Science-Based Guidance and Framework for the Evaluation and Identification of PBTs and POPs: Summary of a SETAC Pellston Workshop

Edited by
G.M. Klečka
The Dow Chemical Company

D.C.G. Muir
Environment Canada

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Authored by
Steering Committee Members and Workgroup Chairs

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Preface

“Science-Based Guidance and Framework for the Evaluation and Identification of PBTs and POPs” summarizes the outcome of a workshop and consensus-building process. The workshop was conceived by a small group of people in the public and private sectors who met informally as a steering committee for more than a year to discuss the need for improving the scientific foundation for the criteria and process for the evaluation of persistent, bioaccumulative, and toxic substances (PBTs) and persistent organic pollutants (POPs). The workshop builds on the outcome of a previous Pellston workshop, held in 1998, which focused on the evaluation of persistence and long-range transport of organic chemicals in the environment, and is linked to other recent Pellston workshops, among them the “Tissue Residue Approach for Toxicity Assessment” workshop held in 2007.

The urgency and impact of the workshop topic are well established. The current regulations define PBTs and POPs in terms of fairly strict criteria that are based on the state of the science in the late 1970s and early 1980s. Since then, an evolution in the state of the science has produced new insights into persistence, bioaccumulation, and toxicity of chemical substances and an array of new methods to identify PBT chemicals. The development of regulatory criteria has not kept up with the rapid development in environmental chemistry and toxicology, and as a result, scientists often find themselves in the situation where guidance on PBT and POPs criteria is limited and sometimes out of date.

With this background, the workshop organizers brought together experts from academia, business, and government to reach consensus on where we stand today and what we can accomplish with the current scientific understanding, as well as what should be done in the future as we address this issue. From the dialog will come a final proceedings, of which this is the summary.

If the results of this workshop help bring together those who devote their energies to the science, regulation, and management of chemicals to work together more effectively towards a common goal of deciding how we must manage chemicals on our planet, it will have been a success.
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Introduction

Several national regulations and regional or global conventions aim to identify and prioritize hazardous substances, including the Canadian Environmental Protection Act (CEPA), European Union (EU) Existing Chemicals and Registration Evaluation Authorization of Chemicals (REACH) programs, United States Toxic Substances Control Act (TSCA) and Toxics Release Inventory (TRI) under the Emergency Planning and Community Right to Know Act (EPCRA), United Nations Economic Commission for Europe (UNECE) Convention on Long-Range Transboundary Air Pollution (LRTAP), and the United Nations Environment Programme (UNEP) Stockholm Convention on POPs. The criteria for evaluating persistence, bioaccumulation, and toxicity characteristics of substances under the various regulations are not harmonized but show large similarities.

Regulations focusing on PBTs and POPs are generally supplementary to existing regulations covering other chemicals. Their aim is to identify substances that may cause unexpected problems, such as those that persist and bioaccumulate and ultimately may lead to adverse effects in organisms, particularly in remote areas where the substances are not directly emitted or used.

The current regulations define candidate PBTs and POPs in terms of fairly strict criteria that are based on the state of the science in the late 1970s and early 1980s. Since then, the evolution in environmental and analytical chemistry, computational chemistry, information technology, and environmental toxicology has produced new insights into the persistence, bioaccumulation, and toxicity of chemical substances and an array of new methods to identify PBT chemicals. The development of regulatory criteria has not kept up with the rapid development in environmental chemistry and toxicology. As a result, businesses, regulators, and academics find themselves in a situation where guidance on PBT and POPs criteria is sometimes available, but it is often too limited and sometimes out of date. These limitations have produced some major challenges. One key challenge is the interpretation of substance information in the form in which it is usually provided in the risk profile against the criteria as they are formulated in the various regulations. Very often these do not match. Another challenge is to identify PBTs and POPs at an early stage, sometimes when information is still limited. Equally challenging is the need for accuracy in the process of identification: False negatives may cause environmental problems when impacts are discovered at a late stage, whereas false positives may cause significant business and societal consequences and may unduly deny society beneficial products. Overall it is of key importance that
current legislation is applied effectively, taking advantage of the current state of the science.

**Workshop Purpose and Goals**

To foster the advancement of a sound scientific foundation for identifying and evaluating PBTs and POPs, an international workshop, sponsored by the Society of Environmental Toxicology and Chemistry (SETAC), was held 28–31 January 2008, to address scientific issues related to persistence, long-range transport, bioaccumulation, and environmental toxicity, and the potential for significant adverse effects. The workshop had broad, tripartite participation from academia, government, and business.

The specific objectives of the workshop were to discuss, reach consensus, and develop guidance on how to evaluate substances that may fulfill PBT and/or POPs criteria using scientific information such as experimental data, monitoring data, and computer models. PBT and POPs criteria are intended here in the broadest sense, including criteria defined in regulations around the world, as well as recommendations for new criteria. The workshop participants addressed the information required to provide a weight of evidence for substance evaluation under these criteria. After thorough discussions of each criterion and an evaluation of several case studies, the participants derived a framework with detailed guidance and recommendations on how to interpret substance-specific scientific information related to such PBT and POPs criteria.

Ultimately, the goal of the workshop is to provide timely input into national and international assessments of PBTs and POPs. Among the key work products is a state-of-the-science review. In addition to disseminating the final report, SETAC will communicate the workshop results to the scientific community and to policy makers by all appropriate means.

**Workshop Participation and Format**

The workshop followed the format of previous SETAC Pellston Workshops and was limited to about 50 participants with broad international perspective and recognized expertise in environmental chemistry, toxicology, multimedia modeling, and risk assessment (see List of Participants). To address the objectives, the workshop was organized into 9 individual sessions. A general plenary was held on the first day, during which invited, authoritative discussion papers were presented to stimulate dialogue. On the basis of his or her expertise, each participant was assigned to a small workgroup, although interaction among
the workgroups was encouraged. Each workgroup was to develop a summary of their deliberations, including discussions of the state of the science pertinent to that workgroup, a critical analysis of available approaches, and methods to integrate these approaches into a framework for assessing PBTs and POPs. Key points from the discussions are summarized in the following sections. The complete workshop proceedings document is in preparation.

**Workgroup Discussions**

**Evaluating environmental persistence**

The persistence of organic compounds is governed by the rates at which they are removed by chemical and biological processes such as biodegradation, hydrolysis, atmospheric oxidation, and photolysis. This workgroup focused on evaluating persistence of organic compounds in environmental media (air, water, soil, sediment) in terms of their single-medium degradation half-lives. The findings built upon the results of a previous Pellston workshop, as well as recent guidance developed for other chemicals assessment programs. The primary aim was to provide guidance to authors and reviewers of chemical dossiers in the government and private sectors. A second objective was to provide a summary of the current state of the science with respect to fate assessment for POPs.

Environmental persistence is influenced by many factors. Chemical structure ultimately determines which transformation processes may be significant for a given compound and which are not likely to be important. The structure also determines inherent properties, such as water solubility, which influence degradation rates. Characteristics of the receiving environment are also important, including hydroxyl radical concentrations in air, as well as temperature, salinity, pH, oxygen concentration, redox status, test chemical concentration, and nutrient status, which directly or indirectly impact rates of transformation in the other media. Transformation processes can significantly reduce the potential for exposure and significant adverse effects. In contrast, physical processes such as dilution and advection do not impact persistence because they do not reduce the environmental burden of the chemical.

After careful consideration of international and national POPs and PBTs regulatory frameworks, the workgroup developed guidance that identifies the information that a risk profile should contain in order to conclude whether a chemical is persistent. Specific attention is given to addressing uncertainty and conflicting data, as part of a weight-of-evidence assessment.
In general, fate testing should be conducted under relevant environmental conditions with respect to temperature, pH, substance concentration, etc. In weight-of-evidence assessments, preference should be given to valid test data over non-test data, such as information derived using quantitative structure–activity relationships (QSARs). Further, it is important to understand the mechanisms by which loss of parent material or intermediate degradation products occurs.

Higher-tier biodegradation studies, often termed “simulation studies,” can be difficult to interpret. Although the tests were originally designed to generate kinetic information (e.g., first-order rate constants) on the biodegradation of a chemical, which can be converted into the corresponding half-life for comparison with criteria, the different mechanisms involved in removal of the parent compound may complicate the analysis of results. For example, when the fate of certain chemicals is examined in soils or aquatic sediments, the results often yield dissipation times that combine removal due to biodegradation, sorption, and bound residue formation.

Critical issues for studies using soil or sediment are whether residues in soil or sediment are extractable by exhaustive extraction methods, and whether those that are not, that is, the non-extractable residues, are covalently bonded to the matrix. The challenge thus lies in interpreting the output of such studies in terms of a chemical’s behavior in the real world. A number of studies suggest that residues that cannot be extracted by aggressive techniques (e.g., Soxhlet extraction, supercritical fluid extraction) are unlikely to be bioavailable to soil organisms. The workgroup concluded that where non-extractable residues can be shown to be covalently bonded to the soil matrix, rates of dissipation (including bound residue formation) can be included with degradation for comparison to the half-life criteria.

It is generally acceptable to take the sum of process-specific first-order rate constants for a given compartment (i.e., the sum of the rate constants for biodegradation, hydrolysis, etc.). This cumulative rate constant can be used to derive a compartmental degradation half-life for comparison to persistence criteria or as input to models, as appropriate. However, rate constants for primary and ultimate degradation should not be combined.

In general, it is not sound scientific practice to use the Arrhenius equation ($Q_{10}$ rule) to quantitatively correct biodegradation data to a common environmental temperature (e.g., 10 °C). This is true because microbial populations generally are adapted to prevailing environmental conditions, and the transformations that they perform cannot be scaled directly with temperature as is the case for abiotic reactions.
No single half-life value can adequately describe degradation in the environment or any environmental compartment. Typically, where multiple degradation studies have been conducted, a range of half-lives is observed. In such cases it is not appropriate to use the slowest or most conservative half-life.

**Multimedia partitioning, overall persistence, and long-range transport potential**

An important feature of chemicals released to the environment is that they can redistribute between media. For example, a substance may be released to either air, water, or soil, and then subsequently move between these phases. It is important to assess the ability of a compound to undergo multimedia partitioning because this behavior will affect the compound's ability to be transported in air or water over long distances, its susceptibility to degradation in a particular compartment, its potential to transfer into living systems, and its overall persistence \( (P_{ov}) \) in the environment.

The distribution of a compound between environmental media is controlled by its physical and chemical properties, and by certain features of the environment (e.g., compartment volumes, and properties such as temperature, pH, and organic matter content). Evaluative models have been developed to make predictions about chemical distribution in a defined multimedia environment. Such models are important tools in behavior profiling. Key physical–chemical property data required for such profiling are solubility in water, vapor pressure, and information on partitioning between media, including the Henry's law constant, and the \( n \)-octanol–water \( (K_{ow}) \) and \( n \)-octanol–air \( (K_{oa}) \) partition coefficients. Different experimental or estimation methods used to derive these properties may give different results. Chemical property data reported in the literature are often inconsistent and incomplete. Because the quality of the data determines the reliability of any PBT or POPs assessment, such data should be compiled carefully. Partitioning properties should be checked for internal consistency, and outliers should be identified and removed from the dataset.

The environmental behavior profile is further developed by combining assessments of the multimedia distribution of the chemical with information on its degradation kinetics in the different media. Environmental half-lives can be determined by various experimental methods; when measured half-lives are unavailable, a number of predictive methods (QSARs) can be employed. Uncertainty ranges for measured or estimated half-lives should be considered.

In current regulations, persistence is often assessed against criteria for single-media half-lives, typically for the relevant environmental compartments,
that is, those in which the compound resides. However, such approaches can overlook important features of chemicals that undergo re-distribution in a multimedia environment. For example, if a chemical released to water or soil is persistent in air and can readily undergo surface-to-air exchange, it could potentially be transported in air and reach remote environments. Similarly, persistent and water-soluble compounds may travel great distances in rivers and oceans. Chemicals should therefore be assessed with respect to their \( P_{ov} \) in an evaluative multimedia regional or global environment.

Several multimedia models have been developed to evaluate the \( P_{ov} \) of chemicals. The Organisation for Economic Co-operation and Development (OECD) has supported the development and inter-comparison of such approaches, which led to the adoption of the OECD \( P_{ov} \) and Long-Range Transport Potential (LRTP) Screening Tool. The OECD LRTP Screening Tool allows comparison of the test chemical against a series of reference chemicals, with well-defined properties and well-known environmental behavior. Hence, it is possible to define a \( P_{ov} \) value that ensures no net accumulation of a chemical in the environment. Such evaluations enable the management of chemicals in a consistent way, irrespective of the particular combination of half-lives. For example, if 100 units of chemical with a \( P_{ov} \) half-life of 90 days are released into a multimedia environment, the levels will decline to about 6 units within a year, while a chemical with a \( P_{ov} \) half-life of 200 days will systematically accumulate. Because \( P_{ov} \) depends on the environmental conditions, it may be inappropriate to define a specific \( P_{ov} \) cut-off value. Rather, \( P_{ov} \) should be used as part of the weight of evidence compiled to screen and evaluate chemicals.

Atmospheric transport is usually the primary mode for conveying persistent substances to remote regions. For this reason, the UNEP and UNECE Conventions define a criterion for half-life in air of >2 days. The original intent of this value was to highlight those chemicals that are sufficiently persistent to be able to travel through the atmosphere to remote regions. Two days is a convenient metric that might apply to substances emitted in parts of the temperate world, which may travel with some efficiency to reach the Arctic. With the 2-day criterion, typically <3% of the chemical will be transported a distance of 1000 km or more. The OECD LRTP Screening Tool permits an assessment of the long-range transport potential for a candidate substance, which can be compared and ranked against other well-studied compounds.

Regulatory approaches often acknowledge the usefulness of monitoring data, often from remote locations, in highlighting potentially problematic chemicals. The occurrence of these problematic chemicals in remote regions is often taken as evidence of their persistence and long-range transport potential. However, detection of a chemical in a remote area is not evidence, per se, of these prop-
properties. Detection in remote environments must be assessed according to the amounts and patterns of usage and emission and the sensitivity of analytical methods, if a robust, scientifically sound risk profile is to be developed.

### In vitro and in silico approaches for bioaccumulation assessment

Predictive tools are critical components of an overall strategy for assessing the potential of chemicals to bioaccumulate within the environment. The prioritization and assessment of chemicals is increasingly moving into the realm of data inadequacy. Consequently, there is and will continue to be a reliance on predictive tools to complete regulatory requirements in a timely, humane, and cost-effective manner.

The toxicokinetic processes of absorption, distribution, metabolism, and elimination (ADME) determine the extent to which chemicals bioaccumulate in living organisms (Figure 1). Mechanistic models of bioaccumulation explicitly consider these ADME processes, but we lack the data needed to specify critical model input parameters, particularly for compounds that are extensively metabolized, that exhibit restricted diffusion across biological membranes, or that do not partition simply to tissue lipid.

A variety of in vitro systems are available for estimating ADME properties, and the workshop participants explored the applicability of these assays to estimating input parameters for bioaccumulation models. Several in vitro assays have been developed by the pharmaceutical industry to predict the membrane permeation of drug candidates. Well-known examples include the Caco2 cell line and the parallel artificial membrane permeability assay (PAMPA). Both assays depend on the ability to measure chemical concentrations in water. As such, they are poorly suited for use with hydrophobic materials. An adaptation of the PAMPA assay that employs silicon disks for both dosing and sampling holds promise for use with high log $K_{ow}$ compounds.

**Figure 1** Conceptual diagram of ADME processes and related kinetic rate constants for fish

\[
\begin{align*}
\text{Gill uptake } k_1 & \quad \text{Gill elimination } k_2 \\
\text{Dietary uptake } k_D & \\
\text{Fecal egestion } k_E & \\
\text{Metabolic transformation } k_M
\end{align*}
\]
The in vivo rate of xenobiotic metabolism ($k_M$) can be estimated using in vitro systems derived from liver tissue (e.g., isolated hepatocytes, microsomes, and S9 fraction) in combination with a physiologically based prediction model. These procedures explicitly consider chemical distribution within the animal, which can be represented as an apparent volume of distribution at steady state ($V_{SS}$). Using this approach, $k_M$ may be viewed as a quotient that integrates information about metabolic clearance (CL) and chemical distribution: $k_M = \frac{CL}{V_{SS}}$. Limited studies have shown that incorporating in vitro metabolism data into models of chemical bioconcentration substantially improves the accuracy of steady-state bioconcentration factor (BCF) predictions.

Efforts are also being made to predict metabolic rate constants from an in silico analysis of chemical structure. Current models use metabolic maps based on well-studied pathways in rodents to predict likely metabolic products in fish. These reactions operate against the base-line extent of accumulation predicted from simple partitioning considerations, and the probability of a specific reaction can be estimated by modeling to measured steady-state chemical concentrations.

A critical issue in bioaccumulation assessment is the question of whether there are molecular-size cut-offs for ADME processes. Size has a gradual effect on membrane permeation, but this effect is driven by the kinetics of permeation and is not partitioning based. Several size cut-offs have been estimated from model-based evaluations of chemical uptake and accumulation in fish. These operationally defined cut-offs depend on the structure of the model used for their estimation and on the conditions under which the data were collected (e.g., fish size and water temperature). As such, they are highly context specific. Similar considerations apply to the estimation of metabolism rate cut-offs for bioaccumulation.

The workgroup developed guidance for the use of bioaccumulation prediction methods within the context of a weight-of-evidence approach. Important to this usage is the “domain of applicability” of results generated from in silico modeling efforts and in vitro assays. The workgroup agreed on an approach which provides the basis for evaluating predictions from multiple models. The reviewed in vitro approaches are promising tools for identification and prioritization of chemicals in bioaccumulation assessment. Their application in regulatory assessment schemes is relatively new, however, and will require continued research to elucidate potential advantages and limitations.
Evaluation of bioaccumulation using whole organism laboratory and field studies

The objective of this workgroup was to prepare guidance on the collection and evaluation of bioaccumulation data from whole organisms in laboratory and field studies. Although applicable for national and regional chemical management programs, the guidance is specifically framed to support the development of the screening information required under Annex D of the Stockholm Convention on POPs, and the risk profiles drafted in accordance with Annex E.

A primary concern for chemicals is to identify whether they biomagnify to concentrations sufficient to pose health concerns to humans or wildlife. Historically, markers of in vivo exposure (e.g., egg shell thinning, bill deformities) have retrospectively led to the identification of POPs. Today, many bioaccumulation metrics from lab and field studies are available to help us understand and predict the bioaccumulation potential of a possible POP.

A variety of laboratory procedures have been described for exposing aquatic species (e.g., fish, invertebrates) and, on occasion, other species (e.g., mammals, birds) to a chemical and for measuring the resulting tissue residues. Exposures to the test compound can be accomplished via multiple routes, for example, aqueous, dietary, or soil–sediment. A number of standard guidelines are available for measuring bioconcentration, bioaccumulation, and other metrics such as biomagnification and biota–sediment accumulation factors (BMF, BSAF) in the laboratory (e.g., OECD, USEPA, ASTM). Results of laboratory bioaccumulation studies should be critically evaluated, and only high-quality data should be used in the screening analysis and resulting risk profile. Further, care should be taken when evaluating the results of laboratory studies conducted using $^{14}$C-labeled test chemicals, because the results often are based on total radioactivity, which can include metabolites present in the test organism.

Field monitoring data may come from studies with free or caged organisms and associated bioaccumulation metrics (e.g., trophic magnification factor (TMF), bioaccumulation factor (BAF)), non-standard tests, and data from tests conducted for other purposes (e.g., toxicity feeding study of birds with measured tissue residues, critical body burdens). The work group considered the advantages and disadvantages of the various lab and field tests and recommended that the relative merits of the metrics are transparent and can be applied in a weight-of-evidence case. Also, the various bioaccumulation metrics and methods used to normalize data (e.g., concentrations based on wet weight, lipid weight, or dry weight) need to be clearly defined. Guidance is provided on how to interpret data uncertainty, and on how to evaluate data reliability so that the most credible data support decisions in screening and risk profiles.
Benchmarking of proposed POP candidates was also recommended because comparisons of test compounds to chemical class analogues that may or may not be listed as POPs may prove useful. This step may prove advantageous in identifying trends in chemical structure and class, in understanding factors that might compromise test results (e.g., highly volatile substances), and in evaluating data consistency.

Based on the bioaccumulation information shared in eight draft risk profiles for candidate POPs, the workgroup developed recommendations for the types of information that are critical, or at least beneficial, to significantly aid transparency and certainty in decision making. The group noted that there is a need to clearly state the bioaccumulation metric and units, data quality, identity of location and species (or sample types), isomers or congeners of greatest concern, references to primary and recent literature, comparison to established POPs, and linkage of the bioaccumulation and/or exposure metric to a significant adverse effect and long-range transport.

**Revisiting bioaccumulation criteria**

Currently, bioaccumulative (B) substances are defined in terms of criteria, expressed in the form of the BAF, BCF, or $K_{ow}$. In view of the absence of a recognized definition, we have defined a B substance as one that biomagnifies in the food-web, that is, increases in normalized concentration (or fugacity) with increasing trophic position. If a chemical biomagnifies, it bioaccumulates to a greater degree than would a chemical that does not biomagnify. Biomagnifying substances have therefore a greater potential to reach high concentrations in upper trophic-level organisms (including humans) and cause adverse effects within the food-web.

The workgroup concluded that the most relevant B criterion is the TMF (also referred to as a “food-web magnification factor”) and that the most conclusive evidence to demonstrate that a chemical substance biomagnifies is a TMF $> 1$. TMF is derived from a correlation between an appropriately normalized chemical concentration in biota and a trophic position. It is crucial for the characterization of TMF that both aquatic and terrestrial food-webs are considered. This is true because chemicals can exhibit fundamentally different TMFs in aquatic and terrestrial food-webs due to differences in the bioaccumulation mechanisms between water- and air-breathing organisms.

In the absence of data on the TMF, the BMF (either derived in the laboratory or based on field data) is a reliable indicator. The BMF is expressed as the ratio of a normalized chemical concentration in a specific organism to that in the organism’s diet or prey at steady-state. A BMF $> 1$ indicates the capability of
the chemical to biomagnify. For the differences noted above, BMFs in both air- and water-breathing organisms must be considered. For laboratory-based BMF measurements, we recommend the use of rainbow trout and rats (or mice) because of the long-term experience with these commonly used test species and because of access to data previously collected for these animals.

The workgroup concluded that the BCF is not a good surrogate for BMF or TMF in terrestrial food-webs, and that in many cases, the BCF is not even a reliable indicator of biomagnification for aquatic food-chains. This is the case because the BCF quantifies chemical bioaccumulation from water but not from the diet. This conclusion is supported by our analysis of draft risk profiles, which identified 5 substances to be bioaccumulative in the environment, although the BCF criteria were not met. Despite these difficulties, the workgroup concluded that the BCF can be a useful indicator of biomagnification if the route of exposure (water) does not affect the biotransformation rate of the chemical in the organism, and if bioavailability issues are not significant experimental artifacts.

Because empirical data regarding the TMF and BMF are available for only a small fraction of chemicals in commerce, it is important to propose surrogate criteria to identify potentially biomagnifying substances. For non-ionizable, non-polar organics, chemicals with a log $K_{ow} < 4$ normally do not biomagnify in aquatic food-webs, and there is no evidence that these substances exhibit BCFs $> 5000$. For the evaluation of chemical biomagnification potential in terrestrial food-webs involving air-breathing organisms, we expect chemicals with a log $K_{oa} < 5$ will not biomagnify in terrestrial food-webs. These substances may not require BMF tests. For substances whose $K_{ow}$ and $K_{oa}$ exceed these criteria, there is the potential for including in vivo biotransformation rate constants ($k_M$) because chemicals that are rapidly degraded in organisms cannot bioaccumulate or biomagnify to a high degree. Modeling studies have suggested that chemicals with biotransformation rate constants on the order of 0.1 d$^{-1}$ cannot biomagnify in food-webs, although further work is needed. Screening assessments also can benefit from the use of food-web bioaccumulation models to calculate BMFs and TMF. Such models have benefits over using chemical property data alone because they can be parameterized to make use of available biotransformation rate data.

The workgroup recognized several research needs to support and improve B assessments. They include 1) technical guidance for the determination of TMF, 2) development of a standard protocol for BMF tests in rats and fish, 3) guidance on the use of field studies for the development of BMF in mammalian or bird and submerged aquatic species, 4) investigation of the potential application of currently available rat and fish dietary data, and 5) investigation of the
possibility of deriving a single biotransformation half-life criterion to identify non-biomagnifying chemicals. We further recommend gathering additional information on the relationships among the BCF, the BMF, and the TMF.

To ensure that B assessments are carried out on the basis of the current state of the science, it is essential that dietary magnification and an assessment of both water- and air-breathing organisms are included. A framework for B assessment is presented in Figure 2.

<table>
<thead>
<tr>
<th>Stage</th>
<th>Description</th>
<th>Evaluation</th>
<th>Outcome</th>
</tr>
</thead>
<tbody>
<tr>
<td>Step 1</td>
<td>Food-web assessment</td>
<td>What food-webs should be considered?</td>
<td>Aquatic Terrestrial</td>
</tr>
<tr>
<td>Step 2</td>
<td>TMF-assessment</td>
<td>Is TMF &gt; 1?</td>
<td>B status Confirmed</td>
</tr>
<tr>
<td>Step 3</td>
<td>BMF-assessment</td>
<td>Is BMF &gt; 1?</td>
<td>B status Probable</td>
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<tr>
<td>Step 4</td>
<td>BCF/BAF-assessment</td>
<td>Is BCF or BAF &gt; 5,000?</td>
<td>B status Possible</td>
</tr>
<tr>
<td>Step 5</td>
<td>Phys-Chem, ADME, Food-Web Model Assessment</td>
<td>Log Kow &gt; 4, log Koa &gt; 5 BMF &gt; 1, TMF &gt; 1</td>
<td>B status Potential</td>
</tr>
</tbody>
</table>

Figure 2 Framework for bioaccumulation assessment

**Use of measurement data in evaluating exposure of human and wildlife to POPs and PBTs**

The Stockholm Convention on Persistent Organic Pollutants recognized that POPs resist degradation, undergo long-range transport (LRT), and accumulate in remote terrestrial and aquatic ecosystems. The convention also acknowledged that indigenous communities, particularly in the Arctic, were at risk because of the biomagnification of POPs and the contamination of their traditional foods. This recognition was largely based on environmental monitoring data, and demonstrates the need for adequate guidance on data collection and use. Indeed the Stockholm Convention (Annex E) requires monitoring data for “exposure in local areas and, in particular, as a result of long-range environmental transport.”

Figure 3 depicts a variation of the exposure–effect continuum. The first part of the continuum, the exposure portion, depicts the “environmental chemical”
originating from a source, moving into the environment where it may undergo various fate and transport steps, coming into contact with humans via the environmental media, and entering the body by one or more exposure routes (ingestion, inhalation, and dermal).

For the so-called “legacy POPs,” including those on the list of the Stockholm Convention, the primary route of human exposure is, and has been, dietary ingestion. However, for some of the new candidate POPs such as polybrominated diphenyl ethers and perfluorooctane sulfonate, the exposure routes include not only dietary ingestion but also non-dietary ingestion of household dust as well as potential inhalation of that dust.

To develop robust data sets on the extent of exposure of wildlife species to POPs requires careful consideration of many factors because of the potentially wide range of possible species and habitats. Based on more than 30 years of extensive measurements of the legacy POPs in biota, there is lot of information available, and the need to monitor compliance with the Stockholm Convention has stimulated recent comprehensive reviews of the issues and publication of a UNEP guidance document. However, there is relatively little guidance on the most appropriate environmental measurement approaches, particularly for new candidate POPs, and on how to create a weight of evidence based on such data.
As we move beyond the “legacy POPs,” there are technical challenges associated with developing robust datasets of new candidate POPs. Many candidates are, or were until recently, high production-volume chemicals, used in a wide variety of industrial and consumer products. Background contamination during lab analysis or field collection (that could yield false positives), and lack of certified analytical methods and standards, are measurement challenges that must be recognized in risk and exposure assessments. In addition to quality assurance issues, development of robust datasets also requires appropriate study designs, incorporating consideration of statistical power, geographical (local, regional, and remote sites) and temporal scope, and key environmental media and tissues, to develop the weight of evidence for exposure. Studies that combine measurements of new candidates with benchmark chemicals such as PCBs are particularly useful for comparative assessment.

The recommended matrix for assessing human exposure to POPs is blood or its components, such as serum or plasma. The primary reason is that exposure to most POPs can be assessed by analyzing blood. Analyzing breast milk has the advantage of directly assessing exposure to the nursing infant, however, this information can be ascertained by analyzing the blood of the mother, both post-partum and during pregnancy. Of course, analyzing milk or serum does not in general give us knowledge about the pathway and, specifically, the route of exposure; these analyses integrate exposure and absorption through all routes.

In developing guidance for global environmental monitoring of legacy POPs, the UNEP Guidance for a Global Monitoring Programme recommends focusing on air, human milk or blood, as well as widely measured biota such as mussels, marine mammals, bird eggs, and fishes as most appropriate types of samples because of past extensive studies and assuming that species close in taxonomy and trophic levels to existing well established programs, seem most appropriate also for new candidate POPs.

For assessing exposure in humans and top predators, the working group recommends using direct measurements of the compound of concern from a significantly and uniquely exposed population (indigenous populations, remote populations), as well as data that demonstrate biomagnification and time trends, if possible. These data must be from the appropriate sample matrix type, must be collected and analyzed using accepted methodologies, must be reviewed for quality assurance, and must be interpreted correctly if they are to be used to assess exposure.
Modeling exposure to persistent chemicals in hazard and risk assessment

Fate and exposure models are used routinely in regulatory applications to inform decision making, and they have helped improve the understanding of POPs and PBT chemical fate, hazards, and potential risks. Using fate and exposure models could significantly improve the risk profile evaluation of significant adverse effects in either the UNEP Stockholm or UNECE LRTAP Conventions. Therefore, the goal here is to motivate the use of models in preparing the risk profile in the POPs assessment procedure and to provide strategies and guidance for their application.

The goal of an exposure assessment for POPs and PBTs is to establish the link between chemical emissions to the environment and exposure in the target organisms of concern. To accomplish this goal, several models are generally needed. First, an environmental fate model is required to describe the fate and presence of the chemical in the various environmental compartments as a result of emissions. Second, bioaccumulation models are needed to predict the resulting exposures in target organisms of various food webs arising from the concentrations in the physical media. These models can be either separate or linked within a modeling package. Further, in the context of preparing a risk profile for a candidate POP, an additional goal is to predict chemical exposures in remote regions that result from long-range transport. Currently there is no standardized consensus model for use in the risk profile context. Therefore, to choose the appropriate model, the risk profile developer must evaluate how appropriate an existing model is for a specific setting, and whether the assumptions and input data are relevant under the conditions of the application.

Fate and exposure models can improve and inform the development of a risk profile in a variety of ways. Comparing model-based exposure predictions to existing monitoring data can establish whether the monitoring data and the exposure predictions are reasonable, representative, and consistent. Confidence in the predictions of many existing models is possible because of their fundamental physical and chemical mechanistic underpinnings and the extensive work already done to compare model predictions and empirical observations. Sensitivity analysis of the model can identify the key processes and most important model parameters that impact the exposure, thereby allowing, when desired, focused research or measurement to improve the risk profile. In the absence of quantitative emission information, benchmarking can be performed, in which the ratio of exposure and emissions of candidate chemicals is compared to the same ratio for known POPs. Such approaches make it possible to combine the relative magnitude of this ratio with the relative emissions.
and relative hazard to arrive at a measure of relative risk. Models can also be used in the risk management context for predicting future time trends, including how quickly exposure levels in remote areas would respond to reductions in emissions.

To illustrate the application of models to predict human exposures in support of the risk profiling process, the workgroup considered a variety of candidate POPs that have been nominated for consideration under the Stockholm Convention. Models were initially used to benchmark the candidates against a series of acknowledged POPs and non-POPs. Additional simulations were performed for one of the candidates in order to compare predicted data to concentrations measured in the environment. On the basis of sensitivity and uncertainty analyses of the findings, it was clear that accurately estimating emission rates is a prerequisite to obtaining useful estimates of exposures and risks. Further, the biotransformation half-lives were shown to be the most sensitive parameter and the most influential for determining predicted human body burden.

The working group recommends developing a model benchmarking tool for human and wildlife exposure in remote regions. This tool would be analogous to the benchmarking tool for persistence and LRT developed for the initial stage of the POP review process. Such a tool would allow a non-expert to do a model-based exposure assessment with confidence, and would contribute to lowering the barriers to exploiting the potential of models. Furthermore, the working group suggests developing a second model benchmarking tool for the recovery time of remote environments following the cessation of chemical emissions. Such a tool would provide transparent, readily comprehensible information on an important motive underlying the concern about POPs, namely the reversibility of potential risks.

**Use of (eco)toxicity data as screening criteria for identification and classification of PBT and POP compounds**

Characterizing significant adverse ecotoxicological effects (SAE) of POPs and PBTs presents particular challenges. In the various international conventions, guidance on the definition and criteria for evaluating toxicity are not detailed, and in some cases, they are unclear. This section focuses on several key issues related to selection of assessment endpoints, use of appropriate effect measures, and methods to address uncertainty in the face of limited data.

The protection goal of POPs and PBT regulations is to prevent significant adverse effects (SAE) on humans and the environment. For humans, the pro-
tection goal is aimed at the individual, and the standards of acceptable risk are well defined, particularly for substances that may cause serious effects such as cancer or reproductive dysfunction. In contrast, significant adverse effects endpoints for most environmental species are mostly at the level of the population, although community-level effects and overall ecological function and sustainability must also be considered. Additional protection may be appropriate for some rare and endangered species for other than strict ecological reasons.

In principle, a large array of standardized guideline studies is available to assess the toxicity of POPs and PBTs. However, only a limited number of substances have sufficiently robust datasets for characterizing adverse effects on the diversity of environmental species. The best database for characterizing toxicity of organic chemicals is for pesticides, for which a large number of acute and chronic tests are available for a number of taxa, including mammals. For many industrial chemicals, the database is more limited, and indirect methods for characterizing toxicity, such as the use of QSARs or extrapolation within modes of action, are necessary. Further, the question of differential sensitivity has been raised, particularly for organisms found in polar regions. While few data address such differential sensitivities, there is no reason to suggest that, if differences exist, they are sufficiently large that data from temperate organisms cannot be used to assess adverse toxicological effects for arctic species. However, recovery from disturbances may take longer time in polar conditions than in temperate or tropical conditions.

Because POPs are persistent and bioaccumulative, the assessment of toxicity generally should not be based on concentrations in environmental matrices but rather on body or tissue residues that are causally linked to adverse responses. The exception is the existence of clear correlations between matrix concentration and adverse effects. Because such information generally is not obtained when existing guideline protocols are used, toxicity testing methods may need to be modified or substantiated by toxicokinetic information to ensure that substances with PBT-like properties are adequately characterized. These data can more easily be matched to environmental monitoring measurements of body or tissue residues for the purposes of assessing whether adverse effects are occurring in the environment. In the face of persistence and accumulation in the food chain, and considering the extent and suitability of data available, a suitable policy on the use of uncertainty factors may need to be applied when judgments about toxicity are made.

When toxicological data are limited, a variety of approaches can be taken assessing a chemical, including the use of structure–activity relationships (SARs) and the mode of toxic action. Various SARs and QSARs have been developed and tested for a variety of chemical classes. Further, understanding the mode
of action of a chemical enables a reasonable extrapolation of potential sensitivity and effect responses across taxonomically diverse groups of organisms. When such information is used to supplement experimental data, a weight-of-evidence approach can inform decisions in a rigorous and scientifically defensible manner. In this context, “weight of evidence” is defined as the use of all available data in conjunction with expert knowledge to reach a conclusion. In the case of PBTs, a weight-of-evidence approach would include incorporating information on tissue residues and critical body burdens with documentation of historical effects and traditional toxicological studies. Given the data limitations for toxicity or measured environmental effects for most PBTs, a well-documented weight-of-evidence approach is preferred for characterizing the ecotoxicity of these substances.

The workgroup reviewed a series of draft risk profile reports for candidate POPs to assess whether the information on various endpoints of concern supported the conclusion that the substances met the criterion of causing significant adverse effects. From the analysis, it was apparent that the profiles lacked consistency in the type of endpoint considered, and there was no clear evidence that a consistent, generally accepted decision-making process was followed. We recommend using an evaluative scheme (Figure 4) based on a tiered approach to ensure that all of the same endpoints are considered in each assessment, and that the amount and type of data used from these endpoints is uniform. We anticipate that use of such approaches will lead to consistent, well-formulated and informed decisions as to whether the substance in ques-

![Figure 4 Framework for assessment of significant adverse ecological effects](image-url)
tion may cause significant adverse effects at environmentally relevant concentrations.

**Framework for identification and assessment of PBTs and POPs**

Several national regulatory programs and regional or global agreements address the assessment and ultimate control of PBT and POP substances. Reviews of substances generally involve an initial priority-setting phase, followed by a more in-depth assessment phase of the properties of prioritized substances and their potential for adverse effects. The ultimate basis for decisions as to whether a substance is a PBT or POP, and whether risk management decisions are required, will depend on the goal and mandate of the initiative. For example, under the Stockholm Convention, decisions about potential POPs are based on “whether the chemical is likely, as a result of its long-range environmental transport, to lead to significant adverse human health and/or environmental effects, such that global action is warranted.” The existing frameworks for evaluating POPs and PBTs provide adequate flexibility to introduce additional, new and emerging scientific evidence into the processes.

In assessing any of the properties associated with potential PBTs or POPs (P, B, T, LRT, SAE), a range of approaches, including the use of empirically derived and model-derived information, can be considered and applied as appropriate. In so doing, both quantitative and qualitative lines of evidence can be used, but the reporting of results should recognize and communicate uncertainties associated with both of these. Although this workshop concentrated on scientific issues, it is important to note that public and other stakeholder views, plus legislation in force in different national jurisdictions, will also influence the way in which POPs and PBTs are evaluated, as will the particular requirements of those commissioning the evaluation. For example, there is a fundamental difference in the methods used to rank and prioritize chemicals for PBT or POP properties when compared to detailed PBT or POP assessment of chemicals that have already been prioritized. In the former case, well-defined prioritization criteria are used at first to filter out substances that are likely neither PBTs nor POPs, or to identify substances with potential for being PBTs or POPs (e.g., Canadian DSL Categorization, US New Chemicals PBT modeling, and EU PBT work group). In this first, priority-setting phase, rapid and efficient approaches should be used, and generally will be developed to minimize the probability of false negative results. Substances that are identified as priorities or as potential PBTs or POPs by this process need to be assessed in more detail in a second, assessment phase by collating empirical and other robust data. The use of more specific models, consideration of data for
analogous chemicals and weight-of-evidence approaches, as discussed in this workshop summary, are recommended in this assessment phase.

The basic framework for PBT or POP assessment is shown in Figure 5, and can be enhanced as new scientific approaches and information arise. The main question that should be asked of any new approach or information is this: Will it help to appropriately identify potential PBTs or POPs for further assessment, or is it designed to help evaluate a small number of chemicals accurately and precisely? The answer to this question will determine whether the information or approach is of use primarily in the priority-setting phase or in the assessment phase of the framework.

Many of the approaches and methods discussed at this workshop are most appropriate for application in the assessment phase of this framework. However, there was some discussion of appropriate, rapid prioritization for P, B, T and LRT through use of QSARs and software programs such as the OECD Toolbox or the OECD Long Range Transport Tool. It should be noted that Annex D of the Stockholm Convention on POPs discusses “screening criteria”, which partly overlap with the approaches proposed for the priority-setting phase of this framework. However, the Stockholm Convention screening criteria also provides for consideration of empirical data from experimental and monitor-
ing studies, which generally might better apply in the assessment phase of the proposed framework.

The following conclusions from the workshop are relevant to the use of rapid tools in the priority-setting phase of the proposed framework:

**General**

- **General**
  - Reliable data from empirical studies should carry more weight in an assessment than should results from predictive tools or estimates. However, empirical data are unavailable for many substances, so reliance on modeling is usually inevitable during priority setting.
  - The advantages and disadvantages of predictive approaches (e.g., QSARs) need to be understood by users, including the domain of applicability (boundary conditions), so that application in assessment regimes is informed.

**Persistence**

- **Persistence**
  - Uncertainty ranges for estimates of chemical half-life based on QSARs and degradation studies may vary by a factor of 5 to 10.
  - In current legislation, persistence is often assessed against criteria for single-media half-lives for the most relevant environmental compartments. However, some structure-activity approaches can overlook important features of chemicals that undergo redistribution in a multimedia environment. Chemicals should therefore also be assessed with respect to their overall environmental persistence \(P_{ov}\) in an evaluative, multimedia regional or global environment. Tools such as the OECD \(P_{ov}\) and LRTP Screening Tool are available for performing this type of evaluation.
  - For volatile and semivolatile compounds, atmospheric transport is usually the primary mode for conveying persistent substances to remote areas. The UNEP and UNECE criterion of a half-life in air of >2 days is an appropriate threshold for prioritizing these compounds.

**Bioaccumulation**

- **Bioaccumulation**
  - Non-ionizable, non-polar organic chemicals with a \(\log K_{ow} < 4\) do not normally biomagnify in aquatic food webs via enrichment in fat tissues, and there is no evidence that these substances exhibit BCFs >5000. In terrestrial food webs with air-breathing organisms, chemicals with a \(\log K_{oa} < 5\) are not expected to biomagnify.
- If molecules of a substance are larger than 1.5 nm, they are not likely to exceed a BCF of 5000. However, this observation is context specific; no size threshold can be defined for BMF, for which additional uptake routes are possible.

**Toxicity**

- When toxicological data are limited, a variety of approaches can be used to assess a chemical, including the use of SARs and consideration of the mode of toxic action. Various QSARs have been developed and tested for a variety of chemical and organism classes. Furthermore, understanding the mode of action of a chemical enables a reasonable extrapolation of potential sensitivity and effect responses across taxonomically diverse groups of organisms.

The following conclusions from the workshop are relevant to the use of more detailed tools and empirical approaches in the assessment phase of the proposed framework:

**Persistence**

- Fate testing should be conducted under relevant environmental conditions with respect to temperature, pH, substance concentrations, etc. It is important to understand the mechanisms by which degradation or distribution of the parent material or intermediate degradation products occurs.

- Higher-tier biodegradation (simulation) studies can be difficult to interpret because of the different mechanisms involved in removal and distribution of the parent compound. One critical issue for sediments and soils is whether residues are bound in a way that might reduce their bioavailability. Another critical issue for water-sediment simulation studies is the unrealistic ratio between water and sediment in the test vessels compared to that in natural water bodies.

- No single half-life value can adequately describe degradation in the environment or any environmental compartment. Typically, where multiple degradation studies have been conducted, there is a range of observed half-lives, all of which might be considered when degradation in the relevant compartment is assessed. In such cases it is not appropriate to use the slowest or most conservative half-life. Instead, care should be taken when such data are compiled: Partitioning properties should be checked for internal consistency, and outliers should be identified and not taken into consideration.
- Detection of a chemical in a remote area is not evidence, per se, of persistence and long-range transport potential. Detection in remote environments needs to be assessed in the context of amounts and patterns of usage and emission and the sensitivity of the analytical methods.

**Bioaccumulation**

- Bioaccumulation models and studies can be improved substantially by incorporating information on ADME. Methods for estimating these properties from in vitro studies are developing rapidly. The mechanistic nature of more recent in silico models makes them more transparent and interpretable, and affords the opportunity to incorporate in vitro–derived ADME information.

- According to recent findings, the most relevant B criterion is the TMF, and the most conclusive evidence to demonstrate that a chemical substance biomagnifies is a TMF >1. TMF is derived from a correlation between appropriately normalized chemical concentration in biota and trophic position. It is crucial for the characterization of TMF that both aquatic and terrestrial food-webs are considered. Such consideration is crucial because chemicals can exhibit fundamentally different TMFs in aquatic and terrestrial food-webs because of differences in the bioaccumulation mechanisms between water- and air-breathing organisms. However, a high BCF is also a strong indicator for a high bioaccumulation potential of a chemical, including secondary poisoning effects in food webs.

**Exposure and effects**

- The recommended matrix for monitoring and assessing human exposure to POPs is blood, or its components such as serum or plasma: Human breast milk may also be used in some jurisdictions.

- Diet-based or tissue-based approaches are direct, accurate, and site-specific methods for assessing the risks to top predators from secondary poisoning by PBTs and POPs. The method uses diet to estimate the ingestion of POPs by predators. The advantage of this approach is that the only requirements for exposure assessment are samples of the predator’s diet, realistic estimates of dietary composition, ingestion rates, and measured concentrations in the prey. Even more direct is the tissue-based approach, which uses measurements of PBT or POP concentrations in the tissues of receptor species (top predators) to determine internal exposure directly, and compares this exposure concentration to tissue-based effect concentrations ("toxicity threshold values") to determine
risk. The advantage of this approach is that estimates of PBT or POP transfer to top predators from lower trophic levels, which often have high uncertainty, are not required. In practice, availability of dose–response and internal exposure–response relationships is limited for PBTs and POPs in top predators, so dose–response relationships for surrogate species must often be used. Ideally, these surrogate species data are supported by field biomarker data on PBT or POP exposure and biological responses in the receptor species of interest.

- In developing guidance for global environmental monitoring of legacy POPs, UNEP Guidance for a Global Monitoring Programme recommends focusing on air, human milk, or blood, as well as widely measured biota (mussels, marine mammals, bird eggs, and fishes) as the most appropriate types of samples because of past extensive studies. This is also the most appropriate approach for new candidate POPs.

- The overall recommendation for assessing exposure in humans and top predators is to use or obtain direct measurements of the compound of concern from a significantly and uniquely exposed population (indigenous populations or remote populations), as well as data demonstrating biomagnification and time trends, if possible.

Exposure and long-range transport

- A consensus modeling tool should be developed for benchmarking a PBT–POPs exposure-to-emissions metric. This model or modeling system should 1) have the ability to couple models describing environmental fate, bioaccumulation, and LRT potential; 2) incorporate the ability to include metabolic loss and transformation of the chemical at all trophic levels; 3) allow for incorporation of new partitioning mechanisms such as those observed for ionizable chemicals; and 4) include the ability to model non–steady-state conditions to allow time trend concerns to be scientifically addressed in a risk profile. Such model development should build on the consensus approach used in developing and gaining acceptance for the current LRT models.

Risk characterization, defined in existing risk assessment frameworks and paradigms as an integration of exposure and effects assessments, is a useful model in assessing PBTs and evaluating the potential for significant adverse effects resulting from long-range transport in POPs assessments. While risk profiles or assessments of PBTs or POPs may not necessarily be fully quantitative risk assessments, inclusion of information on risks and uncertainties is desirable at the assessment phase, notably in helping producers, importers, and users of chemicals, or regulatory authorities (such as the Stockholm Convention POP
Review Committee, the Conference of the Parties, or national authorities) to set priorities and make decisions. Lack of scientific certainty about currently available approaches and tools (such as models) should not prevent their use in providing an integrated risk characterization that considers the weight of multiple lines of evidence and associated uncertainties.

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SETAC Pellston Workshop Participants

Workshop Chairmen
Derek Muir *
Environment Canada, Canada
Gary Klečka *
The Dow Chemical Company, USA

Workshop Advisors
Jim Bridges
University of Surrey, United Kingdom
Steve Eisenreich *
European Chemicals Bureau, Italy
Don Mackay *
Trent University, Canada
Jose Tarazona *
INIA, Spain

Evaluating Environmental Persistence Workgroup
Robert Boethling †
USEPA, USA
Kathrin Fenner
Eawag/ETH Zurich, Switzerland
Mick Whelan
Cranfield University, United Kingdom
Phil Howard
Syracuse Research Corporation, USA
Torben Madsen
DHI-Water and Environment, Denmark
Jason Snape †
AstraZeneca, United Kingdom

Multimedia Partitioning, Overall Persistence and Long-Range Transport Workgroup
James Franklin
CLF Consulting, Belgium
Kevin Jones * †
Lancaster University, United Kingdom
Michael Matthies
University of Osnabrueck, Germany
Martin Scheringer †
ETH Zurich, Switzerland
Stacy Simonich
Oregon State University, USA
Dik van de Meent
RIVM, The Netherlands

In Vitro and In Silico Approaches for Bioaccumulation Assessment Workgroup
Mark Bonnell
Environment Canada, Canada
Beate Escher †
Eawag/ETH Zurich, Switzerland,
Sabcho Dimitrov
University of Zlatarov, Bulgaria,
Xing Han
DuPont Company, USA
Nynke Kramer ^
Utrecht University, The Netherlands
John Nichols †
USEPA, USA

Evaluation of Bioaccumulation using Whole Organism Lab and Field Studies Workgroup
Albert Koelmans
Wageningen University, The Netherlands
Anne McElroy
Stony Brook University, USA
Tom Parkerton
Exxon Mobil Biomedical Sciences, USA
Anne Weisbrod †
The Procter & Gamble Company, USA
Kent Woodburn †
Dow Corning Corporation, USA
Revisiting Bioaccumulation Criteria Workgroup
Lawrence Burkhard
USEPA, USA
Watze de Wolf†
DuPont Company, Belgium
Frank Gobas* †
Simon Fraser University, Canada
Kathy Plotzke
Dow Corning Corporation, USA
Eric Verbruggen
RIVM, The Netherlands

Use of Measurement Data in Evaluating Exposure of Human and Wildlife to POPs and PBTs
Derek Muir*
Environment Canada, Canada
Larry Needham
CDC/NCEH/DLS/OAT, USA
David Powell
Dow Corning Corporation, USA
Deborah Swackhamer†
University of Minnesota, USA

Modeling Exposure to Persistent Chemicals in Hazard and Risk Assessment Workgroup
Jon Arnot^
Trent University, Canada
Christina Cowan-Ellsberry†
The Procter & Gamble Company, USA
Matthew MacLeod
ETH Zurich, Switzerland
Thomas McKone
University of California-Berkeley, USA
Michael McLachlan†
Stockholm University, Sweden

Use of (Eco)toxicity Data as Screening Criteria for Identification and Classification of PBT and POP Compounds Workgroup
Peter Dohmen* †
BASF SE, Germany
Anne Fairbrother
Parametrix, Inc., USA
Marcelle Marchand^
University of Johannesburg, South Africa
Lynn McCarty
L.S. McCarty Scientific Research & Consulting, Canada
Keith Solomon†
University of Guelph, Canada

Framework Workgroup
Robert Chenier†
Environment Canada, Canada
Tala Henry
USEPA, USA
Maria Dolores Hernando
REACH Reference Center, Spain
Christoph Schulte
UBA, Germany
Dolf van Wijk* †
EuroChlor, Belgium

* Steering Committee Members
† Session Chairpersons
^ Graduate Student Participant
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If you desire further information, contact the Pensacola Office if you are in Latin America, Asia/Pacific, or North America or the Brussels Office if you are in Europe or Africa.

1010 North 12th Avenue
Pensacola, Florida, 32501-3367 USA
T 850 469 1500 F 850 469 9778
E setac@setac.org

Avenue de la Toison d’Or 67
B-1060 Brussels, Belgium
T 32 2 772 72 81 F 32 2 770 53 86
E setac@setaceu.org

www.setac.org
Environmental Quality Through Science®