Identification of POP candidates among chemicals in plastic

Screening for LRTP using the Emissions Fractions Approach

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ABSTRACT

There is considerable interest in identifying chemicals which have the potential to undergo long-range environmental transport (LRTP), accumulate in remote regions, and represent a possible risk to environmental and human health. In this report, we have screened a list of 1,000 organic chemicals, as well as selected brominated dioxins and furans (PBDD/Fs), for their potential to be dispersed, transferred to, and accumulated in remote regions. This screening was carried out applying a new set of LRTP metrics, collectively referred to as the emissions fractions approach (EFA), as implemented in a modified version of the OECD P_{OV} and LRTP (long-range transport potential) Screening Tool (The Tool).

NORWEGIAN TITLE

Identifisering av POP kandidater blant kjemikalier i plast.

KEYWORDS

Long-range environmental transport | Screening | Emissions Fractions Approach

ABSTRACT (in Norwegian)

Det er betydelig interesse for å identifisere kjemiske stoffer med potensiale til å transporteres over lange avstander (LRTP) samt akkumulere i uberørte områder, så som i Arktis. Gitt det betydelige antall kjemikalier som produseres globalt og/eller nydannes ved f.eks. forbrenningsprosesser vil måledata alltid være begrenset. Matematiske modeller kan her spille en viktig rolle for å gi en indikasjon hvorvidt et kjemisk stoff har iboende egenskaper som tilsier at det har potensiale til å kunne akkumulere i det fysiske miljø i avsidesliggende områder. I denne rapporten har vi benyttet en modifisert utgave av «The OECD P_{OV} and LRTP (long-range transport potential) Screening Tool (The Tool)» hvor vi har implementert et nytt sett av indikatorer for LRTP som beregner spredning, avsetning og akkumulering i avsidesliggende områder. Modellen har blitt anvendt for 1000 kjemiske stoffer samt utvalgte bromerte dioksiner og furaner (PBBD/Fs). Resultatene tilsier at samtlige PBBD/Fs og 75 andre forbindelser kan ha POP-liknende egenskaper. Flere av disse stoffene er velkjente miljøgifter.

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Preface

The Norwegian Environment Agency asked NILU to carry out an assessment of the long-range environmental transport potential of brominated dioxins and furans (PBBD/Fs) as well as 1,000 other chemicals associated with plastics in 2023. This report presents the main findings from the project.

The authors would like to thank Christina Charlotte Tolfsen, Mitsuko Komada, and Christel Moræus Olsen at the Norwegian Environment Agency for expressing an interest in our research and their support.

We would additionally like to acknowledge support from the Research Council of Norway that allows us to continue our research on screening chemicals for POP-like behaviour (343110).

Contents

Summary

There is considerable interest in identifying chemicals which may undergo long-range environmental transport (LRET), accumulate in remote regions, and represent a possible risk to environmental and human health. As empirical data will always remain limited when considering the large number of chemicals in commerce, the use of mathematical models play an important role in screening chemicals for LRTP.

In this report, we have screened a list of 1,000 organic chemicals used in plastic, as well as selected brominated dioxins and furans (PBBD/Fs), for their potential to be dispersed, transferred to, and accumulated in remote regions. The screening was carried out applying a new set of LRTP metrics, collectively referred to as the emissions fractions approach (EFA), as implemented in a modified version of the OECD P_{OV} and LRTP (long-range transport potential) Screening Tool (The Tool).

All PBBD/Fs and 75 additional discrete chemicals in the screening data set exceeded the threshold for POP-like accumulation in remote regions using the EFA, many of which are already known environmental contaminants, when relying on thresholds defined as the lowest values predicted for a set of 14 legacy POPs. We also show that many of the chemicals that were predicted to be POP-like in terms of their potential accumulation in the remote region would not have been recognized as POP-like using the existing metrics in The Tool. Substances with insufficient monitoring data could then have been neglected as POP candidates (false negative decisions) as the EFA predicts that there are many chemicals on the screening list which have the potential to accumulate in a remote region in the context of Annex E without meeting the screening criteria under Annex D of the Stockholm Convention.

In this report, we furthermore expand on the mechanistic nature of the EFA to identify and discuss opportunities for higher tier LRTP assessments of chemicals of potential interest, using representative chemicals for various chemical categories as examples. The utility of the EFA is furthermore highlighted for 10 more chemicals in the screening data set, some of which have already attracted regulatory interest in recent years.

As The Tool is a relatively simple multimedia model and many of the chemicals in the screening data set fall outside the domain of applicability of the model, we finalize the report with a discussion of some of the more critical model assumptions in The Tool and their implications for LRTP assessments.

Identification of POP candidates among chemicals in plastic. Screening for LRTP using the Emissions Fractions Approach.

1 Introduction

The Stockholm Convention (SC) on Persistent Organic Pollutants (POPs) is a global treaty to protect human health and the environment from chemicals that are persistent (P), bioaccumulative (B), toxic (T), and have the potential for long-range environmental transport (LRTP) to remote areas of the globe, such as the Arctic. The SC includes provisions for Parties to nominate new chemicals for potential amendment to the Convention and the number of chemicals listed as POPs has greatly increased since the SC came into effect. Norway has nominated several substances / substance groups (Penta-BDE, HBCD, and deca-BDE, PFHxS and Dechlorane Plus) to the SC that are now regulated under this global treaty.

Among the tens of thousands of chemicals in commerce, only a small fraction has been analysed in environmental samples. Most POPs and organic Contaminants of Emerging Arctic Concern (CEACs) that are measured and/or monitored in remote areas were initially discovered by analytical chemists who observed unknown signals during the trace analysis of environmental samples collected elsewhere. However, most empirical approaches have a fundamental weakness, as they generally only identify contaminants that are similar to known contaminants because trace analytical methods exclude all chemicals except those that are similar to the analyte in focus. For the development of rational chemical management strategies aiming to protect remote regions from chemical pollution caused by LRET, it is imperative to understand the hazardous properties of a much larger number of chemicals and ultimately, the quantitative relationship between chemical emissions and the resulting exposure.

Simple LRTP screening criteria such as atmospheric half-lives do not differentiate substances according to the dominant mechanisms which dictate their LRTP and their potential for transfer to, and possible accumulation in, surface media of remote regions, such as the Arctic. Due to the variety of the processes involved, mathematical models are required to assess a chemical's LRTP. In response to the need for science-based LRTP assessment, a number of modelling approaches and metrics have been developed. Several years ago, the OECD instituted an expert group that was tasked with providing guidance on LRTP and P assessment by comparing the different model approaches / LRTP metrics and recommending a consensus modelling tool. This initiative led to The OECD P_{OV} and LRTP Screening Tool for assessing chemicals for P and LRTP.

Here, we have applied a modified version of The OECD P_{OV} and LRTP Screening Tool to screen a list of about 1,000 chemicals, as well as selected brominated dioxins (PBDDs) and furans (PBDFs), for LRTP. The list of 1,000 chemicals was provided by the Norwegian Environment Agency and included a wide range of chemicals, including naturally organic compounds. More than 10,000 substances have been identified as used or associated with plastic by Wiesinger et al.[1] From this list, the list of 1,000 to be screened in this project, was generated by filtering out substances with use volumes below 1,000 tonnes, UVCBs, ionic substances, substances without SMILES (simplified molecular-input line-entry system), low confidence of assignment.

2 Methods

2.1 The OECD Tool

The OECD P_{OV} and LRTP Screening Tool for assessing chemicals for P and LRTP is a relatively simple steady-state multimedia model. This software, commonly referred to as "The Tool", is a consensus-based model largely motivated by regulatory needs for screening the hazard potential of non-ionizing organic chemicals.[2] The Tool is parameterized to reflect the environmental characteristics of the global environment and it includes one air, one water, and one soil compartment. For example, the area fractions selected for water and soil mirrors the area fractions for oceans and the terrestrial environment for the entire globe. A detailed description of the existing version of The Tool (version 2.2) can be found in Wegmann et al.[2]

2.2 Metrics

The main outputs from the existing version of The Tool are predictions of a chemical's potential for (i) transport/dispersion in each mobile media (CTD – Characteristic Travel Distance), and (ii) transfer from air to surface media in the remote region divided by the mass flux emitted in the source region (TE – Transfer Efficiency), as well as overall persistence (P_{OV}) (see Fig. 1a and Table 1 for definitions). The alternative LRTP metrics, collectively referred to as the Emissions Fractions Approach (EFA) includes one dispersion-oriented metric (ϕ1), one transfer-oriented metric (ϕ2), and one accumulation oriented-metric (ϕ3)[3] (see Fig 1b and Table 1).

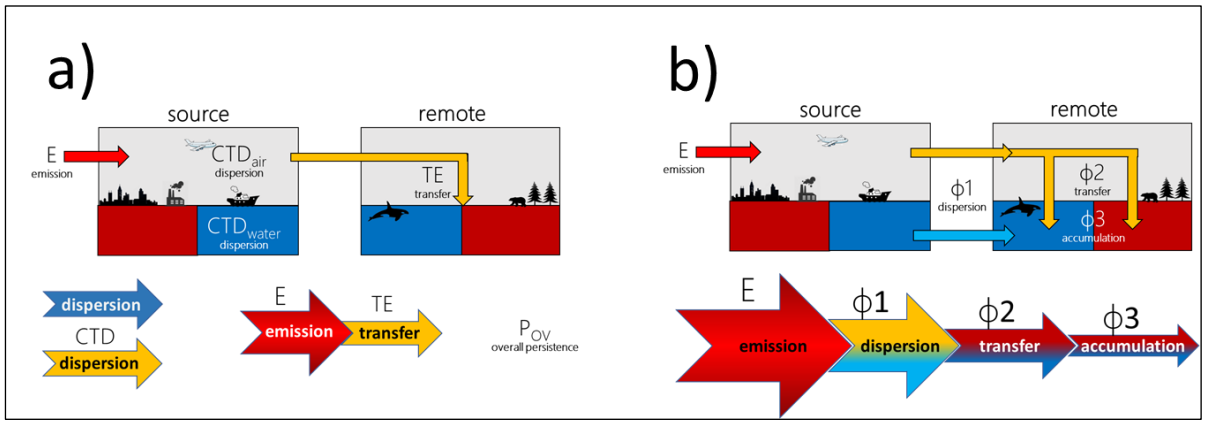


Figure 1: Simplified graphical representation of the existing metrics (panel a) and alternative metrics (panel b) in the modified version of The Tool. The coherence of the alternative EFA metrics is highlighted and the definition of each metric is given in Table 1.

Table 1: Definitions of existing (CTD, TE, and P_{OV})[2] and alternative metrics (φ1, φ2, and φ3)[3].

CTD (km)	The distance from a point source at which the concentration of a chemical has been reduced to ~37%.
TE (%)	TE as defined in The Tool represents the (unidirectional) mass flux from air to surface compartments, divided by the emission mass flux in a source region.
P_{OV} (days)	Overall persistence. P_{OV}, unlike single-media half-life criteria, considers how chemicals distribute in the environment, accounting for the mode of entry of a chemical into the environment.
ϕ1	The environmentally dispersed fraction (ϕ1) quantifies the relative extent to which a chemical can reach remote regions.
ϕ2	The remotely transferred fraction (ϕ2) expresses to what relative extent a chemical can reach surface media in remote regions.

ϕ3	The remotely accumulated fraction (ϕ3) assesses the fraction of chemical emissions accumulating in the surface media of remote regions.

Note that any mechanistic model-based LRTP assessment targeting a chemical's potential for accumulation in a remote region must include surface compartments. Hence, ϕ3 can only be estimated using multimedia models.

2.3 Model input data

A model simulation using The Tool requires information on a chemical's molecular weight (g/mol), the equilibrium partition ratio between water and octanol (log K_{OW} – dimensionless), the equilibrium partition ratio between air and water (log K_{AW} – dimensionless), as well as the degradation half-lives in air, water, and soil (in hours). The required input parameters for each of the 1,000 substances, as well as selected brominated dioxins and furans (PBDD/Fs), were retrieved from EPI Suite using SMILES.[4] For PBDD/Fs, we chose the same 11 congeners as studied by Bjurlid et al.[5, 6] EPI Suite outputs both experimental and predicted property values, and the experimentally measured values were selected whenever available. 105 substances had to be excluded from further assessment because discrete structures were only available for 895 out of 1,000 chemicals in the screening data set. It should be noted that all 895 discrete structures were simulated using the modified version of The Tool, irrespective of whether these were (i) duplicated, (ii) within or outside the domain of applicability of the model, and/or (iii) natural substances.

2.4 Thresholds for POP-like behavior

Thresholds for POP-like behavior for each of the metrics were defined as the lowest values predicted for a set of 14 legacy POPs based on any of the three default emission scenarios (100% to air, 100% to water, and 100% to soil)[3], see Table 2.

Table 2: Thresholds for POP-like behavior, including the number of chemicals exceeding each threshold among the 895 discrete chemicals (with duplicates included).

Bold heading	ϕ1 (-)	ϕ2 (-)	ϕ3 (-)	CTD (km)	TE (%)	P_{OV} (days)
Threshold	7.67e-4	8.41e-5	8.19e-6	1,021	0.32	480
Threshold (log)	-3.12	-4.08	-5.09	3.01	-0.49	2.68
Chemicals>threshold	187	261	94	190	258	32

2.5 Screening for empirical data

An initial screening of empirical data for each of the short-listed chemicals (i.e., those with a log ϕ3 above the threshold in Table 2, with duplicates removed) was conducted using SciFinder. The CAS number was used as the unique substance identifier for this part of the study. The total number of publications was seen as an indication of the available knowledge. However, it should be cautioned that many of these publications do not necessarily fall within the domain of environmental science (ethanol serves as an example).

For each discrete chemical, the title, abstract, and keywords were searched for the word "Arctic". Whenever "Arctic" was mentioned for a specific chemical, a more detailed search for actual findings in different types of matrices was conducted: air (A), water (W), soil/sediment (S), biota (B), and/or humans (H). It should be noted that no further analysis was carried out regarding the levels, the number of studies, the frequency of detection, nor the accuracy or precision of the quantitative data, as this would require a far more extensive analysis.

3 Results

3.1 Brominated dioxins (PBDDs) and furans (PBDFs)

6 PBDDs (2,3,7,8-TeBDD; 1,2,3,7,8-PeBDD; 1,2,3,4,7,8-HxBDD; 1,2,3,6,7,8-HxBDD; 1,2,3,7,8,9-HxBDD; and 1,2,3,4,6,7,8-HpBDD) and 5 PBDFs (2,3,7,8-TeBDF; 1,2,3,7,8-PeBDF; 2,3,4,7,8-PeBDF; 1,2,3,4,7,8-HxBDF; and 1,2,3,4,6,7,8-HpBDF) were simulated. Log ϕ3 of each of the individual PBDD/Fs was well above the threshold for POP-like ϕ3 (-5.09: Table 2), ranging from -2.68 (2,3,7,8-TeBDF) up to -2.57 (1,2,3,4,6,7,8-HpBDD). Four of these congeners were analyzed in more detail in the following.

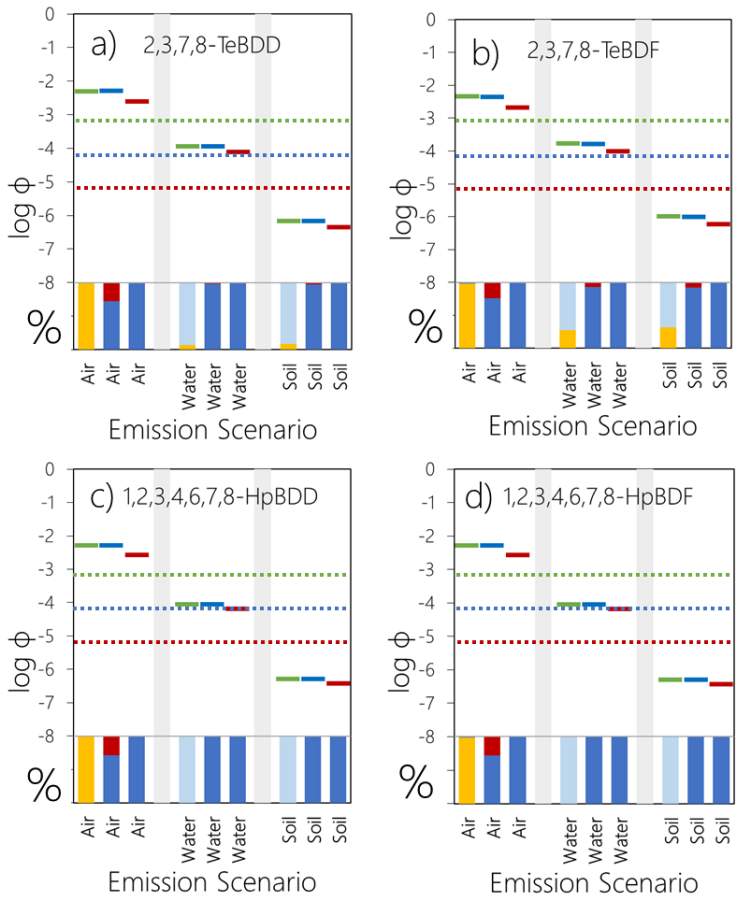


Figure 2: Standard figures for selected PBDD/Fs (see text for explanation).

Each of the four panels in Figure 2 are referred to as standard plots. These types of plots were introduced by Breivik et al.[3] to facilitate a more comprehensive mechanistic interpretation of model predictions on the basis of information embedded in the model's code. In Figure 2, we show standard plots for the congeners among the PBDDs and PBDFs with the highest and lowest value for ϕ3. Each standard plot shows predictions for each of the three default emission scenarios (100% to air, 100% to water, and 100% soil; see x-axis). A standard plot furthermore includes two plots that are stacked on top of each other; The upper part shows results for each metric (ϕ1 – green markers, ϕ2 – blue markers, and ϕ3 – red markers) with log ϕ along the y-axis. The stipulated lines show the thresholds for POP-like behavior according to Table 2. The lower part of each figure contains stacked bars (0 to 100 %). Choosing the emission scenario for air as an example (to the left in each panel in Fig. 2), the left bar displays the relative significance of long-range atmospheric transport (LRAT, yellow) and long-range water transport (LRWT, light blue) in controlling the predicted total dispersion (ϕ1). The middle bar discriminates between the relative importance of net transfer (ϕ2) to water (blue) and soil (red), whereas the right bar highlights the portion accumulating (ϕ3) in soil (red) and water (blue). As model

predictions for each of the three default emission scenarios are covered in Fig. 2[3], a model user with insights into the likely mode of emission of a specific chemical may then choose to rely on the model outputs for the emission scenario(s) that are likely to be more plausible.

As a first observation we note that the upper part of the plots in each of the four panels (Fig. 2) appear similar, i.e., that the LRTP of individual PBDD/Fs are likely to be similar (ϕ1, ϕ2, and ϕ3). When looking at the emission scenario to air only (to the left in each panel in Fig. 2), we note that both ϕ1 and ϕ2 are virtually identical for each of the four congeners. This is because PBDD/Fs are predominantly associated with particles in air ("non-volatiles") which, in turn, are predicted to readily deposit to surface media in the remote region. The relative fractions that are transferred to surface media in the remote region (ϕ2) therefore reflect the area fractions for soil (29%) and water (71%) in the model. However, the potential for accumulation in the remote region for each of the congeners is attributed to accumulation in water, irrespective of the emission scenario considered (i.e., the lower part of the plots in each of the four panels in Fig 2.).

If these chemicals are emitted to water (middle of each panel in Fig. 2), we note that there are subtle differences between the lighter PBDD/Fs (Fig. 2 a, b) versus the heavier congeners (Fig. 2 c, d) when it comes to the predicted mode of dispersion from the source region into the remote region (lower part of the plots in each of the four panels). Specifically, the model suggests that the lighter PBDD/Fs do have a limited potential to evaporate from water and undergo LRAT into the remote region, although LRWT dominates the total dispersion (ϕ1) for the lighter PBDD/Fs.

Overall, the model results suggest that each of the congeners are predicted to exceed the threshold for POP-like accumulation in the remote region (ϕ3) if emitted to air or water, but not soil (Fig. 2).

3.2 LRTP assessment of the screening data set

We have previously shown that LRTP assessments based on the existing (i.e. CTD, TE, and P_{OV}) and alternative metrics (ϕ1, ϕ2, and ϕ3) could lead to different outcomes.[7] To evaluate whether this could also be the case for the screening data set (*N*=895, i.e., without any duplicates removed), we first plot results in a similar way to that recommended by the OECD. The main results are presented in Figure 3. From these results we find that the CTD-P_{OV}-combination flags 24 chemicals as POP-like (Fig. 3a), whereas the TE-P_{OV}-combination flags 28 chemicals (Fig. 3b).

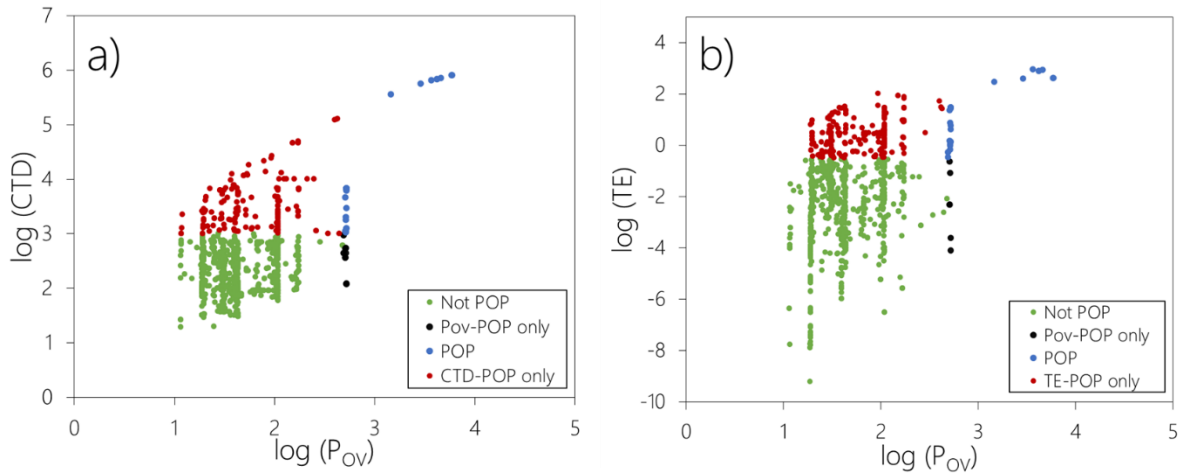


Figure 3: Plots of CTD versus P_{OV} (left panel) and TE versus P_{OV} (right panel) from The Tool for 895 organic chemicals with discrete structures. Chemicals identified as POP-like are located in the upper right quadrant (blue markers).

We have previously pointed out that the existing metrics in The Tool suffer from limitations.[3] These include a lack of (i) integrated treatment of LRT in air and water, (ii) coherency, and (iii) consideration of a chemical's potential to undergo reversible atmospheric deposition ("grass-hopping") when calculating TE. The existing version of The Tool does neither include a metric to assess a chemical's potential to accumulate in surface media of the remote region (Table 1). This may be seen as a major shortcoming because accumulation in surface media is a prerequisite for assessing a chemical's potential to lead to possible adverse effects due to LRT. It is only the EFA which includes a metric for accumulation (ϕ3).

Figure 4 illustrates how the categorization based on the LRTP-P_{OV} combinations compares with a categorization based on ϕ3 for the 895 chemicals. From this we see that ϕ3 flags 94 chemicals as having a potential for accumulation in the remote region due to LRT.

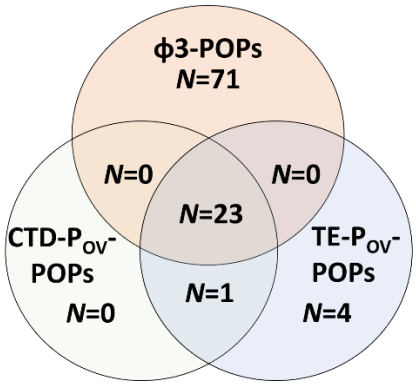


Figure 4: Comparison of the number of chemicals in the screening data set which exceed the criteria for CTD-P_{OV}, TE-P_{OV}, and φ3 (duplicates included).

It is of interest to assess the relative ranks for each of the EFA, as this offers insights into the "discriminatory power" of each metric. For example, a metric that does not lead to a wide range of numerical results will have a limited ability to distinguish between those chemicals that are predicted to have LRTP and those that do not. Figure 5 shows the relative ranks for each EFA metric.

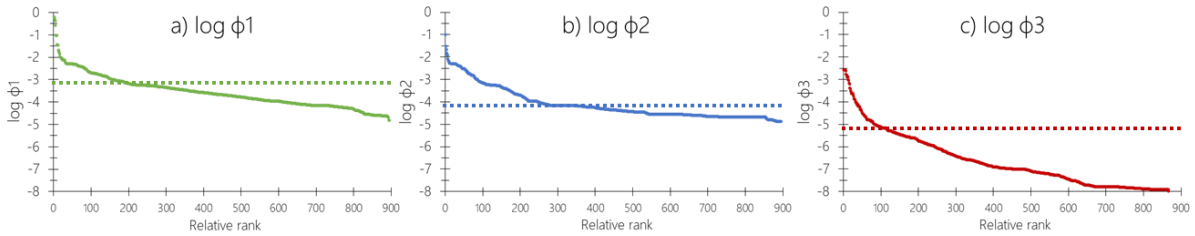


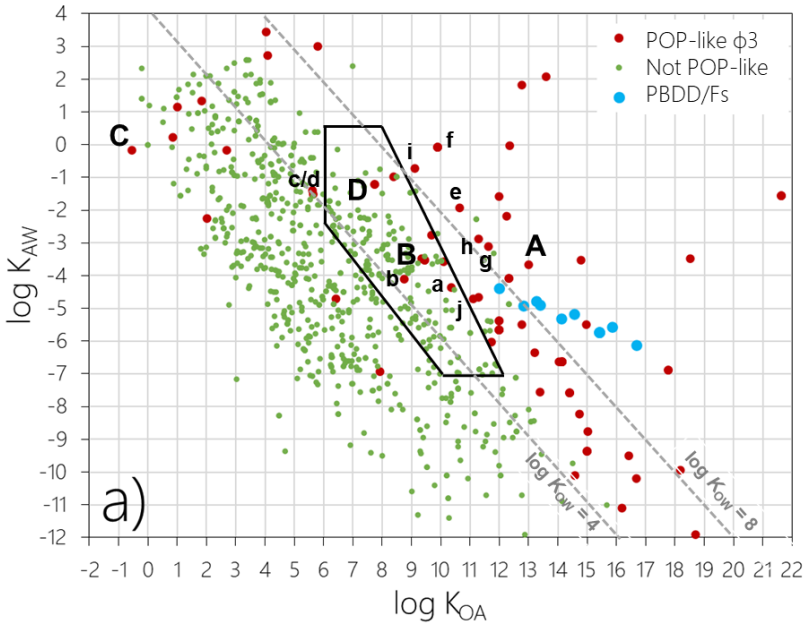
Figure 5: Relative ranking of 895 organic chemicals for LRTP (φ1, φ2, and φ3). The threshold for POP-like LRTP are indicated using dashed lines.

In this data set ϕ1 and ϕ2 vary over ~4 orders of magnitude, whilst ϕ3 varies by close to six orders of magnitude. This shows that the EFA does have the potential to discriminate between chemicals with low and high LRTP, which may be particularly true in the specific case of predicting a chemical's potential for accumulation in the remote region due to LRT (ϕ3).

Up to this point, we have assessed all 895 chemicals with discrete chemical structures without eliminating any duplicates. While 94 out of these 895 chemicals (or structures) exceeded the threshold for POP-like behavior according to ϕ3, only 75 discrete chemicals remained after removal of duplicates. These 75 are listed in Appendix A, which includes a table of CAS numbers, chemical names, and chemical fate properties (model input data), as well as the predicted value for ϕ3, ranked from highest to lowest ϕ3.

The search for empirical data in SciFinder revealed that about half (or more) of the 75 discrete chemicals that exceeded the threshold for ϕ3 have been detected in the environment (Appendix B). A minimum of 20 chemicals have, furthermore, been studied in the Arctic. Note that there are both POPs and POP-like chemicals, as well as naturally occurring substances among these 20 chemicals.

To better understand what separate chemicals that exceeded the threshold for ϕ3 compared to those chemicals that did not, we show two diagnostic plots to facilitate further analyses of the model results, with an emphasis on the roles of partitioning and degradation, respectively. From Figure 6a, we first observe that the chemicals with a POP-like potential for accumulation (ϕ3) are scattered across the partitioning space. From Figure 6b, we furthermore see that there are chemicals which exceed the threshold for ϕ3 (red markers) in each of the four quadrants, i.e., the model predicts that there are chemicals in the screening data set with a POP-like ϕ3 that may or may not exceed an atmospheric half-life > 2 days (LRTP criteria) and/or a half-life in water > 2 months (P criteria). In other words, the chemicals that are predicted to exceed the threshold for ϕ3, as listed in Appendix 1, exhibit a large variability in terms of chemical fate properties (Fig. 6).



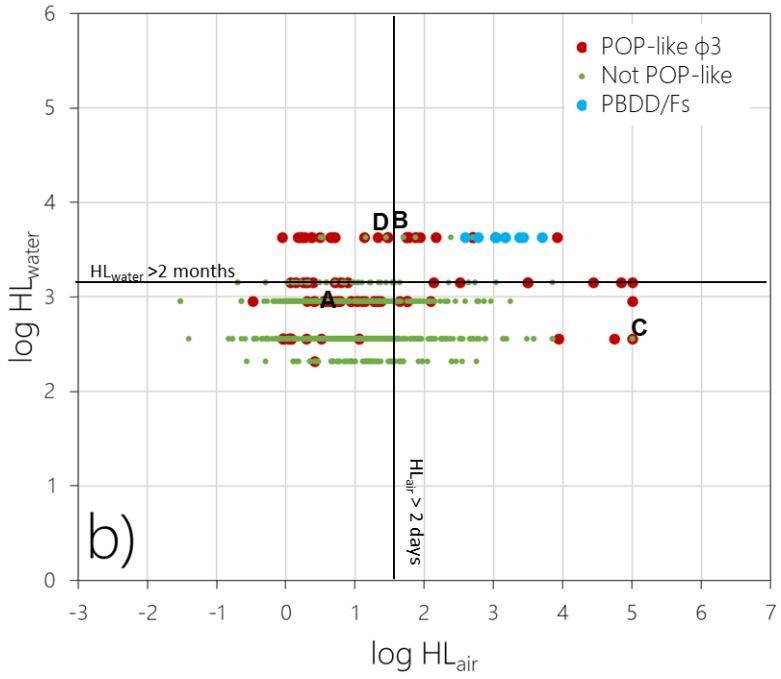


Figure 6: Diagnostic plots for those chemicals that exceeded the threshold for $\phi 3$. Chemicals in the screening data set (N=94) are highlighted with red markers, whereas the selected PBDDs/PBDFs are shown with blue markers. Chemicals falling below the threshold for $\phi 3$ are shown with green markers. Panel a) shows model predictions in a chemical partitioning space (some chemicals in the screening data set are outside the boundaries of the partitioning space and thus, omitted from plot). Panel b) shows the results when plotting degradation half-lives in air (hours) against degradation half-lives in water (hours) for the entire data set. The black outline close to the centre of Panel a) is added for context; It delineates the equilibrium partitioning property combinations that are predicted to result in elevated potential for accumulation in the Arctic physical environment and the Arctic human food-chain using a higher-tier modelling approach.[8] Selected chemicals which exceeded the threshold for POP-like $\phi 3$ are labelled by letters and analysed in further detail below and in Appendix C.

To illustrate how the model may be applied to further analyze the data set, we have selected four chemicals with highly divergent fate properties that exceeded the threshold for ϕ3, as examples. These four chemicals are labelled A, B, C, and D in Figure 6. Chemical A is diisodecyl phenyl phosphite (ranked #20 in Appendix A), Chemical B is o,p'-DDT (ranked #37 in Appendix A), Chemical C is phosgene (ranked #42 in Appendix A), and Chemical D is 1,1-bis(tert-butylperoxy)-3,3,5-trimethylcyclohexane (ranked #77 in Appendix A). In the interest of brevity, we refer to them as A, B, C, and D in the following discussions.

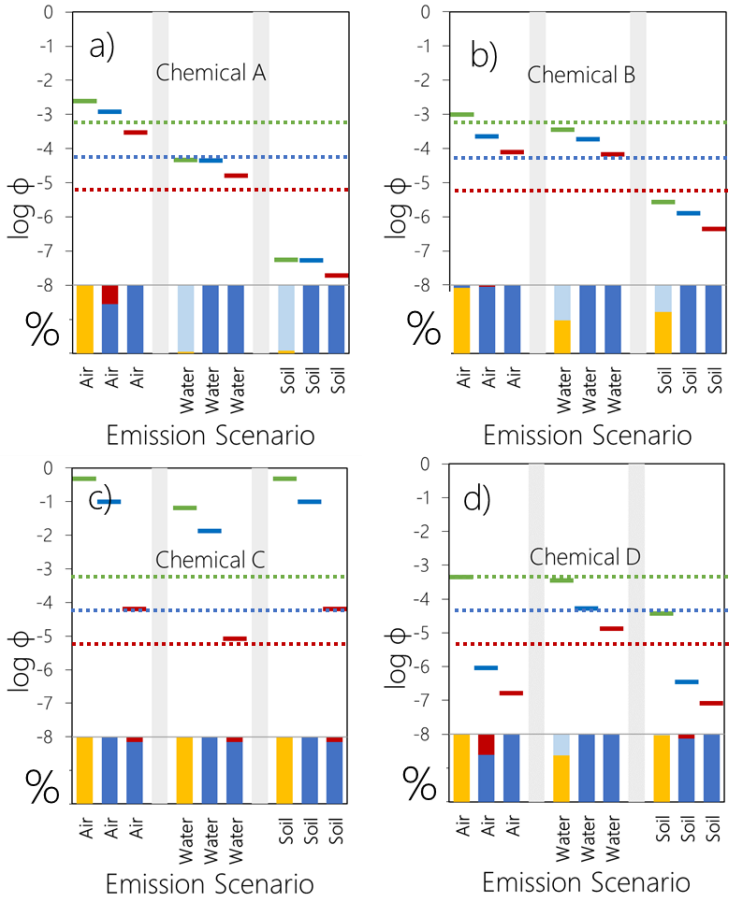


Figure 7: Standard figures for four selected chemicals with highly divergent fate properties that exceeded the threshold for φ3: a) diisodecyl phenyl phosphite, b) o,p'-DDT, c) phosgene, and d) 1,1-bis(tert-butylperoxy)-3,3,5-trimethylcyclohexane.

Chemical A is a fairly non-volatile chemical (log K_{OA} ≈ 13, Fig 7a) that does not exceed the half-life criteria for air or water, i.e., Chemical A falls into the lower left quadrant in Fig. 6b. For Chemical A, the emission scenario to air is what leads to the highest ϕ3 and thereby determines the final value for ϕ3. As Chemical A is predicted to be almost exclusively sorbed to particles in air, similar to the lighter PBDD/Fs (Fig 2a,b), it largely behaves as any other "single-hopper" compound by not undergoing reversible atmospheric deposition (unless it undergoes resuspension, but this is not accounted for in The Tool). However, while ϕ1 was found to be equal to ϕ2 for the PBDD/Fs for the emission scenario to air, this was not the case for Chemical A, because ϕ1 was somewhat higher than ϕ2. This can only be explained by atmospheric reactions in the gas phase.

As noted earlier, it is assumed in The Tool that the fraction of chemical that is predicted to be sorbed to atmospheric particles does not degrade. The implication of this assumption is that the degradation half-life in air is not considered for any perfectly non-volatile chemical in a model calculation using The Tool. While Chemical A is almost exclusively sorbed to particles in air, the tiny fraction that remains in the gas phase is rapidly degraded, as Chemical A has a degradation half-life in air of less than 4 hours.

The difference between the PBDD/Fs versus Chemical A illustrates three key points:

i) Any perfectly non-volatile chemical has the same potential for LRAT if emitted to air, and
ii) This assumption in The Tool implies a risk towards overestimating LRTP of non-volatile chemicals that degrade on particles (false positive decisions).

iii) An accurate estimate of gas-particle partitioning is crucial when assessing the LRTP of chemicals which may exist in both gaseous state and sorbed to particles in air.

Gas-particle partitioning in the Tool is calculated based on log K_{OA}, which in turn, is estimated as log K_{OW} – log K_{AW}. The transition zone, which distinguishes a chemical from being predominantly in the gas phase to being mainly sorbed to particles in air in The Tool, occurs when log K_{OA} ~ 11. If a chemical has a log K_{OA} < 9, then sorption to solids in air can largely be ignored. If a chemical has a log K_{OA} > 13, then reaction in air will play a very minor role in limiting LRAT (unless the chemical in question is relatively reactive in the gas phase, such as Chemical A). Clearly, the default model assumptions governing reaction in air, as well as the description of gas-particle partitioning in The Tool, have potential significant implications for the LRATP assessment of semi-volatile and non-volatile chemicals.

The factors discussed above largely explain why we observe that there are many non-volatile chemicals that are predicted to exceed the threshold for ϕ3 in Figure 6a despite not being very persistent in surface media. It has immediate relevance for the interpretation of results from this screening exercise because any chemical that is ranked #35 and higher has a log K_{OA} > 12.7 (Appendix A).

Opportunities for improved characterization of (i) gas-particle partitioning, (ii) possible degradation on atmospheric particles, (iii) deposition velocities, (iv) atmospheric transport, and (v) impact of environmental variability are thus, important issues to consider for any higher-tier LRTP assessments of chemicals which sorb onto particles in air in appreciable amounts.

Chemical B (o,p'-DDT; Fig. 7b) belongs to the group of legacy semi-volatile organochlorine pesticides, and thereby falls into the center of the chemical partitioning plot which is often referred to as the multi-media region (Figure 6a). Chemical B also exceeds both half-life criteria in Figure 6b. Hence, Chemical B is a key example of a multimedia pollutant for which a multimedia model should be the preferred choice when assessing chemicals for LRTP (e.g., to account for reversible atmospheric deposition). Indeed, much of our mechanistic understanding of the overall environmental fate and LRT behavior of persistent semi-volatile organic contaminants (SVOCs) has been obtained from multimedia models. Because the environmental fate and LRET behavior of individual multimedia pollutants could be dictated by a multitude of processes (in contrast to e.g., the atmospheric dispersion and gross deposition of single-hoppers), any higher-tier model-based LRTP assessments of non-dissociating SVOCs should consider the use of more sophisticated multimedia models and notably, models which accounts for environmental variability. The latter is because factoring in spatial and temporal variability (e.g., temperature) has been demonstrated to have a significant impact on the LRET behavior and fate of SVOCs (e.g., the "dirty dozen").

Chemical C is a volatile chemical ("flyer") which is very persistent in air, but not in water (i.e., falling into the lower right quadrant in Figure 6b). Chemical C is predicted to exceed the threshold for ϕ3 irrespective of the emission scenario considered (Figure 7c). Hence, if a persistent flyer is emitted to surface media (water or soil), an accurate representation of volatilization in the model becomes critical. Clearly, opportunities for higher-tier LRTP assessments of Chemical C and related substances in the context of accumulation in a remote region may involve further efforts to improve the understanding of air-surface exchange. If the chemical is highly persistent in air, it should be noted that a sophisticated description of atmospheric transport may not be required when targeting accumulation in a remote region, as this type of chemical is likely to be well-mixed in the atmosphere of a remote region. HCB offers an example.

Chemical D (Figure 7d) is another chemical which is located within the multimedia region of the plot, yet it is more volatile than Chemical B (Fig. 6a). Chemical D only exceeds the threshold for ϕ3 if is emitted to water, whereas the other two emission scenarios lead to a very low potential for

accumulation in the remote region. Interestingly, the predominant mode of dispersion into the remote region (ϕ1) is attributed to LRAT, rather than LRWT for any of the emission scenarios, even if Chemical D is emitted to water. This suggests that Chemical D has the potential to evaporate after being emitted into water (or soil) in the source region. Yet, it is predicted to be too volatile to have any appreciable deposition from the atmosphere to surface media in the remote region (ϕ3), unless emitted to water. In other words, the predicted potentials for transfer (ϕ2) and accumulation (ϕ3) in the remote region are associated with the water compartment (lower part of Fig. 7d). This indicates that efforts to undertake any higher-tier model-based assessment of Chemical D may involve specific attention to the description of water transport, the degradation half-life in water, as well as the value used for log K_{OW} (which are used to predict sorption to solids in water and in turn, affects the potential for sinking). A more sophisticated multimedia model that accounts for environmental variability may be an obvious choice for any higher-tier model-based assessments for this type of chemical.

Other chemicals exceeding the threshold for ϕ3 There are a large number of non-volatiles that exceeded the criteria for ϕ3, including chemicals which are fairly reactive in surface media. This is a result of the coherency of the EFA. Any perfectly non-volatile chemical is predicted to have high ϕ1 and ϕ2 if emitted to air (Fig 2c,d). Hence, ϕ3 may easily exceed the threshold for POP-like accumulation even if the fraction of deposited chemical that is retained in surface compartments is relatively limited. It is more difficult to anticipate the LRET behavior of chemicals that fall within or in the vicinity of the black outline in the center of Figure 6a because SVOCs and related chemicals are often influenced by a multitude of fate processes. To illustrate some of this variability, we have included 10 more standard plots in Figure S1 (Appendix C) for chemicals that were labelled a to j in Figure 6a.

Chemicals falling below the threshold for ϕ3 Here we have defined a bright-line cut-off criteria to discriminate between chemicals in the screening data set that have POP-like potential to accumulate in surface media in a remote region or not. Given the various uncertainties in model inputs, as well as the simplicity of the model, it may be prudent to expand attention towards chemicals also falling below the threshold in Table 2 for a more detailed LRTP assessment. A list of ~100 chemicals that fell immediately below the threshold for POP-like ϕ3 is included in Appendix D, along with an initial assessment of empirical data included in Appendix E.

4 Discussion

When assessing the model-based results, the reader should be reminded that The Tool is a relatively simple multimedia model for which the domain of applicability is restricted to non-ionizing organic chemicals, irrespective of the LRTP metrics applied. Here, we have applied the model to 895 discrete structures without considering the potential of individual substances to be ionized under environmental conditions, yet we believe this represents a conservative approach for acids.

The Tool represents a hazard-based approach to LRTP assessments, relying on a unit emission rate. Hence, the model is not capable of predicting actual concentrations and thus, exposure. As the model is steady-state and non-spatially resolved, it does not account for environmental variability, which could have a significant influence on the LRT behavior of chemicals. For example, the environmental temperature is 25°C across compartments, which means that the elevated potential for deposition and possible enhanced persistence in cold environments is not captured.

In the context of this study, it should also be kept in mind that the model does not include a description of plastics as a vector for contaminant transport. We have recently also cautioned that The Tool assumes that any non-volatile chemical does not undergo reactions in the particle phase, and that there are possibilities that non-volatile chemicals may be incorrectly classified as undergoing LRAT.

Despite the limitations of what a relatively simple model, such as The Tool, can do, we believe these model predictions offer some useful insights beyond identifying chemicals with LRTP. For example, the EFA offers a mechanistic approach to help identify rational ways forward if possible higher-tier LRTP assessments are desirable, as indicated for Chemicals A to D. This type of analysis could readily be expanded to address specific chemicals of regulatory interest. Another major advantage of the EFA is the ability to identify chemicals which are clearly not POP-like in terms of their potential to accumulate in surface media of the remote region at an early stage of a model-based screening, i.e., chemicals with a log ϕ3 well below the threshold for POP-like behavior (Table 2) which could be important for priority settings.

We envisage that further, in-depth assessments may include consideration of one or more of the following elements, such as:

i) Model sensitivity analyses to identify the more decisive chemical fate properties which dictate the predicted LRTP for a subset of chemicals that are highly ranked and of regulatory concern, followed by exploration of opportunities to refine the more decisive inputs on a chemical-by-chemical basis. The latter can be approached by using more sophisticated *in silico* approaches and/or by reviewing the literature on empirical determination of individual properties (e.g., K_{OW}).
ii) Further exploration of the list of chemicals listed below, with metrics close to the threshold(s) for POP-like behavior (Appendix D).
iii) Assessment of available information / data on production, use, and/or emissions on a chemical-by-chemical basis to make possible inferences regarding potential exposures. This should include an assessment of which of the three emission scenarios that could be more realistic (e.g., down-the-drain-chemical versus chemicals that are more likely to be emitted into air) as this may have profound implications for a chemical's LRTP, as illustrated in the standard plots herein.
iv) Assessment of alternative screening methods for chemicals that are judged to fall outside the model domain for which the Tool was developed (e.g., ionic or inorganic chemicals).
v) A more in-depth review of the literature on empirical studies for chemicals of interest.

For chemicals of elevated interest, there are additional opportunities for higher-tier assessments, such as the application of more sophisticated LRTP models, accounting for environmental variability. In this

context, the EFA metrics offer an additional advantage because they are not tied to The Tool but can be implemented in higher-tier models as well. If reliable information on the actual emissions exists, this additionally offers opportunities to predict concentrations and exposure, which may guide possible empirical efforts. An in-depth assessment should also consider opportunities for screening chemicals of interest in environmental samples from remote regions.

5 References

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Appendix A

Chemical fate properties for 75 discrete chemicals with POP-like ϕ3

Appendix A: Model input parameters for 75 chemicals exceeding the threshold for ϕ3, including their rank order. While the rank order was calculated based on all 895 structures, any duplicates have been removed in this table. It should also be noted that some of the chemical names on the screening list were not complete or understandable.

CAS	Chemical Name	MW (g/mol)	log K_{AW}	log K_{OW}	HL_{air} (hours)	HL_{water} (hours)	HL_{soil} (hours)	log ϕ3	Rank (ϕ3)
12738-64-6	Sucrose benzoate	1175	-31.9	11.22	3.08	4320	8640	-2.57	1
26741-53-7	bis(2,4-Di-tert-butylphenyl)pentaerythritol diphosphite (Irganox 242)	604.7	-6.88	10.9	2.33	4320	8640	-2.57	2
63843-89-0	Bis(1,2,2,6,6-pentamethyl-4-piperidyl) [[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]butylmalonate	685.1	-14	10.03	1.48	4320	8640	-2.57	4
13560-89-9	Dechlorane Plus	653.7	-3.52	11.27	13.6	4320	8640	-2.57	5
32687-78-8	2',3-bis[[3-[3,5-di-tert-butyl-4-hydroxyphenyl]propionyl]]propionohydrazide	552.8	-16.3	7.79	4.69	4320	8640	-2.61	6
3806-34-6	o,o'-Dioctadecylpentaerythritol bis(phosphite)	733.1	-3.48	15.05	1.38	1440	2880	-2.76	7
96-69-5	4,4'-Thiobis (6-t-butyl-m-cresol)	358.5	-9.95	8.24	1.98	1440	2880	-2.79	8
41556-26-7	bis(1,2,2,6,6-Pentamethyl-4-piperidyl) sebacate	508.8	-9.5	6.92	1.6	4320	8640	-2.81	9
26523-78-4	tris(Nonylphenyl) phosphite	689	-1.57	20.05	5.58	900	1800	-2.88	10
79-94-7	Tetrabromobisphenol A	543.9	-8.22	6.53	86.8	4320	8640	-3.02	13
52829-07-9	Bis(2,2,6,6-tetramethyl-4-piperidyl) sebacate	480.7	-10.2	6.5	1.69	4320	8640	-3.04	14
68109-88-6	2-Butenedioic acid, 1,1'-(dioctylstannylene) 4,4'-diethyl ester	631.4	-6.62	7.41	4.39	900	1800	-3.15	15
75627-12-2	Xanthylium, 3,6-bis(ethylamino)-9-[2-(methoxycarbonyl)phenyl]-2,7-dimethyl-, molybdatesilicate	430.6	-11.9	6.83	1.17	1440	2880	-3.21	16
189-55-9	Benzo(r,s,t)pentaphene	302.4	-5.49	7.28	5.13	4320	8640	-3.38	17
78-42-2	tris(2-Ethylhexyl)phosphate	434.7	-5.49	9.49	2.62	208	416	-3.40	18
6505-28-8	2,2'-[(3,3'-dimethoxy[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[3-oxo-N-phenylbutyramide] (Pigment Orange 16, C.I. 21160)	620.7	-22.9	5.93	4.39	4320	8640	-3.49	19
25550-98-5	Diisodecyl phenyl phosphite	438.6	-3.67	9.32	3.59	900	1800	-3.53	20
21652-27-7	(Z)-2-(8-heptadecenyl)-4,5-dihydro-1H-imidazole-1-ethanol	350.6	-6.64	7.51	0.9	360	720	-3.61	21
95-38-5	2-(2-heptadec-8-enyl-2-imidazolin-1-yl)ethanol	350.6	-6.64	7.51	0.9	360	720	-3.61	21
119-47-1	6,6'-di-tert-butyl-2,2'-methylenedi-p-cresol (Antioxidant A02246)	340.5	-8.76	6.25	6.28	1440	2880	-3.67	26
13323-63-2	Dibutylbis(palmitoyloxy)stannane	743.8	1.81	14.56	3.91	900	1800	-3.74	27
110-25-8	(Z)-N-methyl-N-(1-oxo-9-octadecenyl)glycine	353.6	-7.57	6.83	1.18	360	720	-3.87	28
27178-16-1	Diisodecyl adipate	426.7	-2.18	10.08	8.67	900	1800	-3.93	31
3590-84-9	Tetraoctyltin	571.6	4.36	17.23	3.23	360	720	-4.01	32

Appendix A: Model input parameters for 75 chemicals exceeding the threshold for ϕ3 including rank order (continued).

CAS	Name	MW	log K_{AW}	log K_{OW}	HL_{air} (hours)	HL_{water} (hours)	HL_{soil} (hours)	log ϕ3	Rank (ϕ3)
57-11-4	Stearic acid	284.5	-4.09	8.23	11.4	360	720	-4.02	33
85391-79-3	Dibutylbis(octadeca-9(Z),12(Z)-dienoyloxy)stannane	791.8	2.07	15.67	0.33	900	1800	-4.06	35
133-14-2	bis(2,4-Dichlorobenzoyl) peroxide	380	-4.36	6.01	146	4320	8640	-4.10	36
789-02-6	o,p'-DDT	354.5	-3.52	6.79	74.7	4320	8640	-4.10	37
2374-14-3	2,4,6-Trimethyl-2,4,6-tris(3,3,3-trifluoropropyl)cyclotrisiloxane	468.5	5.23	9.84	54.9	4320	8640	-4.18	39
376-06-7	Perfluoromyristic acid (PFTDA)	714.1	4.89	8.83	494	4320	8640	-4.19	41
75-44-5	Phosgene (Carbon dichloride oxide)	98.92	-0.17	-0.71	100000	360	720	-4.20	42
72629-94-8	Pentacosafluorotridecanoic acid (PFTrDA)	664.1	4.17	8.16	494	4320	8640	-4.22	43
71-55-6	1,1,Trichloroetane (Chlorten)	133.4	-0.18	2.49	27000	1440	2880	-4.26	44
307-55-1	Perfluorododecenoic acid (PFDOA)	614.1	3.45	7.49	494	4320	8640	-4.34	45
117-08-8	Tetrachlorophthalic anhydride	285.9	-4.11	4.65	8120	4320	8640	-4.36	46
56803-37-3	tert-Butylphenyl diphenyl phosphate	382.4	-5.38	6.61	21.3	900	1800	-4.36	47
10213-78-2	2,2'-(Octadecylimino)diethanol	357.6	-6.36	6.85	1.99	360	720	-4.43	49
634-66-2	1,2,3,4-Tetrachlorobenzen	215.9	-1.51	4.6	3120	1440	2880	-4.50	50
79-74-3	2,5-di-tert-Pentylhydroquinone	250.4	-7.55	5.83	4	900	1800	-4.52	51
25448-25-3	Triisodecyl phosphite	502.8	-0.04	12.31	2.46	1440	2880	-4.53	52
95-94-3	1,2,4,5-Tetrachlorobenzene	215.9	-1.39	4.64	3120	1440	2880	-4.55	53
540-97-6	Dodecamethylcyclohexasiloxane (D6)	444.9	3.01	8.87	137	1440	2880	-4.57	54
2162-74-5	Bis(2,6-diisopropylphenyl)carbodiimide	362.6	-1.93	8.72	7.74	1440	2880	-4.57	55
72-54-8	Dichlorodiphenyldichloroethane (DDD)	320.1	-3.57	6.02	59.1	4320	8640	-4.63	56
1330-78-5	Tris(methylphenyl) phosphate	368.4	-5.66	6.34	18.7	900	1800	-4.63	57
78-32-0	tri-p-Tolyl phosphate	368.4	-5.66	6.34	18.7	900	1800	-4.63	57
72-55-9	DDE	318	-2.77	6.51	21	4320	8640	-4.68	59
2058-94-8	Perfluoroundecanoic acid (PFUnDA)	564.1	2.73	6.82	494	4320	8640	-4.68	60
75-45-6	Chlorodifluoromethane	86.47	0.22	1.08	54600	360	720	-4.70	61
53-19-0	Dichlorodiphenyl)dichloroethane, (2,4-DDD, Mitotane)	320.1	-3.48	5.87	59.1	4320	8640	-4.78	62
65143-89-7	Benzenesulfonic acid, hexadecyl(sulfophenoxy)-, disodium salt	598.7	-13.1	5.28	10.5	900	1800	-4.79	63
25550-98-5	Diisodecyl phenyl phosphite	438.6	-1.58	10.41	3.51	900	1800	-4.80	64
22984-54-9	2-Butanone, o,o',o''-(methylsilylidyne)trioxime	301.5	-0.07	9.83	55.7	900	1800	-4.80	65

Appendix A: Model input parameters for 75 chemicals exceeding the threshold for ϕ3 including rank order (continued).

CAS	Name	MW	log K_{AW}	log K_{OW}	HL_{air} (hours)	HL_{water} (hours)	HL_{soil} (hours)	log ϕ3	Rank (ϕ3)
6683-19-8	Pentaerythritol tetrakis(3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate),	1178	-26	1.36	1.85	4320	8640	-4.80	69
26544-23-0	Isodecyl diphenyl phosphite (DPDP)	374.5	-3.11	8.52	6.12	900	1800	-4.81	70
27554-26-3	Diisooctyl phthalate	390.6	-2.89	8.39	12.5	900	1800	-4.82	71
124-28-7	Dimantine (N,N-Dimethyl-1-octadecanamine)	297.6	-0.73	8.39	2.52	900	1800	-4.83	72
119313-12-1	2-Benzyl-2-dimethylamino-4'-morpholinobutyrophenone	366.5	-10.1	4.5	0.89	4320	8640	-4.83	73
93-83-4	N,N-bis(2-Hydroxyethyl)oleamide	369.6	-9.37	5.62	1.11	360	720	-4.88	74
6731-36-8	1,1-bis(tert-Butyldioxy)-3,3,5-trimethyl cyclohexane	302.5	-1.21	6.53	29.6	4320	8640	-4.88	77
1025-15-6	Triallyl isocyanurate	249.3	-11.1	5.12	2.02	900	1800	-4.95	79
1330-78-5	Tris(methylphenyl) phosphate	368.4	-5.66	6.34	10.8	900	1800	-4.96	80
101-02-0	Triphenyl phosphite (TPP)	310.3	-4.66	6.62	23.7	900	1800	-4.98	81
74-90-8	Hydrogen cyanide	27.03	-2.26	-0.25	8560	360	720	-5.00	82
36788-39-3	7-[2-(2-Hydroxymethylethoxy)methylethoxy]tetramethyl-3,6,8,11-tetraoxa-7-phosphatridecane-1,13-diol	430.5	-15	-1.34	2.07	1440	2880	-5.00	83
603-35-0	Triphenylphosphine	262.3	-6.03	5.69	43.9	900	1800	-5.02	85
75-71-8	Dichlorodifluoromethane	120.9	1.15	2.16	100000	900	1800	-5.02	86
80-51-3	4,4'-Oxydi(benzenesulfonohydrazide)	358.4	-15.3	0.08	122	900	1800	-5.03	87
112-69-6	Hexadecyldimethylamine (Armeen DM 16D)	269.5	-0.98	7.41	2.6	900	1800	-5.03	88
108-77-0	2,4,6-trichloro-1,3,5-triazine (Cyanuric chloride)	184.4	-4.7	1.73	68800	1440	2880	-5.06	89
76-13-1	1,1,2-Trichlorotrifluoroethane (Freon-113)	187.4	1.33	3.16	100000	1440	2880	-5.06	90
2451-62-9	1,3,5-tris(oxiranylmethyl)-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	297.3	-18.4	1.21	13.8	900	1800	-5.06	91
1330-78-5	Tris(methylphenyl) phosphate	368.4	-5.66	6.34	8.94	900	1800	-5.08	92
75-87-6	Trichloroacetaldehyde (Chloral)	147.4	-6.92	0.99	321	1440	2880	-5.08	93
215-58-7	Dibenz[a,c]anthracene	278.4	-4.7	6.41	5.13	1440	2880	-5.08	94

Appendix B

Empirical information for 75 unique chemicals with POP-like φ3

Appendix B: Empirical information for 75 unique chemicals exceeding the threshold for ϕ3.

CAS	Chemical Name	Detected in the environment	Detected in the Arctic	Compartments	References (SciFinder)	Group	Rank (ϕ3)
12738-64-6	Sucrose benzoate	No	No		339		1
26741-53-7	bis(2,4-Di-tert-butylphenyl)pentaerythritol diphosphite, (Irganox 242)	Yes	No		4257	Phosphate	2
63843-89-0	Bis(1,2,2,6,6-pentamethyl-4-piperidyl) [[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]butylmalonate	No	No		883		4
13560-89-9	Dechlorane Plus	Yes	**Yes**	A, W, B	876		5
32687-78-8	2',3-bis[[3-[3,5-di-tert-butyl-4-hydroxyphenyl]propionyl]]propionohydrazide	Yes	No		2193		6
3806-34-6	o,o'-Dioctadecylpentaerythritol bis(phosphite)	Yes	No		2713		7
96-69-5	4,4'-Thiobis (6-t-butyl-m-cresol)	Yes	No		4177		8
41556-26-7	bis(1,2,2,6,6-Pentamethyl-4-piperidyl) sebacate	?	No		3177		9
26523-78-4	tris(Nonylphenyl) phosphite	Yes	No		3466	Phosphate	10
79-94-7	Tetrabromobisphenol A	Yes	**Yes**	A	6545		13
52829-07-9	Bis(2,2,6,6-tetramethyl-4-piperidyl) sebacate	No	No		6321		14
68109-88-6	2-Butenedioic acid, 1,1'-(dioctylstannylene) 4,4'-diethyl ester	No	No		1	Sn	15
75627-12-2	Xanthylium, 3,6-bis(ethylamino)-9-[2-(methoxycarbonyl)phenyl]-2,7-dimethyl-, molybdatesilicate	No	No		38		16
189-55-9	Benzo(r,s,t)pentaphene	Yes	**Yes**	S	1255		17
78-42-2	tris(2-Ethylhexyl)phosphate	Yes	Yes	A, W, S, B	4937	Phosphate	18
6505-28-8	2,2'-[(3,3'-dimethoxy[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[3-oxo-N-phenylbutyramide] (Pigment Orange 16, C.I. 21160)	No	No		165		19
25550-98-5	Diisodecyl phenyl phosphite	No	No		359	Phosphate	20
21652-27-7	(Z)-2-(8-heptadecenyl)-4,5-dihydro-1H-imidazole-1-ethanol	No	No		115		21
95-38-5	2-(2-heptadec-8-enyl-2-imidazolin-1-yl)ethanol	No	No		123		21
119-47-1	6,6'-di-tert-butyl-2,2'-methylenedi-p-cresol, (Antioxidant A02246)	Yes	**Yes**	B	7002		26
13323-63-2	Dibutylbis(palmitoyloxy)stannane	No	No		11	Sn	27
110-25-8	(Z)-N-methyl-N-(1-oxo-9-octadecenyl)glycine	No	No		813		28
27178-16-1	Diisodecyl adipate	No	No		986		31
3590-84-9	Tetraoctyltin	No	No		161	Sn	32

Appendix B: Empirical information for 75 unique chemicals exceeding the threshold for ϕ3.

CAS	Chemical Name	Detected in the environment	Detected in the Arctic	Compartments	References (SciFinder)	Group	Rank (ϕ3)
57-11-4	Stearic acid				212000		33
85391-79-3	Dibutylbis(octadeca-9(Z),12(Z)-dienoyloxy)stannane	No	No		0	Sn	35
133-14-2	bis(2,4-Dichlorobenzoyl) peroxide	No	No		1901		36
789-02-6	o,p'-DDT	Yes	**Yes**	A, W, S, B, H	7314		37
2374-14-3	2,4,6-Trimethyl-2,4,6-tris(3,3,3-trifluoropropyl)cyclotrisiloxane	No	No		677	Si	39
376-06-7	Perfluoromyristic acid (PFTDA)					PFAS	41
75-44-5	Phosgene(Carbon dichloride oxide)						42
72629-94-8	Pentacosafluorotridecanoic acid (PFTrDA)					PFAS	43
71-55-6	1,1,Trichloroetane (Chlorten)	Yes	**Yes**	A	13000		44
307-55-1	Perfluorododecenoic acid PFDOA					PFAS	45
117-08-8	Tetrachlorophthalic anhydride						46
56803-37-3	tert-Butylphenyl diphenyl phosphate	Yes	No		230	Phosphate	47
10213-78-2	2,2'-(Octadecylimino)diethanol	No	No		930		49
634-66-2	1,2,3,4-Tetrachlorobenzen	Yes	**Yes**	A, S, B, H	2053		50
79-74-3	2,5-di-tert-Pentylhydroquinone	Yes	No		481		51
25448-25-3	Triisodecyl phosphite	Yes	No		406	Phosphate	52
95-94-3	1,2,4,5-Tetrachlorobenzene	Yes	**Yes**	A, S, B, H	2714		53
540-97-6	Dodecamethylcyclohexasiloxane (D6)	Yes	**Yes**	A, W, S, B	2181	Si	54
2162-74-5	Bis(2,6-diisopropylphenyl)carbodiimide	No	No		957		55
72-54-8	Dichlorodiphenyldichloroethane	Yes	Yes	A, S, B, H	14000	DDT	56
1330-78-5	Tris(methylphenyl) phosphate	Yes	**Yes**	W, B, S	12000	Phosphate	57
78-32-0	tri-p-Tolyl phosphate	Yes	**Yes**	W, B, S	583	Phosphate	57
72-55-9	DDE	Yes	**Yes**	A, S, B, H	19000	DDT	59
2058-94-8	Perfluoroundecanoic acid (PFUnDA)		?			PFAS	60
75-45-6	Chlorodifluoromethane	Yes	**Yes**	A			61
53-19-0	Dichlorodiphenyl)dichloroethane, (2,4-DDD, Mitotane)	Yes	**Yes**	A, S, B, H	6001	DDT	62

Appendix B: Empirical information for 75 unique chemicals exceeding the threshold for ϕ3.

CAS	Chemical Name	Detected in the environment	Detected in the Arctic	Compartments	References (SciFinder)	Group	Rank (ϕ3)
65143-89-7	Benzenesulfonic acid, hexadecyl(sulfophenoxy)-, disodium salt						63
25550-98-5	Diisodecyl phenyl phosphite	No	No		359	Phosphate	64
22984-54-9	2-Butanone, o,o',o''-(methylsilylidyne)trioxime	No	No		1484	Si	65
6683-19-8	Pentaerythritoltetrakis(3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate),	No	No		46000		69
26544-23-0	Isodecyl diphenyl phosphite (DPDP)	No	No		403		70
27554-26-3	Diisooctyl phthalate	Yes	No		1295		71
124-28-7	Dimantine (N,N-Dimethyl-1-octadecanamine)	No	No		1977		72
119313-12-1	2-Benzyl-2-dimethylamino-4'-morpholinobutyrophenone	Yes	No		5004		73
93-83-4	N,N-bis(2-Hydroxyethyl)oleamide	No	No		1204		74
6731-36-8	1,1-bis(tert-Butyldioxy)-3,3,5-trimethyl cyclohexane				2560		77
1025-15-6	Triallyl isocyanurate	Yes	No		11000		79
1330-78-5	Tris(methylphenyl) phosphate	Yes	**Yes**	W, S, A, B	12000	Phosphate	80
101-02-0	Triphenyl phosphite (TPP)	Yes	**Yes**	B	11000	Phosphate	81
74-90-8	Hydrogen cyanide						82
36788-39-3	7-[2-(2-Hydroxymethylethoxy)methylethoxy]tetramethyl-3,6,8,11-tetraoxa-7-phosphatridecane-1,13-diol	No	No		125		83
603-35-0	Triphenylphosphine	No	No		56000	Phosphate	85
75-71-8	Dichlorodifluoromethane	Yes	**Yes**	A	11000		86
80-51-3	4,4'-Oxydi(benzenesulfonohydrazide)	No	No		2779		87
112-69-6	Hexadecyldimethylamine (Armeen DM 16D)	Yes	No		1940		88
108-77-0	2,4,6-trichloro-1,3,5-triazine (Cyanuric chloride)	Yes	No		16000		89
76-13-1	1,1,2-Trichlorotrifluoroethane (Freon-113)	Yes	**Yes**	A	7316		90
2451-62-9	1,3,5-tris(oxiranylmethyl)-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	No	No		3721		91
1330-78-5	Tris(methylphenyl) phosphate	Yes	Yes	A, W, S, B	12000	Phosphate	92
75-87-6	Trichloroacetaldehyde (Chloral)	Yes	No		7144		93
215-58-7	Dibenz[a,c]anthracene	Yes	Yes	A, W, S, B	1777	PAH	94

Appendix C

Standards plots for 10 chemicals with a log ϕ3 > -5

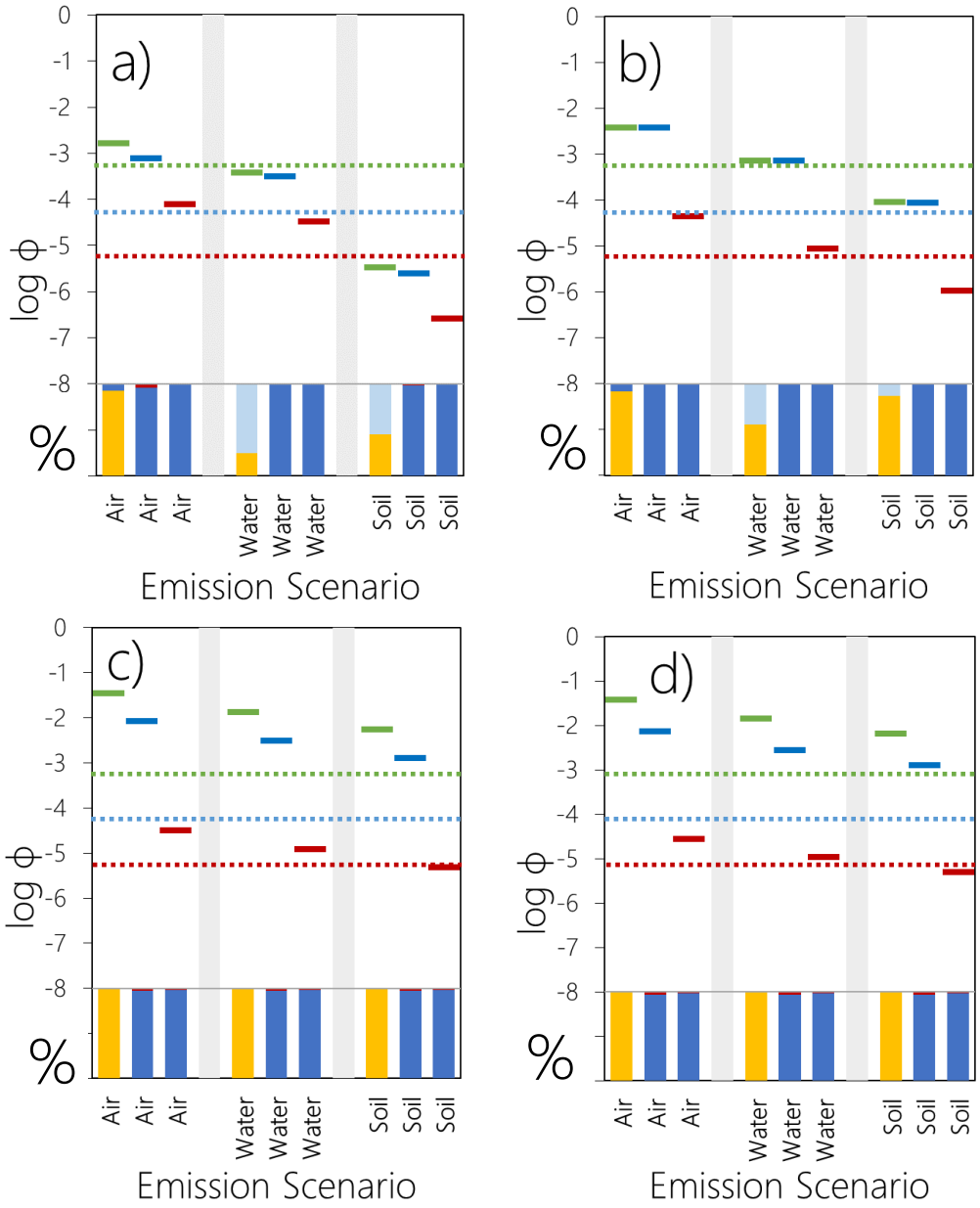

Figure S1: Standard figures for 10 selected chemicals with a log φ3 > -5; a) bis(2,4-Dichlorobenzoyl) peroxide, b) Tetrachlorophthalic anhydride, c) 1,2,3,4-Tetrachlorobenzene, and d) 1,2,4,5-Tetrachlorobenzene. The letter in each panel corresponds to the letter used for labelling the chemical in Figure 6a.

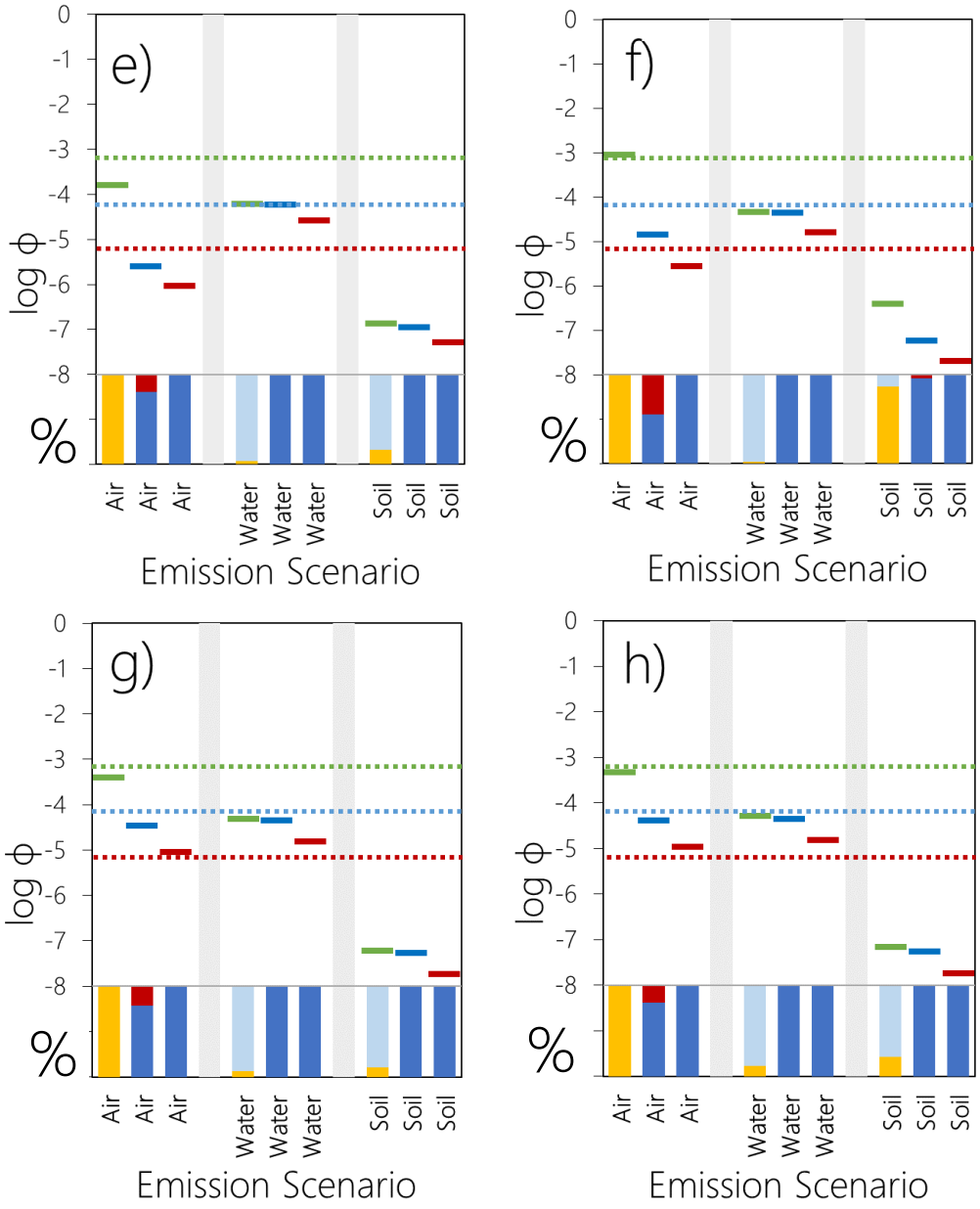

Figure S1 (continued): Standard figures for 10 selected chemicals with a log φ3 > -5; e) bis(2,6-Diisopropylphenyl)carbodiimide, f) 2-Butanone, o,o',o''-(methylsilylidyne)trioxime, g) Isodecyl diphenyl phosphite (DPDP), and h) Diisooctyl phthalate. The letter in each panel corresponds to the letter used for labelling the chemical in Figure 6a.

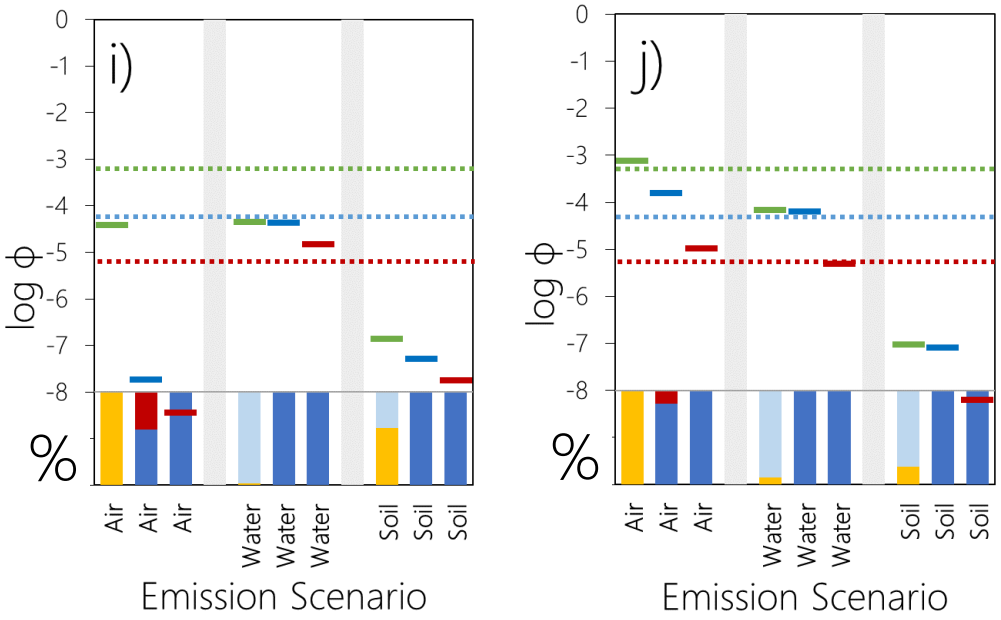

Figure S1 (continued): Standard figures for 10 selected chemicals with a log φ3 > -5; i) Dimantine, j) Triphenyl phosphite (TPP). The letter in each panel corresponds to the letter used for labelling the chemical in Figure 6a.

Appendix D

Model predictions for ~100 chemicals falling below the threshold for ϕ3

Appendix D: Model input parameters and predictions for ~100 chemicals falling below the threshold for ϕ3.

CAS	Name	MW	log K_{AW}	log K_{OW}	HL_{air} (hours)	HL_{water} (hours)	HL_{soil} (hours)	log ϕ3
7621-86-5	2-(4-Aminophenyl)-1H-benzimidazol-2-amine	224.3	-12.8	1.16	0.93	900	1800	-5.10
80-08-0	Dapsone, (4,4'-diaminodiphenyl sulphone)	249.3	-12.4	1.57	8.48	900	1800	-5.11
36788-39-3	7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl-3,6,8,11-tetraoxa-7-phosphatridecane-1,13-diol	430.5	-15	-1.56	1.28	900	1800	-5.12
108-78-1	Melamine	126.1	-12.1	-1.37	389	900	1800	-5.14
1330-78-5	Tris(methylphenyl) phosphate	416.4	-17.6	4.9	1.28	900	1800	-5.15
4067-16-7	3,6,9,12-tetraazatetradecamethylenediamine	232.4	-21.5	-3.67	0.64	360	720	-5.17
320-67-2	2-(β-D-ribofuranosyl)-4-amino-1,3,5-triazin-2-one (Azacitidine)	244.2	-18.8	-2.17	2.64	360	720	-5.17
17540-75-9	4-sec-Butyl-2,6-di-tert-butylphenol	262.4	-3.4	6.43	12.5	1440	2880	-5.17
75-25-2	Bromoform	252.7	-1.66	2.4	1730	900	1800	-5.17
112-57-2	Tetraethylenepentamine	189.3	-17.9	-3.16	0.81	360	720	-5.18
335-76-2	Nonadecafluorodecanoic acid (PFDA)	514.1	0.97	6.15	494	4320	8640	-5.21
79-11-8	Chloroacetic acid	94.5	-6.42	0.22	326	360	720	-5.22
135-57-9	N,N'-dithiodi-o-phenylenedibenzamide	456.6	-12.8	4.59	1.05	1440	2880	-5.25
2921-88-2	Dursban (Chlorpyrifos)	380.9	-3.39	5.4	27.8	4320	8640	-5.27
4645-07-2	2,4-dihydro-4-[(2-methoxyphenyl)azo]-5-methyl-2-phenyl-3H-pyrazol-3-one	308.3	-8.46	4.63	11.1	1440	2880	-5.28
57-50-1	Sucrose	342.3	-19.7	-3.7	2.24	208	416	-5.29
57-41-0	Phenytoin	252.3	-10.7	2.09	13.1	900	1800	-5.29
26444-49-5	Cresyl diphenyl phosphate	356.3	-9.73	4.77	3.6	900	1800	-5.29
1354569-12-2	2-Butenedioic acid, 2-methyl-, 1,4-bis(2-ethylhexyl) ester, (2Z)-	354.5	-3.33	8.49	5.94	208	416	-5.32
100-57-2	Hydroxy(phenyl)mercury	294.7	-9.43	-0.12	123	900	1800	-5.32
13676-54-5	1,1'-(methylenedi-p-phenylene)bismaleimide	358.4	-15.3	2.32	6.59	900	1800	-5.34
118-79-6	2,4,6-Tribromophenol	330.8	-5.84	4.13	540	1440	2880	-5.34
306-83-2	2,2-dichloro-1,1,1-trifluoroethane HCFC-123	152.9	0.02	2.18	7130	1440	2880	-5.35
111-69-3	Adiponitrile	108.1	-7.31	-0.32	360	360	720	-5.35
104-15-4	Toluene-4-sulfonic acid	172.2	-6.94	-0.62	188	360	720	-5.35
58-08-2	1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl- (Caffeine)	196.2	-14.8	-2.57	8.73	360	720	-5.36

Appendix D: Model input parameters and predictions for ~100 chemicals falling below the threshold for ϕ3.

CAS	Name	MW	log K_{AW}	log K_{OW}	HL_{air} (hours)	HL_{water} (hours)	HL_{soil} (hours)	log ϕ3
74-87-3	Chloromethane	50.49	-0.44	0.91	7130	360	720	-5.37
120-78-5	Di(benzothiazol-2-yl) disulphide, (Altax®)	332.5	-11	4.66	0.81	900	1800	-5.38
121-79-9	Propyl gallate, (Propyl 3,4,5-trihydroxybenzoate)	212.2	-14.6	1.8	2.78	360	720	-5.39
88-06-2	2,4,6-Trichlorophenol	197.5	-3.77	3.69	423	1440	2880	-5.39
85-44-9	Phthalic anhydride	148.1	-6.16	1.6	343	360	720	-5.40
80-07-9	Bis(4-chlorophenyl) sulphone, (DDS)	287.2	-5.25	3.9	438	1440	2880	-5.40
1321-74-0	Divinylbenzene-55	350.6	-3.92	4.96	3.38	4320	8640	-5.41
87-90-1	Symclosene (1,3,5-trichloro-1,3,5- triazinane-2,4,6-trione)	232.4	-8.6	0.94	85.6	900	1800	-5.41
3697-24-3	5-Methylchrysene	242.3	-3.65	6.07	1.96	1440	2880	-5.43
35541-81-2	1,4-Cyclohexanedimethanol dibenzoate	352.4	-5.67	6	14.4	900	1800	-5.44
79-07-2	2-Chloracetamide	93.51	-6.79	-0.53	113	360	720	-5.44
10222-01-2	2,2-dibromo-2-cyanoacetamide	241.9	-6.11	0.82	128	900	1800	-5.44
75-12-7	Formamide	45.04	-7.25	-1.51	128	360	720	-5.47
732-26-3	2,4,6-tri-t-Butylphenol	262.4	-3.4	6.06	16	1440	2880	-5.47
1478-61-1	Bisphenol AF	336.2	-7.63	4.47	3.2	4320	8640	-5.47
7575-23-7	Pentaerythritol tetrakis(3-mercaptopropionate), (PETMP®)	488.7	-14.8	2.59	1.47	900	1800	-5.47
115-27-5	Chlorendic anhydride	370.8	-5.44	4.37	74.6	4320	8640	-5.47
514-10-3	Abietic acid, ((1R,4aR,4bR,10aR)-1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,10,10a-decahydrophenanthrene-1-carboxylic acid)	302.5	-3.56	6.46	0.03	900	1800	-5.48
27253-31-2	Neodecanoic acid, cobalt salt	18.02	-3.18	-1.38	100000	360	720	-5.48
144-62-7	Oxalic acid	90.04	-8.23	-1.74	247	208	416	-5.50
100-21-0	Terephthalic acid	166.1	-10.1	2	208	360	720	-5.50
119462-56-5	1,3-bis(3-methyl-2,5-dioxo-1H-pyrrolinylmethyl)benzene	324.3	-16.8	2.69	2.78	900	1800	-5.52
124-30-1	Octadecylamine	269.5	-1.42	7.71	4.74	360	720	-5.53
142-16-5	Bis(2-ethylhexyl) maleate	340.5	-3.52	7.94	8.69	208	416	-5.54
3081-14-9	N,N'-bis(1,4-Dimethylpentyl)-4-phenylenediamine	304.5	-5.4	6.3	2.04	900	1800	-5.55
75-05-8	Acetonitrile	41.05	-2.85	-0.34	1550	360	720	-5.55
26446-73-1	bis(Methylphenyl) phenyl phosphate	354.4	-5.7	5.8	20.1	900	1800	-5.56
7173-62-8	(Z)-N-9-octadecenylpropane-1,3-diamine	324.6	-4.87	7.47	0.82	360	720	-5.56
67-64-1	Acetone	58.08	-2.84	-0.24	1430	360	720	-5.57

Appendix D: Model input parameters and predictions for ~100 chemicals falling below the threshold for ϕ3.

CAS	Name	MW	log K_{AW}	log K_{OW}	HL_{air} (hours)	HL_{water} (hours)	HL_{soil} (hours)	log ϕ3
84-61-7	Dicyclohexyl phthalate	330.4	-5.39	6.2	10.6	900	1800	-5.57
57-41-0	Phenytoin	252.3	-9.38	2.47	24.2	900	1800	-5.58
120-95-6	2,4-di-t-Pentylphenol	234.4	-3.57	6.31	4.99	900	1800	-5.60
51-03-6	Piperonyl butoxide	338.5	-8.44	4.75	2.4	900	1800	-5.60
112-90-3	(Z)-9-Octadecenylamine	267.5	-1.47	7.5	1.12	360	720	-5.60
112-91-4	Oleonitrile	263.5	-0.99	7.5	1.32	360	720	-5.60
13674-87-8	Tris[2-chloro-1-(chloromethyl)ethyl] phosphate (TDCPP)	430.9	-6.97	3.65	14.2	4320	8640	-5.60
110-15-6	Succinic acid	118.1	-10.8	-0.59	92.9	208	416	-5.61
6362-80-7	1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene	236.4	-1.48	6.51	1.38	900	1800	-5.62
552-30-7	Benzene-1,2,4-tricarboxylic acid 1,2-anhydride, (Trimellitic anhydride)	192.1	-8.28	1.95	322	360	720	-5.62
77-09-8	Phenolphthalein	318.3	-13.4	2.89	3.05	900	1800	-5.63
1024-57-3	Heptachlor epoxide	389.3	-3.07	4.98	49.3	4320	8640	-5.64
79-14-1	Glycol acid	76.05	-6.94	-1.11	82.5	208	416	-5.66
108-24-7	Acetic anhydride	102.1	-3.63	-0.58	3040	360	720	-5.67
74-79-3	L-Arginine	174.2	-16.1	-3.92	3.05	360	720	-5.67
75-37-6	1,1-Difluoroethane	66.05	-0.08	0.75	7130	360	720	-5.69
64-18-6	Formic acid	46.03	-5.17	-0.54	570	208	416	-5.75
77-78-1	Dimethyl sulphate (DMS)	126.1	-3.79	0.16	1350	360	720	-5.76
107-12-0	Propionitrile	55.08	-2.82	0.16	735	360	720	-5.76
29570-58-9	2-[[3-[(1-oxoallyl)oxy]-2,2-bis[[(1-oxoallyl)oxy]methyl]propoxy]methyl]-2-[[(1-oxoallyl)oxy]methyl]-1,3-propanediyl diacrylate	578.6	-17.9	3.15	2.85	900	1800	-5.76
2495-25-2	Tridecyl methacrylate	268.4	-0.75	7.17	5.58	360	720	-5.77
91-97-4	3,3'-dimethylbiphenyl-4,4'-diyl diisocyanate	264.3	-4.42	6.05	10.4	900	1800	-5.77
79-20-9	Methyl acetate	74.08	-2.33	0.18	753	360	720	-5.77
65-85-0	Benzoic acid	122.1	-5.81	1.87	207	360	720	-5.77
88-19-7	Toluene-2-sulfonamide	171.2	-4.72	0.84	210	900	1800	-5.78
375-95-1	heptadecafluorononanoic acid (PFNA)	464.1	1.29	5.48	494	4320	8640	-5.79
1461-25-2	Tetrabutyltin (TBT)	347.2	2.39	9.37	4.51	208	416	-5.79

Appendix D: Model input parameters and predictions for ~100 chemicals falling below the threshold for ϕ3.

CAS	Name	MW	log K_{AW}	log K_{OW}	HL_{air} (hours)	HL_{water} (hours)	HL_{soil} (hours)	log ϕ3
103-23-1	bis(2-ethylhexyl) adipate	370.6	-2.27	8.94	10.1	208	416	-5.80
124-04-9	Adipic acid	146.1	-10.1	0.08	45.9	208	416	-5.80
1222-05-5	1,3,4,6,7,8-Hexahydro-4,6,6,7,8,8-hexamethylin-deno[5,6-c]pyran (Galoxolide)	258.4	-2.36	5.9	9.87	1440	2880	-5.82
91-94-1	3,3-Dichlorobenzidine	253.1	-8.94	3.51	6.49	1440	2880	-5.84
120-46-7	1,3-Diphenyl-1,3-propanedione	224.3	-7.27	2.51	62.9	900	1800	-5.85
106-89-8	1-Chloro-2,3-epoxypropane	92.53	-2.91	0.45	583	360	720	-5.85
4712-55-4	Diphenyl phosphonate	234.2	-6.73	4.8	34.8	900	1800	-5.86
26140-60-3	Terphenyl	230.3	-2.89	6.03	27.9	900	1800	-5.89
84-65-1	Anthraquinone	208.2	-6.02	3.39	171	900	1800	-5.90
75-86-5	Acetone cyanohydrin	85.11	-3.27	-0.03	219	900	1800	-5.90
57-39-6	Tris(2-methylaziridin-1-yl)phosphine oxide (METEPA)	215.2	-10.2	0.69	12.5	900	1800	-5.90
5124-30-1	4,4'-methylenedicyclohexyl diisocyanate	262.4	-2.56	6.11	8.33	900	1800	-5.90
74-31-7	Diphenyl-p-phenylenediamine	260.3	-8.08	4.93	1.28	900	1800	-5.91
77-93-0	Triethyl citrate	276.3	-6.8	0.33	35	360	720	-5.92
75980-60-8	Diphenyl(2,4,6-trimethylbenzoyl)phosphine oxide	348.4	-8.48	3.87	7.14	1440	2880	-5.93
106-37-6	1,4-Dibromobenzene	235.9	-1.44	3.79	730	900	1800	-5.93
1675-54-3	Bisphenol A diglycidyl ether	340.4	-8.75	3.84	3.84	1440	2880	-5.94

Appendix E

Empirical information for ~80 chemicals falling below the threshold for ϕ3

Appendix E: Empirical information for ~100 chemicals falling below the threshold for ϕ3.

CAS	Name	Detected in the environment	Detected in the Arctic	Compartments	References (SciFinder)	Group	log ϕ3
7621-86-5	2-(4-Aminophenyl)-1H-benzimidazol-2-amine		N		912	Aniline	-5.10
80-08-0	Dapsone, (4,4'-diaminodiphenyl sulphone)	Y	N		17,000		-5.11
36788-39-3	7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl-3,6,8,11-tetraoxa-7-phosphatridecane-1,13-diol	N	N		125	Phosphate	-5.12
108-78-1	Melamine		N		60		-5.14
1330-78-5	Tris(methylphenyl) phosphate	Y	Y	A W S B	12,000	Phosphate	-5.15
4067-16-7	3,6,9,12-tetraazatetradecamethylenediamine		N		3,316		-5.17
320-67-2	2-(β-D-ribofuranosyl)-4-amino-1,3,5-triazin-2-one (Azacitidine)		N				-5.17
17540-75-9	4-sec-Butyl-2,6-di-tert-butylphenol	Y	N		180		-5.17
75-25-2	Bromoform	Y	Y	A W S B	12,000		-5.17
112-57-2	Tetraethylenepentamine						-5.18
335-76-2	Nonadecafluorodecanoic acid (PFDA)						-5.21
79-11-8	Chloroacetic acid						-5.09
135-57-9	N,N'-dithiodi-o-phenylenedibenzamide	N	N		407		-5.25
2921-88-2	Dursban (Chlorpyrifos)	Y	Y	B W A	24,000	Phosphate	-5.27
4645-07-2	2,4-dihydro-4-[(2-methoxyphenyl)azo]-5-methyl-2-phenyl-3H-pyrazol-3-one	N	N		36		-5.28
57-50-1	Sucrose						-5.29
57-41-0	Phenytoin	Y	N		23,000		-5.29
26444-49-5	Cresyl diphenyl phosphate	Y	Y	S W	1,768	Phosphate	-5.29
1354569-12-2	2-Butenedioic acid, 2-methyl-, 1,4-bis(2-ethylhexyl) ester, (2Z)-	N	N		21		-5.32
100-57-2	Hydroxy(phenyl)mercury	N	N		278	Hg	-5.32
13676-54-5	1,1'-(methylenedi-p-phenylene)bismaleimide	N	N		4,858		-5.34
118-79-6	2,4,6-Tribromophenol	Y	Y	B H	2,767		-5.34
306-83-2	2,2-dichloro-1,1,1-trifluoroethane HCFC-123				3,074	CFC	-5.35
111-69-3	Adiponitrile	N	N		4,603		-5.35
104-15-4	Toluene-4-sulfonic acid						-5.35
58-08-2	1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl- (Caffeine)	Y	Y	H	69,000	Coffee	-5.36

Appendix E: Empirical information for ~100 chemicals falling below the threshold for ϕ3.

CAS	Name	Detected in the environment	Detected in the Arctic	Compartments	References (SciFinder)	Group	log ϕ3
74-87-3	Chloromethane					CFC	-5.37
120-78-5	Di(benzothiazol-2-yl) disulphide, (Altax®)		N		10,000		-5.38
121-79-9	Propyl gallate (Propyl 3,4,5-trihydroxybenzoate)		N		9,539	Natural	-5.39
88-06-2	2,4,6-Trichlorophenol		Y	W	8,262	Natural(?)	-5.39
85-44-9	Phthalic anhydride						-5.40
80-07-9	Bis(4-chlorophenyl) sulphone, (DDS)	Y	Y	B	2,560		-5.40
1321-74-0	Divinylbenzene-55		N		22,000		-5.41
87-90-1	Symclosene ((1,3,5-trichloro-1,3,5- triazinane-2,4,6-trione)		N		3,632	Cyanur-Cl	-5.41
3697-24-3	5-Methylchrysene		Y	W S	716	PAH	-5.43
35541-81-2	1,4-Cyclohexanedimethanol dibenzoate	N	N		130		-5.44
79-07-2	2-Chloracetamide		N		3,919		-5.44
10222-01-2	2,2-dibromo-2-cyanoacetamide		N		1,085		-5.44
75-12-7	Formamide		N		130		-5.47
732-26-3	2,4,6-tri-t-Butylphenol		N		12		-5.47
1478-61-1	Bisphenol AF		N		4,337		-5.47
7575-23-7	Pentaerythritol tetrakis(3-mercaptopropionate), (PETMP®)		N		4,934		-5.47
115-27-5	Chlorendic anhydride						-5.47
514-10-3	Abietic acid, ((1R,4aR,4bR,10aR)-1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,10,10a-decahydrophenanthrene-1-carboxylic acid)		Y	S	4,833		-5.48
27253-31-2	Neodecanoic acid, cobalt salt						-5.48
144-62-7	Oxalic acid						-5.50
100-21-0	Terephthalic acid						-5.50
119462-56-5	1,3-bis(3-methyl-2,5-dioxo-1H-pyrrolinylmethyl)benzene	N	N		387		-5.52
124-30-1	Octadecylamine		N		16,000		-5.53
142-16-5	Bis(2-ethylhexyl) maleate		N		1,017	Ester	-5.54
3081-14-9	N,N'-bis(1,4-Dimethylpentyl)-4-phenylenediamine	Y	N		460	PD	-5.55
75-05-8	Acetonitrile				171,000		-5.55
26446-73-1	bis(Methylphenyl) phenyl phosphate	Y	N		87	Phosphate	-5.56
7173-62-8	(Z)-N-9-octadecenylpropane-1,3-diamine	N	N		369		-5.56
67-64-1	Acetone				352,000	Acetone	-5.57

Appendix E: Empirical information for ~100 chemicals falling below the threshold for ϕ3.

CAS	Name	Detected in the environment	Detected in the Arctic	Compartments	References (SciFinder)	Group	log ϕ3
84-61-7	Dicyclohexyl phthalate		N		2,850	Ester	-5.57
57-41-0	Phenytoin						-5.58
120-95-6	2,4-di-t-Pentylphenol		N		401		-5.60
51-03-6	Piperonyl butoxide		N		5,839		-5.60
112-90-3	(Z)-9-Octadecenylamine		N		14,000		-5.60
112-91-4	Oleonitrile		N		307		-5.60
13674-87-8	Tris[2-chloro-1-(chloromethyl)ethyl] phosphate (TDCPP)	Y	Y	A W S B	1,864		-5.60
110-15-6	Succinic acid						-5.61
6362-80-7	1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene		N		1,035		-5.62
552-30-7	Benzene-1,2,4-tricarboxylic acid 1,2-anhydride, (Trimellitic anhydride)						-5.62
77-09-8	Phenolphthalein				12,000		-5.63
1024-57-3	Heptachlor epoxide	Y	Y	A W S B H	6,629		-5.64
79-14-1	Glycol acid						-5.66
108-24-7	Acetic hydride						-5.67
74-79-3	L-Arginine						-5.67
75-37-6	1,1-Difluoroethane					CFC	-5.69
64-18-6	Formic acid						-5.75
77-78-1	Dimethyl sulphate (DMS)						-5.76
107-12-0	Propionitrile						-5.76
29570-58-9	2-[[3-[(1-oxoallyl)oxy]-2,2-bis[[(1-oxoallyl)oxy]methyl]propoxy]methyl]-2-[[(1-oxoallyl)oxy]methyl]-1,3-propanediyl diacrylate						-5.76
2495-25-2	Tridecyl methacrylate						-5.77
91-97-4	3,3'-dimethylbiphenyl-4,4'-diyl diisocyanate						-5.77
79-20-9	Methyl acetate						-5.77
65-85-0	Benzoic acid						-5.77
88-19-7	Toluene-2-sulfonamide						-5.78
375-95-1	heptadecafluorononanoic acid (PFNA)					PFAS	-5.79
1461-25-2	Tetrabutyltin (TBT)					Sn	-5.79

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