Supplemental information for Solomon et al., 2013

The SI provides definitions of a number of terms that we have used in the main text of the paper. For a more complete list of terms and definitions that are relevant to PPPs please refer to IUPAC glossary of terms [1].

Glossary of terms related to persistence

Degradation – Is when substances in different environmental compartments are transformed into degradation products by processes, such as microbial degradation, hydrolysis, and photolysis. Degradation also includes processes such as oxidation and transformation into microbial biosynthetates or polymerization products, which may result in larger molecules than the parent substance [2].

Degradation products – Are all substances resulting from biotic or abiotic transformation reactions of the test substance including CO_2, microbial biosynthetates, and products that are in bound residues [2].

Half-life - abbreviated as $t_{½}$, is used to characterize the rate of a first order process. It is the time interval that corresponds to an exponential decrease in concentration by a factor of 2 (Figure S1). The half-life and the first-order kinetic rate constant k are related by the equation $t_{½} = \ln 2/k$. Both terms are equivalent and are independent of the initial concentration.

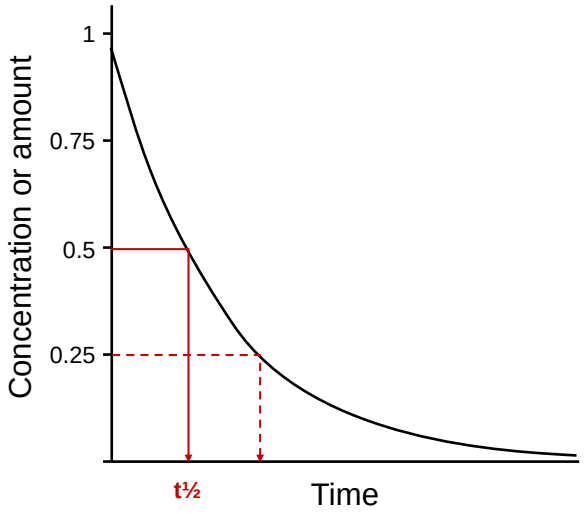

Figure S1. Illustration of half-life of a substance

Disappearance/Dissipation time (DT) **-** Disappearance or Dissipation Time (DT50/90) has no association to any particular type of kinetics and describes the time taken for a 50/90% decline in mass or concentration of a substance to occur by dissipation from the environment after it has been applied to, formed in, or transferred to, an environmental compartment. DT does not differentiate between transfer processes and degradation processes. The first half-life of a substance may be identical to the DT50. The term half-life has been restricted to mean the half-life of a single first-order process to avoid confusion in the use of terminology.

Non-extractable residues (NER) and bound residues (BR) – In general, NER consists of covalently bound and biogenic residues [3] as well as sequestered or entrapped xenobiotic molecules in structural voids and hydrophobic interiors of micelle-like humic aggregates [4]. The first two fractions are considered to be an integral part of the organic soil or sediment matrix. The third fraction of NER might be reversibly sorbed

and slowly released over long time leading to small extractable amounts. This was recently shown by Jablonowsky et al. [5] by means of accelerated solvent extraction and LC-MS/MS analysis of atrazine and 2-hydroxy-atrazine in an agriculturally used outdoor lysimeter 22 years after the last application. However, the particular concern of PBT compounds is the combination of the three characteristics, and in this context the bioavailability, i.e., that they will be present in amounts that are toxic or bioaccumulate, is essential. It is generally considered and shown in many studies, that the bioavailability of NER is low or negligible.

Degradation time (DegT) - Degradation time (DegT50/90) is similar to dissipation time, but the 50/90% decline in mass or concentration of a substance occurs by degradation only. FOCUS defines degradation products as all substances resulting from biotic or abiotic transformation reactions of the test substance including CO_2, microbial biosynthetates, and products that are in bound residues (see above).

Glossary of terms related to bioaccumulation

The uptake of a chemical from the environment by a living organism is a complex process that may occur through different patterns. The term “bioaccumulation” is often improperly used in a generic way. For the sake of clarity we provide the following basic definitions.

Bioconcentration – Is the accumulation of a chemical in the tissues of an organism as a result of direct exposure to the surrounding medium (e.g., water; i.e., it does not include transfer via the food web). [6, 7]. Bioconcentration is expressed by the following equation:

$$d\,C_b/dt = k_1 C_m - k_2 C_b \qquad (1)$$

where C_b is the concentration in the biota, C_m is the concentration in the environmental medium (e.g. water), k_1 and k_2 are uptake and clearance constants, respectively. Bioconcentration is basically a physical-chemical process and involves equilibrium partitioning between the organism and the environmental medium.

Bioconcentration Factor (BCF) – Is defined as the ratio of a contaminant concentration in biota to its concentration in the surrounding medium (e.g., water). At long exposure times (steady state), the BCF also equals the ratio of the uptake and clearance constants [8].
It is expressed by the equation:

$$BCF = C_b/C_m = k_1/k_2 \qquad (2)$$

C_b and C_m must be expressed with the same units (weight/weight) so BCF is a non-dimensional value.

Bioaccumulation – Is defined as the accumulation of chemicals in the tissue of organisms through any route, including respiration, ingestion, or direct contact. [9]. Bioaccumulation may be expressed by the following equation:

$$d\,C_b/dt = k_1C_m + -k_3C_f - k_2C_b \qquad (3)$$

where C_f is the concentration in food, C_m is the concentration in the environmental medium (e.g. water), C_b is the concentration in the biota, k_1 and k_2 are uptake and clearance constants, respectively and k_3 is the food uptake constant. Indeed, this is a simplified expression of bioaccumulation based on the assumption that only one medium is involved in uptake and that only one constant is required for clearance. A more complete equation should consider that clearance occurs through different metabolic processes (respiration, excretion, metabolic transformation, growth dilution, etc.) and that, at least in the terrestrial environment, uptake may occur through respiratory surfaces and through skin contact.

Bioaccumulation Factor (BAF) – Is the ratio of the contaminant in an organism to the concentration in the ambient environment at a steady state, where the organism can take in the contaminant through ingestion with its food as well as through direct contact. [9].

According to this definition, BAF may be expressed as BCF:

$$BAF = C_b/C_m \qquad (4)$$

where C_b is the concentration in the biota, C_m is the concentration in the environmental medium, however, it cannot be expressed as a ratio of uptake and clearance constants.

Biota-Sediment Accumulation Factor (BSAF) – Is the ratio of the contaminant concentration in tissue to the contaminant concentration in sediment.
It is expressed by the equation:

$$BSAF = C_b/C_s \qquad (5)$$

where C_b is the concentration in the biota and C_s is the concentration in sediment. As for BAF above, concentration in the organisms is often normalized to the concentration of lipid. In addition, the concentration of organic carbon in sediment also may influence the bioavailability of contaminants through sorption/desorption, causing increased variability in BSAFs between sites. As a result, BSAFs are also normalized to the concentration of lipid in the organism and the amount of organic carbon in the sediment [10, 11].

Biomagnification – Is the result of the process of bioaccumulation and biotransfer by which tissue concentrations of chemicals in organisms at one trophic level exceed tissue concentrations in organisms at the next lower trophic level in a food chain."[9].

Biomagnification is conceptually different from bioconcentration in that it involves chemical transport against the thermodynamic gradient [i.e., from a low fugacity in the prey to a higher fugacity in the predator, 12].

Biomagnification Factor (BMF) – Is the ratio of concentrations of a compound at two consecutive trophic levels at steady state. BMF can also be expressed in terms of a rate constant-based bioaccumulation model:

$$BMF = C_n/C_{n-1} = \alpha f/k_e \qquad (6)$$

where α is assimilation efficiency, f is feeding rate, and k_e is the first-order elimination constant. BMF can be calculated from field data on assumed trophic relations or from laboratory feeding experiments.

Trophic Magnification Factor (TMF) – Is defined as the average factor by which the normalized chemical concentration in biota of a food web increases per trophic level [12]. It is calculated as the slope of the regression line between the logarithm of the chemical concentration in different organisms (normalized in terms of lipids or fugacities, see below) and the position of the organisms in the trophic chain:

$$\text{Log } C_b = a + bTP \qquad (7)$$

$$TMF = 10^b \qquad (8)$$

where C_b is the concentration in the biota and TP is the trophic position in the considered food chain [13]. TMF is considered the most appropriate measure of biomagnification in a food chain [12].

Normalization and extrapolation - The concentration of chemicals in the biota may be expressed as (weight of chemical)/(weight of organism) (e.g. ng/g). However, there are several possibilities for reporting the concentration in organisms.

> ***Fresh (or wet) weight.*** It is generally applied to organisms intended to be used as food items for humans. Indeed, all standards for the content of dangerous chemicals in food are expressed as fresh weight, considering that edible organisms (fish, meat, vegetables) are usually consumed fresh. Units are ng/g ww.
> ***Dry weight.*** From a scientific point of view, concentrations in dry weight are more significant and easily comparable. Units are ng/g dw.
> ***Lipid weight.*** For lipophilic compounds, which accumulate in fat tissues, this is the best way for expressing concentrations in biota. It is the only possibility to get comparable data for a proper calculation of BMF and TMF. Lipid content in biota is very variable depending upon species. For example, fish can be grouped into four categories according to their fat content: lean fish (<2%), low fat (2–4%), medium fat (4–8%) and high fat (>8%) [14]. Moreover, lipid content may be highly different in the same species as a function of age, seasonal cycle, food

availability, sex, reproductive period, etc. Units are ng/g lipid. However, one must be aware that not all bioaccumulative chemicals are stored in lipids. For example perfluorinated compounds, as well as methyl-mercury, are stored in proteins. In these cases, lipid normalization is inappropriate.

Total organic carbon. For hydrophobic compounds in sediments, two normalizations can be used. As for BMF above, concentration in the organisms is often normalized to the concentration of lipid. In addition, the concentration of organic carbon in sediment may influence the bioavailability of contaminants through sorption/desorption, causing increased variability in BSAFs between samples from different sites. As a result, BSAFs are also normalized to the concentration of lipid in the organism and the amount of organic carbon in the sediment [10, 11]. Units are ng/g lipid/OC.

Fugacity. The fugacity (f) of a chemical in an environmental medium (biotic or abiotic) is:

$$f = C/Z \qquad (9)$$

where C is the concentration in the medium and Z is the capacity constant, depending on the characteristics of the medium and of the chemical [15]. Due to some conceptual difficulties, normalization to fugacity is not very frequently used in the literature. However, for modeling purposes, expressing chemical concentrations in terms of their fugacities is the most appropriate and thermodynamically sound method for comparing data in different organisms and in different environmental media [12, 16].

Glossary of terms related to toxicity

Acute toxicity – The concept of acute toxicity is substantially different in human toxicology and in ecotoxicology. In human toxicology it may be defined as the toxicity produced by a chemical when it is administered in one or more doses during a period not exceeding 24 h. The observed endpoint is usually death. In ecotoxicology, the same concept used in human toxicology is usually applied only for higher terrestrial vertebrates (bird, mammals). In other cases, the definition depends upon the type of organism tested and, in particular, upon the length of the lifecycle. In animals other than terrestrial vertebrates acute toxicity is the effect (death or comparable endpoints, e.g., immobilization) observed after a short term exposure (usually from 24 h up to 14 d, as a function of the lifespan) to a concentration of chemical (not dose) in an environmental medium (water, air, soil). For microorganisms (algae, bacteria) the concept of short term changes substantially. The standard test on algae required by chemical regulations (72 h growth inhibition) covers several generations and must be considered as a test on population dynamics. Actual acute tests must be performed using a time span lower than a life cycle (from 5 minutes to 1 hour) measuring some metabolic endpoints (photosynthesis, luminescence inhibition). For higher plants, the concept of acute toxicity is not applicable. Usually tests measure responses in a relatively long time, generally weeks. Responses include growth, emergence, and germination of seeds and are assumed as chronic effects.

Chronic toxicity – It is the ability of a substance to cause harmful effects over an extended period, usually upon repeated or continuous exposure sometimes lasting for the entire life of the exposed organism. The observed endpoint is usually other than death (e.g., growth, reproduction, etc.). Unless acute toxicity, where most frequently used data is L/EC50, a relevant result of chronic tests is the NOEC (No Observed Effect Concentration). However one must be aware that, unless EC50, the NOEC value is not statistically calculated and is strongly dependent upon the experimental conditions (intervals between tested concentrations, number of individuals, etc.). Low EC values (from 5-25) are often used as a surrogate for NOEC. The advantage is that these are calculated from a concentration-response curve and are less dependent upon the experimental conditions. It is assumed that a response differing less than 10% from the control is not a significant response. However, there are some controversial opinions on this assumption [17].

CMR (Carcinogenic/Mutagenic/Reprotoxic) chemicals – Carcinogenicity and mutagenicity are concepts referred to human toxicology. In ecotoxicology, considering the goals of protection (see above), there is general consensus on assuming that carcinogenicity and mutagenicity are not very relevant for affecting structure and functions of biological communities. On the contrary, reproductive effects, capable to affect population dynamics, are ecologically relevant endpoints. According to REACH (Annex XIII) and to Regulation 1107/2009 [18], CMR chemicals fulfill the T criterion for PBT classification. However, the definition of reproductive toxicity in Regulation 1272/2008 [19] refers to hazard categories describing only human (or mammals) reproductive toxicity. More attention should be devoted to endocrine disrupting chemicals capable to produce effects on reproduction and development of organisms other than mammals.

STOT (Specific Target Organ Toxicants) – Regulation 1272/2008 [19] provides the following definition:

“Target organ toxicity (repeated exposure) means specific, target organ toxicity arising from a repeated exposure to a substance or mixture. All significant health effects that can impair function, both reversible and irreversible, immediate and/or delayed are included.”

Also STOT chemicals fulfill the T criterion for PBT classification. However, in this case too, it is grounded in human toxicology. The concept of “mode of action” has a different meaning in ecotoxicology in comparison with human toxicology and should be referred to broader end-points (such as reproduction impairment, population growth, mortality, etc.) producing ecologically relevant effects on population dynamics and community structure and functions. Moreover, STOT concept is not applicable to the large numbers of species, from bacteria to higher vertebrates, which are the object of ecotoxicologicjabal effect assessment.

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