Supplementary Material - Are Ingredients of Personal Care Products Likely to Undergo Long Range Transport to Remote Regions?

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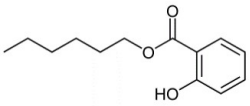
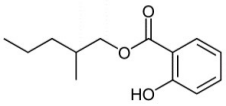
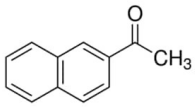
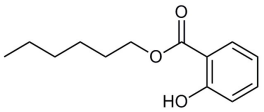
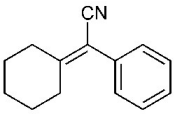
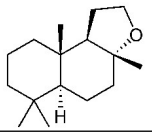
Table S1. Structure, common and IUPAC name, and CAS of selected PCPs.

AmylS (Amyl Salicylate; Pentyl 2-hydroxybenzoate) CAS no: 2050-08-0	
IsoamylS (Isoamyl Salicylate; 3-Methylbutyl 2-hydroxybenzoate) CAS no: 87-20-7	
OraC (Oranger Crystals; 2-Acetonaphthone) CAS no: 93-08-3	
HexS (Hexyl Salicylate; Hexyl 2-hydroxybenzoate) CAS no: 6259-76-3	
Peo (Peonile; 2-Cyclohexylidene-2-phenylacetonitrile) CAS no: 10461-98-0	
Amb (Ambrofix; Dodecahydro-3a,6,6,9a-tetramethylnaphtho[2,1-b]furan) CAS no: 6790-58-5	

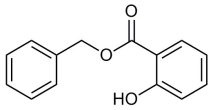
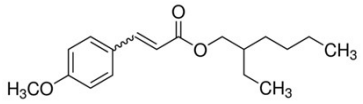
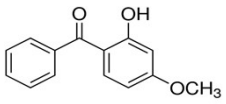
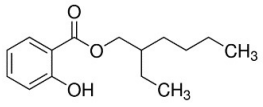
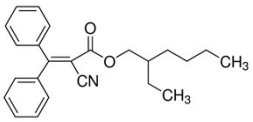
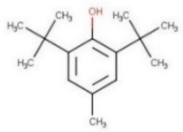
BenS (Benzyl Salicylate; Benzyl 2-hydroxybenzoate) CAS no: 118-58-1	
EHMC (Ethylhexyl methoxycinnamate; 2-ethylhexyl 3-(4-methoxyphenyl)prop-2-enoate) CAS no: 5466-77-3	
BP3 (Benzophenone-3; 2-hydroxy-4-methoxyphenyl)-phenylmethanone) CAS no: 131-57-7	
EHS (Ethylhexyl Salicylate; 2-ethylhexyl 2-hydroxybenzoate) CAS no: 118-60-5	
OCR (Octocrylene; 2-ethylhexyl 2-cyano-3,3-diphenylprop-2-enoate) CAS no: 6197-30-4	
BHT (Butylated hydroxytoluene; 2,6-ditert-butyl-4-methylphenol) CAS no: 128-37-0	

Table S2 Information of 12 PCP chemicals: manufacture and/or import in tonnes/year in European Union (EU) and United States (U.S.), consumer use, price of the chemicals in Euro, and the properties of concern detected so far.

Common name	Manufacture and/or import (tonnes/year)	Consumer use [a]	Price (Euro)	Properties of concern
AmylS	EU ≥ 10 [a] U.S. < 500 (2019) [b]	Air care products, biocides, perfumes, fragrances, polishes and waxes, washing & cleaning products, and cosmetics	< 100 for 1 kg [c]	Development and reproductive toxicity [b]
IsoamylS	EU ≥ 10 to < 100 [a] U.S. < 500 (2019) [b]		76 for 500 mL [d]	Acute toxicity [a]
OraC	EU ≥ 100 to < 1,000 [a] U.S. < 50 (2019) [b]		~ 35 for 100 g [c,d]	Eye irritation [a]
HexS	EU ≥ 1,000 to < 10,000 [a] U.S. < 5,000 (2019) [b]		~ 20 for 100 g [c]	Skin sensitising [a]
Peo	EU ≥ 100 [a] U.S. < 500 (2019) [b]		~ 40 for 100 g [c]	Acute toxicity [a]
Amb	EU ≥ 100 to < 1,000 [a] U.S. < 50 (2019) [b]		205 for 25 g [d]	Reproductive toxicity [a]
BenS	EU ≥ 1,000 to < 10,000 [a] U.S. < 5,000 (2019) [b]		< 15 for 100 g [c]	Skin sensitising [a]
EHMC	EU ≥ 1,000 to < 10,000 [a] U.S. > 500 total Production Volumes between 2016 and 2019 [b]	Cosmetics, personal care products, Washing and cleaning products	~ 50 for 100 mL [d]	Hepatoxicity [b]
BP3	EU ≥ 100 to < 1,000 [a] U.S. < 200 (2019) [b]	Cosmetics and personal care products, coating products, fillers, putties, plasters, modelling clay and finger paints	100 for 500 g [d]	Endocrine Disrupting [a]
EHS	EU ≥ 1,000 to < 10,000 [a] U.S. < 10,000 (2019) [b]	Cosmetics and personal care products and perfumes and fragrances	75 for 500 mL [d]	Reproduction and development toxicity [a]
OCR	EU ≥ 1,000 to < 10,000 [a] U.S. < 10,000 (2019) [b]	Cosmetics and personal care products and perfumes and fragrances	77 for 100 g [d]	Persistent, Bioaccumulative and Toxic [a]
BHT	EU ≥ 10,000 to < 100,000 [a] U.S. < 5,000 (2019) [b]	Washing & cleaning products, lubricants and greases, plant protection products, adhesives and sealants,	30 for 500 g [d]	Endocrine Disrupting [a]

	polishes and waxes, coating products and fertilisers.

a – ECHA Website. Manufactured/Imported values per registrant. (Accessed on 5th January 2025)
b – ChemView – United States Environmental Protection Agency (https://chemview.epa.gov/chemview/#null) (Accessed on 5th January 2025). Reported values refer to the National Aggregate Production Volumes of year 2019 unless otherwise specified.
c – Pellwall website. (https://pellwall.com/) (Accessed on 5th January 2025).
d – TCI Europe website. (https://www.tcichemicals.com/IL/en/) (Accessed on 5th January 2025).

Table S3. Mean blank levels (n=3) with standard deviation, and Method Detection Limits (MDL). Mean detection limits are calculated as three times the standard deviation of the blank signal.

Name	Mean blank [ng abs]	MDL [ng abs]
IsoamylS	0.76 ± 0.09	0.3
AmylS	0.72 ± 0.18	0.6
OraC	0.15 ± 0.01	0.0
HexS	0.84 ± 0.59	1.8
Peo	0.23 ± 0.16	0.5
Amb	0.20 ± 0.15	0.5
BenS	0.33 ± 0.12	0.3
EHMC	0.08 ± 0.03	0.1
BP3	0.14 ± 0.09	0.3
EHS	1.66 ± 0.31	0.9
OCR	1.09 ± 0.31	0.9
BHT	1.53 ± 1.06	3.2

Table S4. Physical and chemical properties used in the calculations for the chemical partitioning space. Log K_{WA} (water-air partition ratio), log K_{IA} (ice-air partition ratio), log K_{SA} (snow-air partition ratio), log K_{OA} (octanol-air partition ratio), log K_P (particle-air partition ratio), A (hydrogen bond acidity descriptor), B (hydrogen bond basicity descriptor), L (solute gas-liquid partition descriptor).

Chemicals	log K_{WA}	log K_{IA} [a]	log K_{SA} [b]	log K_{OA}	log K_P [c]	A [d]	B [d]	L [d]
IsoamylS	3.05	-1.05	-0.27	7.42	-4.83	0.07	0.50	7.29
AmylS	3.19	-1.14	-0.36	7.45	-4.81	0.07	0.50	7.15
OraC	4.63	-1.53	-0.74	7.43	-4.83	0.00	0.50	6.91
HexS	2.96	-0.73	0.05	7.86	-4.40	0.07	0.50	7.79
Peo	3.67	-0.78	-0.05	7.90	-4.35	0.00	0.53	7.84
Amb	2.22	-0.80	-0.07	7.46	-4.79	0.00	0.53	7.81
BenS	4.62	0.50	0.99	8.72	-3.54	0.07	0.67	8.36
EHMC	4.10	1.57	2.04	10.18	-2.08	0.00	0.69	10.26
BP3	5.97	0.58	1.27	9.61	-2.65	0.16	0.55	8.91
EHS	2.79	-0.35	0.47	8.52	-3.73	0.07	0.48	8.55
OCR	6.08	4.12	4.29	13.14	0.89	0.00	0.87	12.83
BHT	2.80	0.39	1.06	8.06	-4.19	0.35	0.55	7.56

[a] Calculated using Eq. (3) by (Lei and Wania, 2004)
[b] Calculated using Eq. (5) by (Lei and Wania, 2004)
[c] Calculated using Eq. (10) by (Harner and Bidleman, 1998)
[d] EAS-E Suite

SI Section 1

Prediction of internal energies

$\Delta U_{AW} = \Delta H_{AW} + RT$ R [J mol^{-1} K^{-1}] = 8.31 T = 298.15 K

$\Delta U_{OA} = -8.75(\pm 0.18) \cdot \log_{10} K_{OA} - 5.07(\pm 1.19)$ (Baskaran et al., 2023).

$\Delta U_{OW} = \Delta H_{OW}$

Table S5 Equations and default parameters used to derive the atmospheric distribution ratios in a cloud at temperatures below and above freezing (Lei and Wania, 2004).

Equations		
$K_{Rain/Air}$	$K_{WA}+3K_{IA}/r$	
$K_{Snow/Air}$	$A_I\rho_W K_{SA}$	
log $K_{Particle/Air}$	$\log K_p * \rho$	
Parameters		
r [mm]	Droplet radius	1
A_I [m^2 g^{-1}]	Specific surface area	0.1
ρ_W [g m^{-3}]	Density of water	10^6
ρ [µg m^{-3}]	Density of particles	1.7×10^{12}

SI Section 2

EFA model equations

Partitioning ratios

K_{AW} = 10 ^ (log K_{AW} + ΔU_{AW} * (1 / 298.15 - 1 / T) / (2.303 * R))

K_{OW} = 10 ^ (log K_{OW} + ΔU_{OW} * (1 / 298.15 - 1 / T) / (2.303 * R))

K_{OA} = K_{OW} / K_{AW}

T is the temperature in Kelvin (298.15 or 273.15). R = 8.314 J K^{-1} mol^{-1}.

Degradation half-lives

The reaction rate of a chemical in the air is a function of temperature (Kelvin) and of the concentration of OH radicals.

The OH radicals were coded in the model in the following way:

OH_{warm} = 1500000# / 2 (24-hour average based on EPIWIN 12 hr average of 1.5E6 radicals / cm^3)

OH_{cold} = OH_{warm} / 10 (assumed to be 10% of the warm region)

Activation Energies (EA)

Activation energies for reaction in J/mol [model input].

kRAref [model input - cm3 molecules-1 sec-1]

kRWref = Log(2) / HalfLife, water [the half-life in water at 25°C is model input]

kRSref = Log(2) / HalfLife, soil [the half-life in soil at 25°C is model input]

T = 25°C

kRA = kRAref * OHwarm * 3600 * Exp (EAair / R * (1 / 298.15 - 1 / 298.15)) [3600 is used for unit conversion]

kRW = kRWref

kRS = kRSref

T = 0°C

kRA = kRAref * OHcold * 3600 * Exp (EAair / R * (1 / 298.15 - 1 / 273.15))

kRW = kRWref * Exp (EAwater / R * (1 / 298.15 - 1 / 273.15))

kRS = kRSref * Exp (EAsoil / R * (1 / 298.15 - 1 / 273.15))

End If

HalfLife, air= Log(2) / kRA

HalfLife, water = Log(2) / kRW

HalfLife, soil = Log(2) / Krs

Table S6 Concentrations (ng L^{-1}), the relative percentage difference (RPD) and the total average RPD of PCP chemicals in duplicate snow samples collected at the Villum Research Station.

	17/12/2018 VRS 1			28/01/2019 VRS 2	11/02/2019 VRS 3			25/02/2019 VRS 4			11/03/2019 VRS 5			25/03/2019 VRS 6			08/04/2019 VRS 7			22/04/2019 VRS 8			06/05/2019 VRS 9			21/05/2019 VRS 10			03/06/2019 VRS 11			Average RPD
	R1	**R2**	**%**		**R1**	**R2**	**%**	**R1**	**R2**	**%**	**R1**	**R2**	**%**	**R1**	**R2**	**%**	**R1**	**R2**	**%**	**R1**	**R2**	**%**	**R1**	**R2**	**%**	**R1**	**R2**	**%**	**R1**	**R2**	**%**	
IsoamylS	1.6	1.1	37	1.2	1.8	2.8	43	5.0	5.3	6	8.2	9.6	16	2.1	3.1	38	7.3	6.9	6	2.4	4.1	52	1.1	0.8	32	185.7	182.5	2	2.2	2.2	0	8%
AmylS	1.3	1.4	7	1.3	1.9	2.4	23	3.9	3.1	23	1.3	1.4	7	1.1	2.7	84	1.9	2.1	10	2.3	2.3		ldl	ldl		113.8	125.7	10	2.4	2.5	4	8%
OraC	0.2	0.2	0	0.5	0.8	1.0	22	2.7	2.2	20	2.3	2.4	4	0.6	1.2	67	3.8	3.2	17	0.5	1.7	109	ldl	ldl		2.0	2.2	10	0.3	0.3	0	14%
HexS	ldl	ldl		ldl	ldl	ldl		11.2	8.9	23	ldl	ldl		3.5	5.7	48	5.2	5.7	9	3.7	5.0	30	ldl	ldl		182.3	193.2	6	6.2	6.1	2	19%
Peo	ldl	ldl		ldl	ldl	ldl		1.3	0.9	36	ldl	ldl		ldl	ldl		ldl	ldl			ldl		ldl	ldl		9.1	11.5	23	ldl	ldl		11%
Amb	ldl	ldl		ldl	ldl	ldl		1.4	0.9	43	ldl	ldl		ldl	ldl		ldl	ldl			ldl		ldl	ldl		31.4	37.5	18	ldl	ldl		7%
BenS	0.9	1.2	29	1.8	1.1	1.8	48	6.1	5.0	20	1.2	1.0	18	0.6	4.2	150	1.3	2.1	47	3.8	5.9	43	ldl	ldl		18.0	20.0	11	1.3	1.3	0	13%
EHMC	0.4	0.8	67	1.5	0.3	0.4	29	0.7	0.3	80	ldl	ldl		0.4	0.3	29	0.6	0.2	100	9.5	6.5	38	0.4	0.3	29	0.3	1.3	125	0.6	0.2	100	32%
BP3	2.2	4.4	67	5.9	1.3	2.1	47	1.9	2.4	23	0.8	1.1	32	0.5	0.6	18	ldl	ldl		1.1	0.8	32	0.7	2.9	122	5.5	9.2	50	0.6	0.8	29	17%
EHS	2.1	4.3	69	3.6	3.1	4.5	37	12.8	11.0	15	1.9	2.1	10	2.7	8.6	104	3.9	5.0	25	31.9	46.9	38	ldl	ldl		79.8	85.6	7	12.6	7.5	51	40%
OCR	2.1	5.0	82	8.5	2.6	4.5	54	3.6	2.1	53	ldl	ldl		ldl	ldl		ldl	ldl		181.8	153.1	17	ldl	ldl		2.9	6.3	74	ldl	ldl		25%
BHT	ldl	ldl		ldl	ldl	ldl		ldl	ldl		ldl	ldl		ldl	ldl		ldl	ldl			ldl		ldl	ldl		11.9	12.9	8	ldl	ldl		28%
																												Total average RPD				12%

ldl – below the detection limit

Table S7 Arithmetic mean concentrations (ng L^{-1}) of PCP chemicals in duplicates snow samples collected at the Villum Research Station. Total load of FMs, UVFs, and PCP chemicals in each sample, and the total amount of each chemical found during the sampling period.

	VRS 1 17/12/2018	**VRS 2 28/01/2019**	**VRS 3 11/02/2019**	**VRS 4 25/02/2019**	**VRS 5 11/03/2019**	**VRS 6 25/03/2019**	**VRS 7 08/04/2019**	**VRS 8 22/04/2019**	**VRS 9 06/05/2019**	**VRS 10 21/05/2019**	**VRS 11 03/06/2019**	**Tot (ng L^{-1})**
BHT	ldl	ldl	ldl	ldl	ldl	ldl	ldl	ldl	ldl	12.4	ldl	12.4
IsoamylS	1.3	1.2	2.3	5.1	8.9	2.6	7.1	3.3	1.0	184.1	2.2	219.2
AmylS	1.4	1.3	2.2	3.5	1.4	1.9	2.0	2.3	ldl	119.8	2.5	138.2
OraC	0.2	0.5	0.9	2.4	2.3	0.9	3.5	1.1	ldl	2.1	0.3	14.3
HexS	ldl	ldl	ldl	10.1	ldl	4.6	5.4	4.4	ldl	187.8	6.2	218.4
Peo	ldl	ldl	ldl	1.1	ldl	ldl	ldl	ldl	ldl	10.3	ldl	11.4
Amb	ldl	ldl	ldl	1.1	ldl	ldl	ldl	ldl	ldl	34.5	ldl	35.6
BenS	1.1	1.8	1.5	5.5	1.1	2.4	1.7	4.9	ldl	19.0	1.3	40.2
EHMC	0.6	1.5	0.3	0.5	ldl	0.4	0.4	8.0	0.3	0.8	0.4	13.2
BP3	3.3	5.9	1.7	2.1	0.9	0.6	ldl	0.9	1.8	7.4	0.7	25.3
EHS	3.2	3.6	3.8	11.9	2.0	5.6	4.4	39.4	ldl	82.7	10.0	166.8
OCR	3.6	8.5	3.6	2.8	ldl	ldl	ldl	167.5	ldl	4.6	ldl	190.5
∑FMs	4.0	4.8	6.8	29.0	13.7	12.4	19.7	16.0	1.0	557.4	12.4	
∑UVFs	10.8	19.4	9.4	17.3	3.0	6.6	4.8	215.8	2.1	95.5	11.1	
Tot (ng L^{-1})	**15.0**	**24.1**	**16.3**	**46.3**	**16.7**	**19.0**	**24.6**	**231.8**	**3.1**	**665.3**	**23.5**	

ldl – below the detection limit

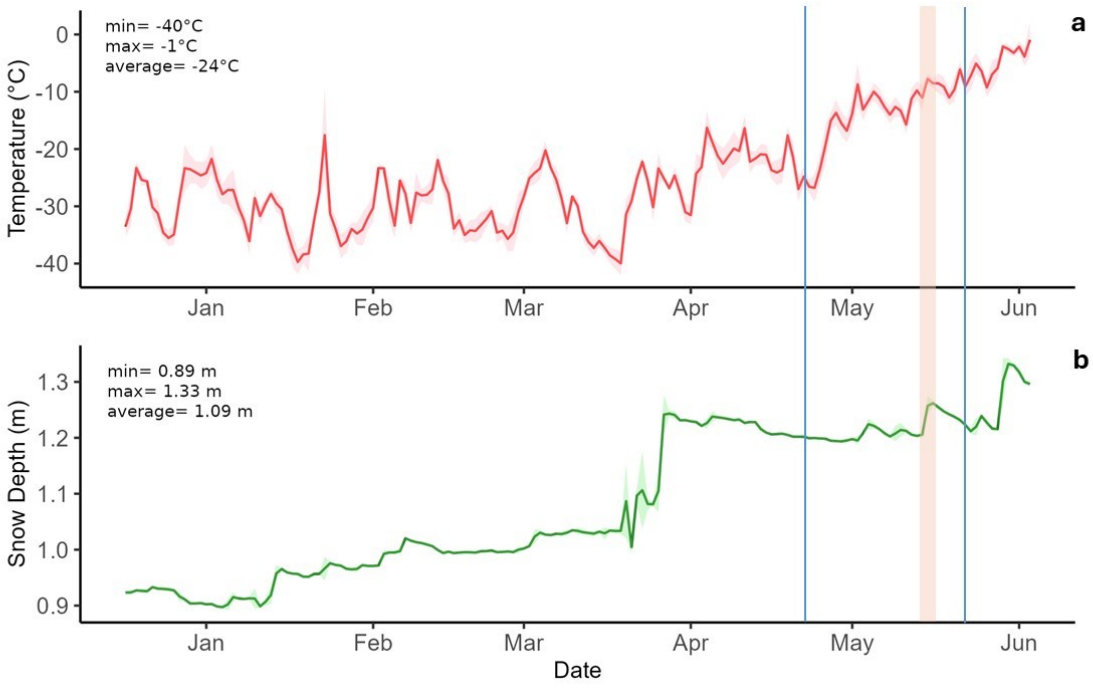


Figure S1. Temperature (a) and snow depth (b) data obtained from in situ observation at an automatic weather station at VRS, showing maximum, minimum, and average values from 18th December 2018 to 3rd June 2019. The plots represent daily averages (with shading indicating the standard deviation) based on five-minute average data collected throughout each day. Vertical blue lines indicate high PCPs concentration events on 22nd April and 21st May 2019, while the shaded orange area highlights the identified snowfall event prior to 21st May 2019.

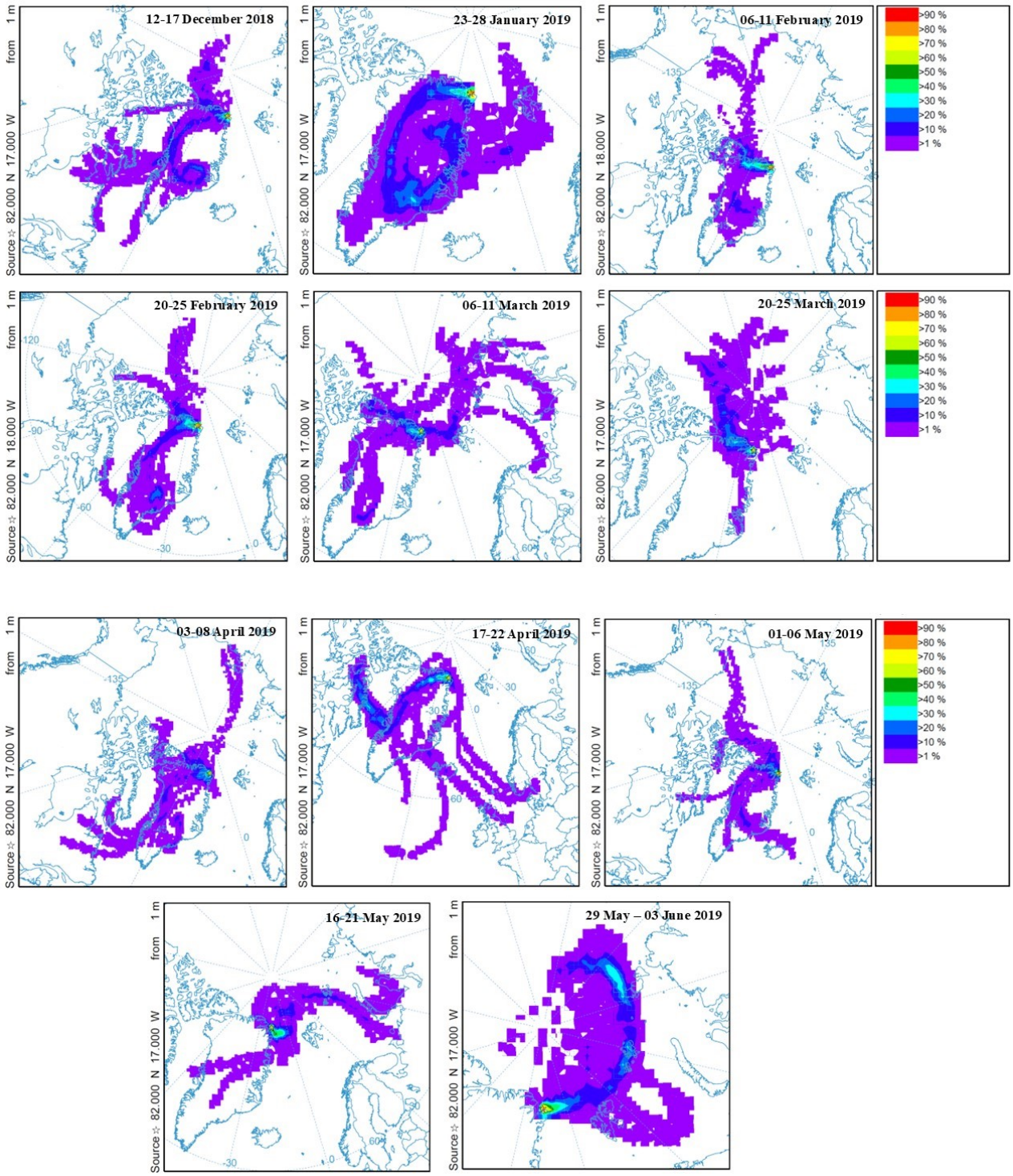


Figure S2 Back trajectory frequencies simulated with HYSPLIT Trajectory Model online version for each sampling date at the Villum Research Station.

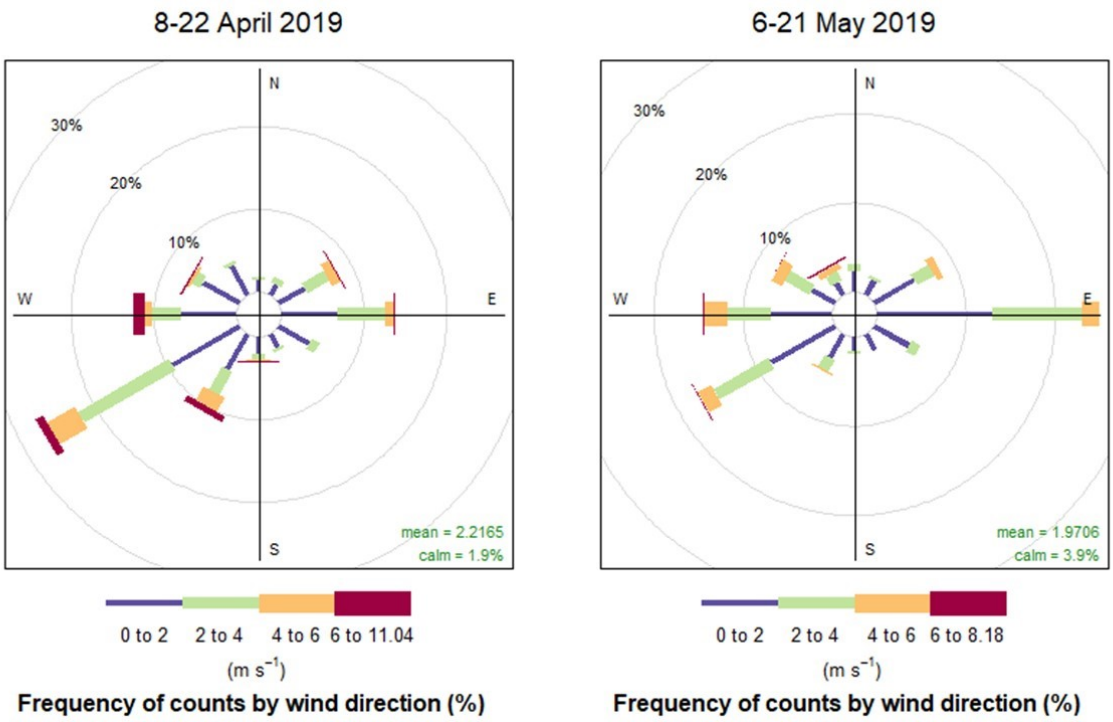


Figure S3 Wind Rose illustrating the distribution of wind directions and associated wind speeds recorded between the 8-22 April and 6-21 May 2019, two weeks before the two events of contamination registered at the Villum Research Station on April 22nd and May 21st. The radial bars indicate the frequency of occurrence of wind from each direction, with longer bars signifying higher frequencies. The coloured segments within each bar represent wind speeds categorized by the legend, with colours ranging from purple (lower speeds) to red (higher speeds). The scale at the bottom shows the wind speed intervals in meters per second (m s^{-1}).

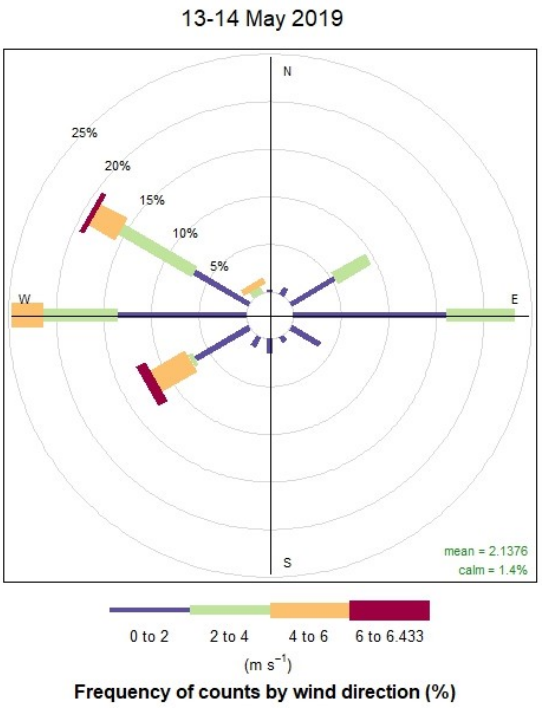


Figure S4 Wind Rose illustrating the distribution of wind directions and associated wind speeds recorded 24 hours before the snow depth increase recorded on May 14th 2019.

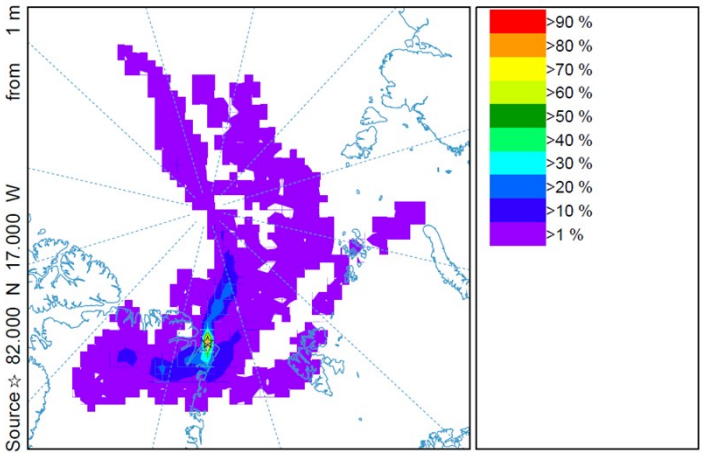


Figure S5 HYSPLIT back trajectories calculated for May 14th 2019, following the identified precipitation event.

Table S8 The mean of the partition ratios estimated at 25°C with UFZ LSER, EAS-E Suite, COSMOtherm, EPI Suite, SPARC. Their adherence to the thermodynamic triangle without OPERA calculations is displayed (closure).

Chemical	**log K_{OW}**	**log K_{AW}**	**log K_{OA}**	**closure**	**abs closure**
Isoamyl Salicylate	4.35	-3.05	7.42	-0.02	0.02
Amyl Salicylate	4.25	-3.19	7.45	-0.02	0.02
Oranger Crystals	2.86	-4.63	7.43	0.06	0.06
Hexyl Salicylate	4.86	-2.96	7.86	-0.04	0.04
Peonile	4.24	-3.67	7.90	0.01	0.01
Ambrofix	5.23	-2.22	7.46	-0.01	0.01
Benzyl Salicylate	4.13	-4.62	8.72	0.03	0.03
EHMC	6.09	-4.10	10.18	0.01	0.01
BP3	3.63	-5.97	9.61	-0.01	0.01
EHS	5.70	-2.79	8.52	-0.03	0.03
OCR	7.14	-6.08	13.14	0.08	0.08
BHT	5.37	-2.80	8.06	0.11	0.11
Average					**0.04**

Table S9 Partition ratios estimated with COSMOtherm at 0 °C and -6.8 °C

Chemical	**COSMOtherm 0 °C**			**COSMOTherm -6.8 °C**		
	log K_{OW}	**log K_{AW}**	**log K_{OA}**	**log K_{OW}**	**log K_{AW}**	**log K_{OA}**
Isoamyl Salicylate	4.68	-3.38	8.17	4.67	-3.75	8.53
Amyl Salicylate	4.68	-3.38	8.17	4.67	-3.75	8.53
Oranger Crystals	2.54	-5.89	8.32	2.50	-6.27	8.66
Hexyl Salicylate	5.26	-3.26	8.65	5.25	-3.64	9.03
Peonile	3.86	-5.19	9.01	3.84	-5.57	9.38
Ambrofix	4.32	-4.77	9.09	4.23	-5.25	9.47
Benzyl Salicylate	4.66	-4.68	9.42	4.68	-5.06	9.83
EHMC	5.94	-6.07	11.99	5.87	-6.66	12.52
BP3	3.60	-6.76	10.33	3.59	-7.21	10.76
EHS	5.98	-3.13	9.27	5.96	-3.56	9.68
OCR	6.55	-7.55	14.07	6.50	-8.19	14.67
BHT	5.62	-2.75	8.56	5.59	-3.16	8.94

Table S10 Input data for EFA model. Molecular weight (MW), environmental degradation half-lives, internal energies of phase transfer, and the environmental activation energies for 12 PCP chemicals.

Chemical	MW (g/mol)	k_{RAref} (cm^3 $molecules^{-1}$ sec^{-1}) [a]	Half-life in water (hours) [b]	Half-life in soil (hours) [b]	ΔU_{AW} [c]	ΔU_{OW} [d]	E_{aAir}	E_{aWater}	E_{aSoil}
BHT	220.35	1.64E-11	1372.7	2745.5	84174	2851	10000	30000	30000
IsoamylS	208.25	1.71E-11	150.03	300.05	70717	-2357	10000	30000	30000
AmylSal	208.25	1.7E-11	266.3	532.6	71474	-1275	10000	30000	30000
OrangerCrystals	170.21	1.11E-11	525.84	1051.7	69459	-1289	10000	30000	30000
HexylSal	222.27	1.77E-11	155.76	311.52	74181	-3476	10000	30000	30000
Peonile	197.27	3.55E-11	451.25	902.49	73184	-3484	10000	30000	30000
Ambrofix	236.38	2.56E-11	3723.9	7447.8	83743	4115	10000	30000	30000
BenzylSal	228.24	1.58E-11	270.93	541.86	75327	-6596	10000	30000	30000
EHMC	290.39	3.48E-11	208.73	417.46	105412	3604	10000	30000	30000
BP3	228.24	1.08E-10	405.43	810.86	81894	-6817	10000	30000	30000
EHS	250.33	1.94E-11	182.14	364.27	81276	-1959	10000	30000	30000
Octocrylene	361.48	1.73E-11	250.94	501.87	120717	1112	10000	30000	30000

[a] Average values calculated using OPERA and EPISuite

[b] Values calculated with OPERA

[c] Average of three prediction techniques: Van't Hoff equation with COSMOtherm data, and ΔU from ΔH ppLFER with UFZ LSER and EAS-E Suite data

[d] Values calculated from thermodynamic triangle $\Delta U_{OA} + \Delta U_{AW}$. Where ΔU_{OA} was calculated using Van't Hoff equation with COSMOtherm data, ΔU from ΔH pplfer with UFZ LSER and EAS-E Suite data, and eq. 2 in table 1 from Baskaran et al. 2023 (Baskaran et al., 2023).

Table S11 Predicted metrics for 12 PCP chemicals and the minimum values predicted for 14 POPs under the Stockholm Convention in the three emission scenarios. All predictions refer to both warm and cold scenarios.

	BHT	**IsoamylS**	**AmylS**	**OraC**	**HexS**	**Peo**	**Amb**	**BenS**	**EHMC**	**BP3**	**EHS**	**OCR**	**Min values POPs**
φ1 warm	-3.63	-3.65	-3.65	-3.49	-3.67	-3.96	-3.68	-3.63	-3.91	-4.43	-3.70	-2.36	-3.3
φ2 warm	-4.23	-4.95	-4.72	-4.40	-4.94	-4.49	-4.29	-4.68	-4.80	-4.51	-4.89	-2.42	-4.1
φ3 warm	-6.20	-8.43	-7.97	-7.45	-8.20	-7.51	-5.94	-7.95	-6.98	-7.65	-7.46	-3.83	-5.1
φ2 cold	-3.92	-3.94	-3.94	-3.66	-3.96	-4.41	-4.02	-3.84	-4.05	-4.51	-4.01	-2.36	-3.4
φ3 cold	-5.47	-6.93	-6.70	-6.10	-6.71	-6.94	-5.26	-6.61	-5.91	-7.17	-6.09	-3.35	-3.9

Table S12 Input data for EFA model. Molecular weight (MW), physical chemical properties at 25°C, environmental degradation half-lives, internal energies of phase transfer, and the environmental activation energies for 14 POPs under the Stockholm Convention.

Chemical	**MW (g/mol)**	**log K_{AW} (-)**	**log K_{OW} (-)**	**k_{RAref} (cm^3 $molecules^{-1}$ sec^{-1})**	**Half-life in water (hours)**	**Half-life in soil (hours)**	**ΔU_{AW}**	**ΔU_{OW}**	**E_{aAir}**	**E_{aWater}**	**E_{aSoil}**
a-HCH	290.9	-3.53 [c]	3.94 [c]	9.95 E-14 [e]	8,760 [h]	2,190 [h]	56,800 [c]	-5,100 [c]	10,000	30,000	30,000
g-HCH	290.9	-3.91 [c]	3.83 [c]	1.19 E-13 [e]	8,760 [h]	2,190 [h]	57,200 [c]	-10,200 [c]	10,000	30,000	30,000
PCB-28	257.54	-1.93 [I]	5.66 [I]	1.04 E-12 [f]	5,500 [k]	10,000 [k]	52,300 [a]	-26,300 [a]	10,000	30,000	30,000
PCB-52	291.99	-1.96 [I]	6.26 [I]	5.90 E-13 [f]	10,000 [f]	17,000 [f]	54,100 [a]	-27,300 [a]	10,000	30,000	30,000
PCB-101	326.43	-2.08 [I]	6.38 [I]	3.00 E-13 [f]	31,000 [k]	100,000 [k]	59,700 [a]	-23,800 [a]	10,000	30,000	30,000
PCB-118	360.88	-2.36 [I]	6.65 [I]	3.00 E-13 [f]	31,000 [f]	100,000 [f]	60,500 [a]	-28,500 [a]	10,000	30,000	30,000
PCB-138	360.88	-1.97 [I]	7.19 [I]	1.60 E-13 [f]	55,000 [f]	170,000 [f]	61,300 [a]	-25,000 [a]	10,000	30,000	30,000
PCB-153	360.88	-2.13 [I]	6.86 [I]	1.60 E-13 [f]	55,000 [f]	550,000 [f]	62,800 [a]	-31,100 [a]	10,000	30,000	30,000
PCB-180	395.32	-2.51 [I]	7.15 [I]	1.10 E-13 [f]	55,000 [k]	1,000,000 [k]	63,600 [a]	-29,100 [a]	10,000	30,000	30,000
HCB	284.8	-3.91 [b]	3.83 [b]	1.29 E-14 [e]	4,320 [d]	8,640 [d]	50,490 [b]	-24,700 [b]	10,000	30,000	30,000
pp-DDT	354.5	-3.34 [b]	6.39 [b]	3.44 E-12 [d]	4,320 [d]	8,640 [d]	68,978 [g]	-24,350 [g]	10,000	30,000	30,000
pp-DDD	321	-3.70 [b]	6.33 [b]	4.34 E-12 [d]	4,320 [d]	8,640 [d]	69,948 [g]	-23,960 [g]	10,000	30,000	30,000
cis-Chlordane	409.8	-2.63 [b]	6.20 [b]	7.09 E-12 [d]	4,320 [d]	4,320 [d]	81,388 [g]	-10,150 [g]	10,000	30,000	30,000
trans-chlordane	409.8	-2.56 [b]	6.27 [b]	7.09 E-12 [d]	4,320 [d]	4,320 [d]	78,368 [g]	-6,640 [g]	10,000	30,000	30,000

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[b] Shen and Wania 2005 Compilation, Evaluation, and Selection of Physical-Chemical Property Data for Organochlorine Pesticides (Shen and Wania, 2005)

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[d] EPISuite

[e] Beyer et al. 2003 Temperature Dependence of the Characteristic Travel Distance (Beyer et al., 2003)

[f] Wania and Su 2004 Quantifying the Global Fractionation of Polychlorinated Biphenyls (Wania and Su, 2004)

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