot be entered unless a representative structure can be determined; and
5. Look for measure data: remember that measured data are preferred over screening-level estimations. Refer to Chapter 3 of this manual "Getting Started by Identifying Existing Data," for help in finding existing data.

7.3 How Does the PBT Profiler Work?

Extensive information on the methodology behind the PBT Profiler is available within the online method at http://www.pbtprofiler.net/Methodology.asp. This information is briefly summarized in this section.

7.3.1 Predictive Methods Incorporated into the PBT Profiler

The PBT Profiler was constructed using some of the same methods incorporated into EPISuite™ and ECOSAR to make its predictions, for example:

- Persistence in Air is estimated using AOPWIN, and persistence in Water / Soil / Sediment using the ultimate biodegradation expert survey module of the BIOWIN.
- Percentage in Each Medium is estimated using Mackay' Level III multimedia mass balance model (also called a fugacity model).
- Bioaccumulation is provided directly from an estimated bioconcentration factor (BCF) generated by BCFWIN.
- Toxicity to fish is estimated using the class-specific fish chronic value (ChV) from ECOSAR.

7.3.2 PBT Criteria

The image to the right shows the both criteria and the color coding which indicates if the criteria have been exceeded. If the criteria are not exceeded the value is in **green** font, if the criteria are exceeded the results are in **orange** font, and if they are greatly exceeded the results are in **red** font. The criteria used by the PBT Profiler are briefly described below. For more details on the criteria used to identify potential PBT chemicals see the PBT Profiler online help at http://www.pbtprofiler.net/criteria.asp. The site has links to the Federal Register Notices describing each of the 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*	> 10 mg/L Or No Effects at Saturation	0.1-10 mg/L	< 0.1 mg/L

*EPA New Chemical Program Criteria
**TRI Criteria

Persistence Criteria
The PBT Profiler combines the persistence criteria used by the New Chemicals Program for water, soil, and sediment and highlights chemicals with an estimated half-life ≥ 2 months and < 6 months in orange text and those with an estimated half-life ≥ 6 months in red. The half-life in air, which is the TRI Reporting criteria, is not used in the PBT Profiler's Persistence summary. The PBT Profiler uses 30 days in a month for its comparisons.

Bioaccumulation Criteria
The PBT Profiler uses a bioconcentration factor (BCF) as the indicator of a chemical's potential to bioaccumulate. Bioconcentration is uptake of a chemical from the surrounding media by an organism living in that media.

Toxicity
The PBT Profiler uses criteria developed in EPA's New Chemical Program to highlight a chemical that may be chronically toxic to fish. These criteria are:

	Low Concern	Moderate Concern	High Concern
Fish ChV (mg/L)	> 10 mg/L	0.1 - 10 mg/L	< 0.1 mg/L

7.4 Interpreting PBT Profiler Predictions

7.4.1 Three Levels of Predictions

The PBT Profiler was designed to be easy to interpret and provide results in three levels of detail. These three levels of detail include:

- P, B, and T estimates compared to EPA criteria with results in color-coded output (Level 1),
- Quantitative results (Level 2), and
- Additional information for P2 assessments (Level 3).

7.5 Cautions Regarding Use of the PBT Profiler

7.5.1 Screening Level Caveats

The PBT Profiler is a screening-level method that, like all screening methods, has certain limitations. The PBT Profiler is best used as a research tool to identify chemicals that may need further evaluation for potential persistence, bioaccumulation and toxicity.

7.5.2 Chemicals That Should Not be Profiled

There are a number of chemical classes that should not be investigated using the PBT Profiler. These chemicals are summarized here but more detailed information on these chemicals and why they should not be profiled is available in the online model at http://www.pbtprofiler.net/Chemicals.asp.

Important classes of chemicals that should not be profiled are provided below.

Chemicals with Experimental Data: Predicted data should not be used in place of experimental data from a well conducted laboratory studies.

Inorganic Chemicals: The estimation methods used in the PBT Profiler were designed and developed for organic chemicals. Inorganic chemicals (chemicals that do not contain Carbon) will not provide reliable results and should *not* be profiled.

Reactive Chemicals: Reactive chemicals, those that have a half-life of less than 60 days under "normal" environmental conditions, should not be profiled. By their nature these chemicals would meet the criteria of the "not persistent" category. Examples of reactive chemicals are provided in the online model.

Salts (Organic Salts): Only salts of Sodium (Na), Potassium (K) salts, and Ammonium (NH4+) can be profiled because the p/chem and fate of these compounds are well documented in the environmental literature.

High Molecular Weight Compounds: Polymers and chemicals with an average molecular weight >1,000 should not be profiled as the physical property estimation methods were not developed for these types of compounds.

Chemicals with Unknown or Variable Composition: Compounds with a variable composition, such as oligomers, natural fats, or a product mixture that changes composition depending on the reaction conditions, should not be profiled.

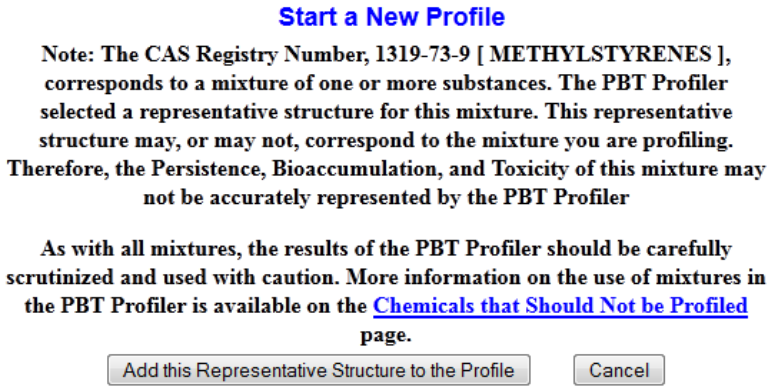
Mixtures: If the chemical you want to profile is a mixture of discrete organic substances, each substance can be run through the PBT Profiler separately and the result can be compared. If there is one component of a mixture that predominates, then it may be used to represent the entire mixture (i.e., a representative structure can be entered), however results should be interpreted with caution.

Surfactants: Surfactants should not be run through the PBT Profiler. Surfactants do not typically dissolve in water; instead, they tend to form micelles (dispersed aggregates of the surfactant molecules). Because they form dispersion, their water solubility and other environmental fate parameters cannot be accurately estimated using the methodology employed by the PBT Profiler.

\Highly Fluorinated Compounds: Many highly fluorinated chemicals (those that have more fluorines than non-fluorine atoms bonded to carbon), including fully fluorinated organics (those that have all hydrogens on carbon replaced with fluorine), have physical/chemical and environmental fate properties that are very different from their non-substituted analogs. The models used by the PBT Profiler do not accurately predict the unique characteristics of these materials, although the estimation methods are continually improving as more data become available.

Built in Flags

The PBT Profiler has built-in flags that are intended to warn the user if an inappropriate chemical has been profiled. These warning flags are displayed when the user enters a chemical that should not be profiled. The flag for mixtures is shown to the right. Other flags and sample CAS Numbers that trigger each flag are listed below.



PBT Profiler Flag	Sample CAS RN that triggers Flag
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

7.5.3 If the Profiler Identifies a Chemical as a Possible PBT

If the chemical being evaluated is identified as a potential PBT, the user should conduct further evaluations of the chemical. These evaluations can include:

- Verifying chemical composition (including structure),
- More extensive data searches,
- Estimations using other methods,
- Estimation of possible releases to the environment and any resulting exposures, or
- Comparing the estimated results with a data-rich chemical that has a similar structure.

If testing is necessary to confirm estimations, EPA's Office of Chemical Safety and Pollution Prevention has developed a series of Harmonized Test Guidelines for use when testing chemicals, and in the development of data submissions to the Agency. Consultation with a scientist who can assist with these evaluations may be helpful.

After running a chemical through the PBT Profiler, the user can click on "P2 Considerations" on the bottom of the "Results" page to get useful information on how the chemical is predicted to behave if released to air, water, or soil. General users are encouraged to work with scientists (chemists,

toxicologists, or risk assessors) to be sure the method is used properly and results are interpreted properly.

7.6 Evaluation / Validation Studies of the PBT Profiler

7.6.1 Beta Test and Peer Review

The PBT Profiler was beta tested and peer reviewed before being released to the public in September 2002. The PBT Profiler Peer Review can be obtained online at www.regulations.gov by searching for Docket ID: EPA-HQ-OPPT-2002-0025. The list of all documents in the docket will be displayed and most can be downloaded as PDFs.

The PBT Profiler Methodology describes the results of two exercises comparing predictions from the PBT Profiler with measured data for known PBT chemicals. The first evaluation compared summary results of the PBT Profiler to organic chemicals generally recognized as being PBTs; the 64 PBT organic chemicals in EPA's final PBT Rule for TRI and the 12 United Nations Environment Programme (UNEP) Persistent Organic Pollutants (POPs). For the 64 chemicals in EPA's TRI Rule, the PBT Profiler flagged 49 as PBTs and 13 as persistent and bioaccumulative with the toxicity "not estimated." As indicated on the "Interpreting the PBT Profiler Results" Page, persistent and bioaccumulate chemicals may accumulate in the environment to relatively high levels. Similar results were obtained for the 12 POPs (using a representative structure for the PCBs, polychlorinated dioxins, and polychlorinated furans). All but 3 of the POPs are listed in the final TRI rule.

The second evaluation compared summary results of the PBT Profiler to a published data set containing evaluated environmental persistence values [Mackay, D; Shiu, W.Y.; Ma, K. Physical-Chemical Properties & Environmental Fate on CD-ROM. CRC Press . ISBN/ISSN: 0849321921 (2000)]. Analysis of these data reveals that, in general, the PBT Profiler summaries were in very good agreement with the published data.

7.6.2 Case Studies Using the PBT Profiler

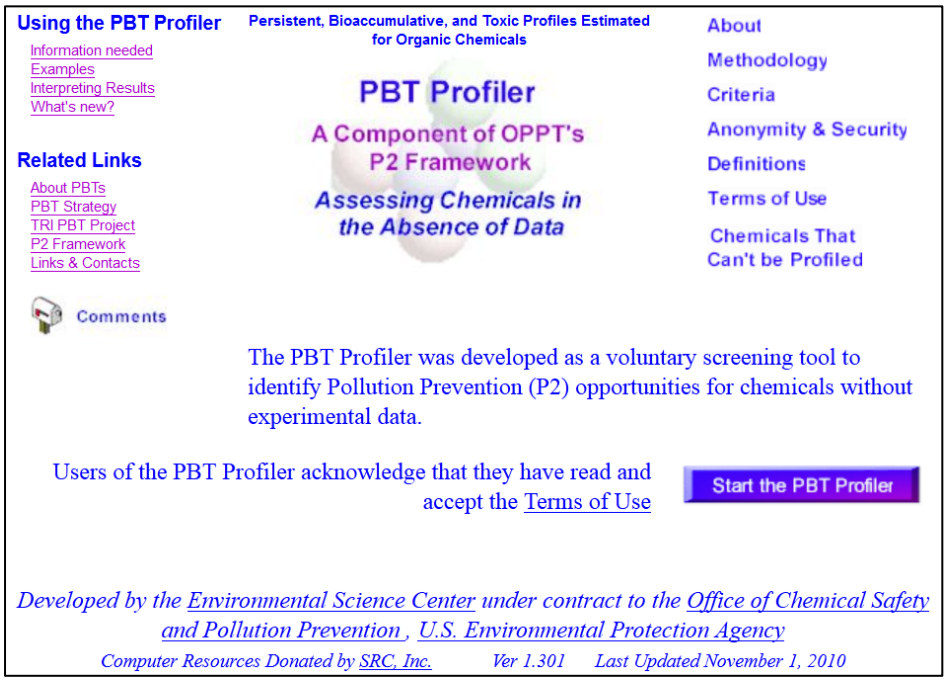
A number of companies participating in Sustainable Futures have conducted case studies in the application of the Sustainable Futures / P2 Framework methods, including the PBT Profiler. These case studies, which are available on the Sustainable Futures web site, include:

- SC Johnson's Use of the EPA PBT Profiler to Screen SC Johnson's Chemical Inventory (PDF),
- Bayer's Experience In The Use And Application Of The PBT Profiler for Predicting Persistence, Bioconcentration and Aquatic Toxicity of Chemical Substances (PDF), and
- Eaton Aeroquip Inc.'s Experience In the Use and Application of the PBT Profiler for Predicting Persistence, Bioconcentration, and Toxicity of Chemical Substances (PDF).

7.7 Running the Sample Chemical in the PBT Profiler

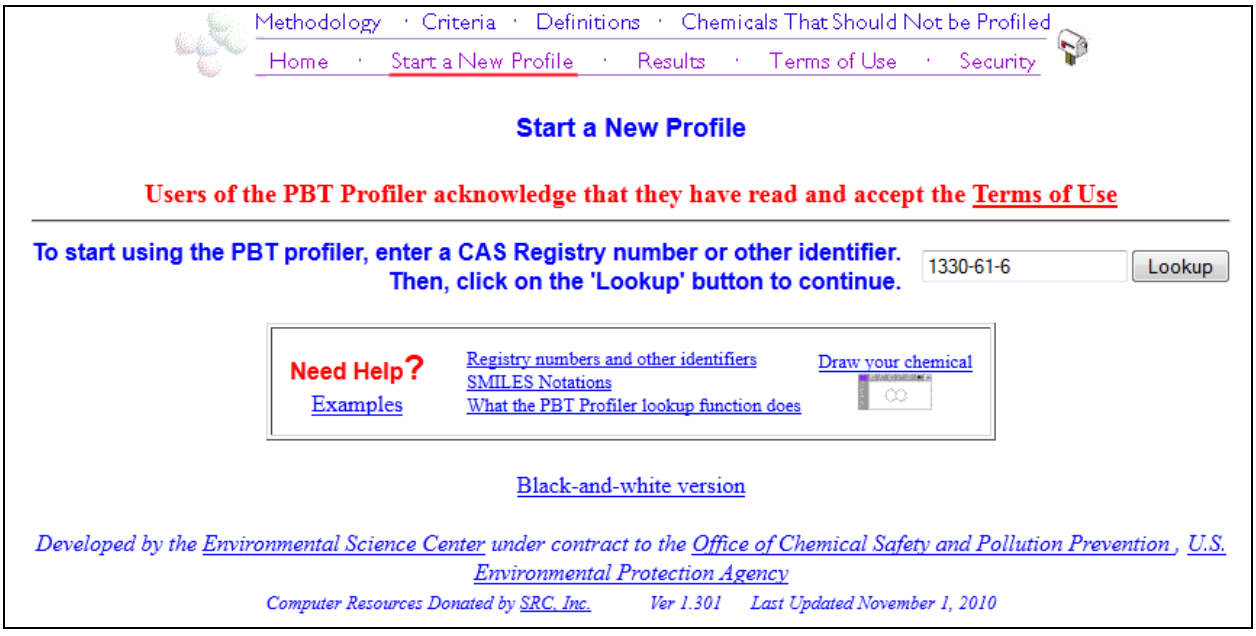
You can access the PBT Profiler online at www.pbtprofiler.net.

The opening screen is shown to the right. When you click on "Start the PBT Profiler" you go to a page that explains the purpose of the PBT Profiler and provides cautions on its use. In order to continue using the PBT Profiler you need to click on a button acknowledging that you have read and understand the issues and considerations relating to the PBT Profiler.

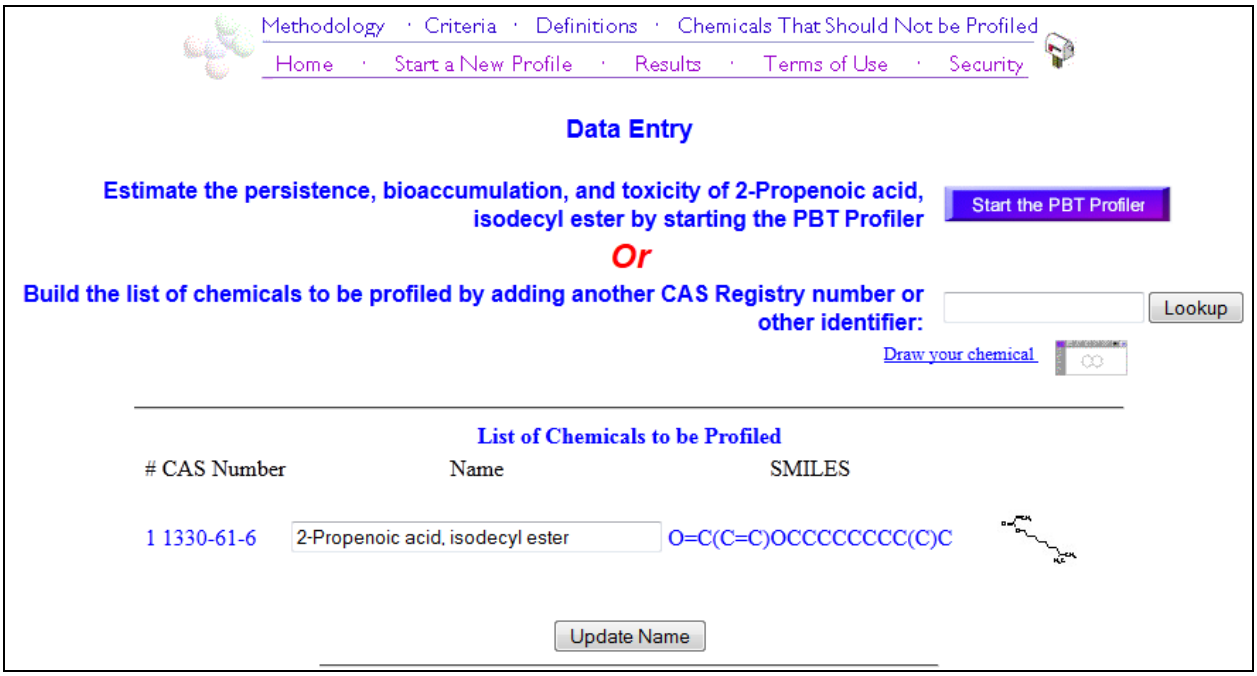


7.7.1 Evaluating Isodecyl Acrylate (CAS 1330-61-6) with the PBT Profiler

Enter the CAS RN for Isodecyl acrylate and click the "look up" button shown in the image below.



This chemical is in the accompanying database of chemical structures so the SMILES Notation for the structure is retrieved and entered in the Profiler (below). You can now click on the "Start the PBT Profiler" button to run the model.

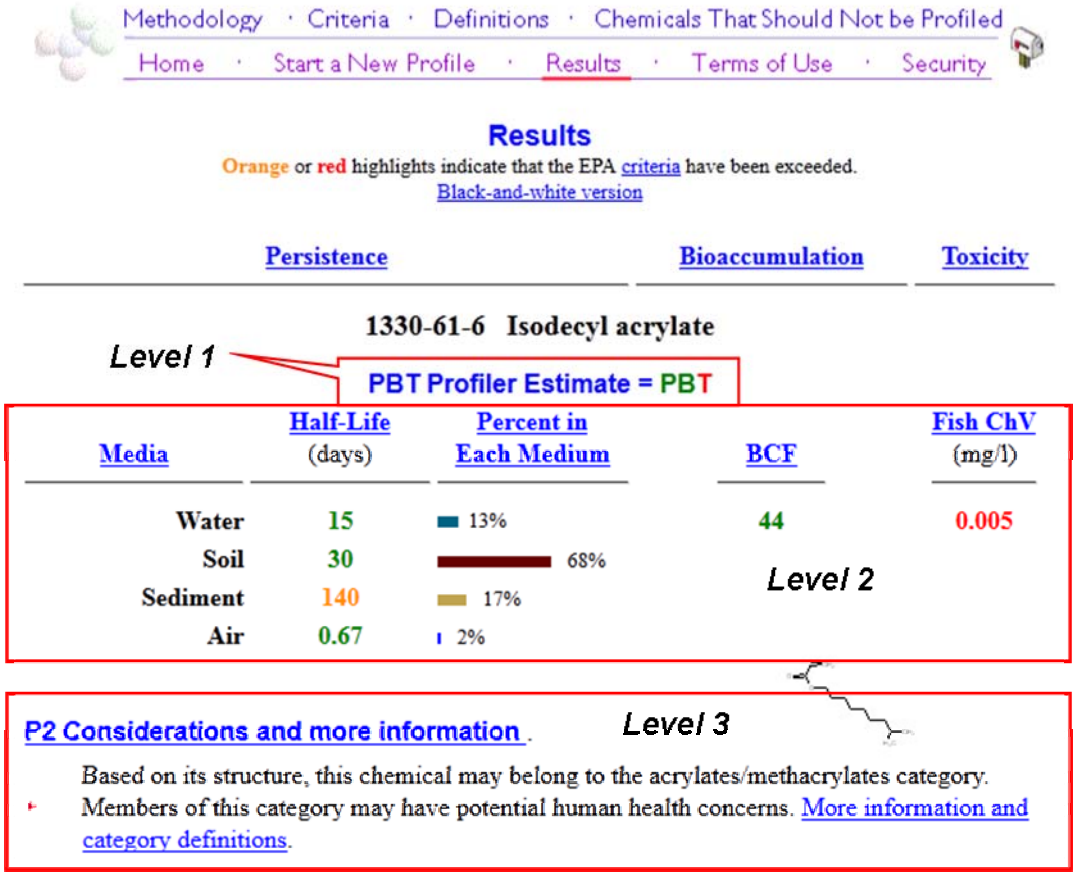


7.7.2 Interpreting PBT Profiler Results for the Sample Chemical

Here are the three levels of results (shown below) for Isodecyl acrylate CAS 1330-61-6.

Level 1 results, **P B T** (P is green, B is green and T is red), show that the chemical is not a PBT. A PBT chemical would be orange or red for all three properties.

Level 2 results describe half-lives in Water, Soil, Sediment, and Air with Percent in Each Medium, Fish BCF, and Fish Chronic Value. Notice that if you click on the name of each property you will go to the online Definition where the property is explained. The predicted values for Isodecyl acrylate show that the half-life in Sediment exceeds the PBT criteria however, since sediment is not the predominant media where the chemical will be found the P call is not based on the Sediment half-life. Results for half-lives in other media do not exceed the criteria. The greatest percentage (68%) will remain in soil. The fish BCF does not excel PBT criteria but the Fish Chronic Value does exceed PBT criteria.



Level 3 results are available by clicking on the "P2 Considerations and more information" link. These results provide a "what if" estimation of how the chemical could behave in the environment and are intended to help the user with pollution prevention considerations. Level 3 results for Isodecyl acrylate include the PBT Profiler Physical/Chemical Property Estimates. Under the Persistence Summary the results indicate that Isodecyl acrylate will partition predominantly to soil and have a half-life in soil of 30 days. If released to water, the chemical will partition to sediment where it may be persistent and if enters a sewage treatment plant, it will likely absorb to sewage sludge. The chemical is not expected to

bioaccumulate in the food chain because it does not exceed the fish BCF criteria. Isodecyl acrylate is predicted to be chronically toxic to fish, and may be toxic to other aquatic organisms. The PBT Profiler has determined that the chemical structure of Isodecyl acrylate indicates that it may be a member of the Acrylates / Methacrylates chemical category as described in the EPA Chemical Categories Report.

7.7.3 Entering Results into the SF Worksheet

The PBT Profiler results are entered into the Sustainable Futures Worksheet on page 2 in the **SUSTAINABLE FUTURES SUMMARY** section (shown below). You enter No in response to the question "Is the chemical predicted to be a PBT by the PBT Profiler?"

SUSTAINABLE FUTURES SUMMARY:			
Concern Level	HIGH	MODERATE	LOW
Persistence			
Bioconcentration			
Cancer Health Hazard			
Non-Cancer Health Hazard			
Aquatic Toxicity Hazard			
Is the chemical predicted to be a PBT by PBT Profiler?	No		

7.8 Obtaining Additional Training Materials on the PBT Profiler

The training materials covering PBT Profiler that were developed by EPA for use in the 3 day Sustainable Futures hands-on training sessions may provide you with additional information. These materials are frequently updated. For PDF copies of the presentations contact Kelly Mayo-Bean, U.S. EPA (mayo.kelly@epa.gov) 202-564-7662.