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Supplementary material

Currently used pesticides, hexachlorobenzene and hexachlorocyclohexanes in the air and seawater of the German Bight (North Sea)

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Table S1. Detailed information on air sampling

Latitude and longitude represent the mean sampling stations. Salinity, wind speed and air temperature are mean values

	Date	Latitude (°N)	Longitude (°E)	Volume (m^3)	Wind speed ($m\ s^{-1}$)	T_A (°C)
H319 A1	04–05-Mar-2010	54.85	7.98	320	6.6	1.2
H319 A2	05–06-Mar-2010	53.93	7.49	294	11.5	0.5
H319 A3	06–07-Mar-2010	54.38	6.35	322	4.6	0.6
H319 A4	08–09-Mar-2010	55.20	7.28	249	3.3	0.8
H319 A5	09–10-Mar-2010	55.43	4.40	399	6.2	2.5
H319 A6	10-Mar-2010	54.68	6.61	119	3.0	1.6
H325 A1	01–02-May-2010	54.13	7.81	86	5.9	7.8
H325 A2	02–03-May-2010	54.56	6.36	307	8.1	7.0
H325 A3	03–04-May-2010	54.15	7.91	349	8.4	8.0
H325 A4	04–05-May-2010	54.68	5.19	267	7.7	6.3
H325 A5	05–06-May-2010	55.28	5.69	324	4.3	6.7
H325 A6	06–07-May-2010	54.80	8.16	348	10.3	7.7
H325 A7	07-May-2010	53.73	6.74	127	13.7	6.6
H331 A2	14–15-Jul-2010	54.85	8.18	331	9.8	20.4
H331 A3	15–16-Jul-2010	53.91	7.48	272	9.3	18.9
H331 A4	16–17-Jul-2010	55.03	6.53	243	8.7	17.3
H331 A5	17–18-Jul-2010	55.32	4.70	322	8.8	15.4
H331 A6	18–19-Jul-2010	54.68	5.42	311	8.2	17.0
H331 A7	19-Jul-2010	55.10	7.75	42	3.9	19.0

Table S2. Detailed information on water sampling

Latitude and longitude represent the mean sampling stations. Wind speed and water temperature are mean values

	Date	Latitude (°N)	Longitude (°E)	Volume (L)	Wind speed (m s^{-1})	T_W (°C)	Salinity (psu)
H319 W1	04-Mar-2010	54.24	8.25	105	10.1	1.0	30.1
H319 W2	05-Mar-2010	54.44	6.37	192	7.5	3.5	34.1
H319 W3	05-Mar-2010	53.98	6.60	152	10.9	2.5	32.6
H319 W4	06-Mar-2010	55.00	7.50	214	8.7	2.1	34.1
H319 W5	06-Mar-2010	55.05	6.70	196	5.3	3.4	34.5
H319 W7	08-Mar-2010	54.72	8.13	106	2.2	0.4	30.9
H319 W8	08-Mar-2010	55.15	7.53	205	1.9	1.9	33.9
H319 W9	09-Mar-2010	55.40	4.56	226	6.7	3.9	34.5
H319 W10	09-Mar-2010	55.75	3.83	201	7.0	3.4	34.5
H319 W11	10-Mar-2010	54.68	6.28	217	2.6	3.6	34.4
H325 W1	01-May-2010	54.10	7.91	94	5.3	7.7	31.9
H325 W2	02-May-2010	54.23	7.09	144	4.9	7.9	32.5
H325 W3	02-May-2010	54.34	6.36	209	6.3	7.7	33.5
H325 W4	03-May-2010	54.45	7.50	202	9.4	7.7	31.7
H325 W5	03-May-2010	54.15	7.91	167	6.6	8.4	30.1
H325 W6	04-May-2010	54.68	6.32	212	10.6	7.0	33.9
H325 W7	04-May-2010	54.68	5.23	138	7.9	7.1	34.5
H325 W8	05-May-2010	55.40	4.49	189	3.0	7.4	34.5
H325 W9	05-May-2010	55.16	5.05	184	2.1	8.2	34.6
H325 W10	06-May-2010	55.13	7.66	164	8.9	7.8	n.a.
H325 W11	06-May-2010	55.05	8.25	146	9.6	9.2	n.a.
H325 W12	07-May-2010	53.77	7.03	65	14.1	9.1	32.1
H331 W1	13-Jul-2010	54.101	7.90	100	2.4	18.6	31.0
H331 W5	15-Jul-2010	54.51	7.50	148	10.5	18.4	30.6
H331 W6	16-Jul-2010	53.90	6.59	126	10.8	18.0	31.9
H331 W7	16-Jul-2010	54.29	6.36	204	10.2	16.8	33.0
H331 W8	17-Jul-2010	55.23	7.14	164	8.2	16.5	33.1
H331 W9	17-Jul-2010	55.33	5.81	196	9.2	16.2	34.1
H331 W10	18-Jul-2010	55.47	4.36	185	7.1	15.3	34.3
H331 W11	18-Jul-2010	55.16	5.01	194	8.8	15.9	34.2
H331 W12	19-Jul-2010	54.68	6.73	153	7.1	17.2	32.4
H331 W13	19-Jul-2010	55.05	7.50	169	5.0	17.6	31.2

Table S3. Detailed information on water sampling in the rivers Elbe and Weser and their estuaries

	Location	Date	Latitude (°N)	Longitude (°E)	Volume (L)	Salinity (psu)
E3	Elbe	22-Feb-2011	53.54	9.88	5	No data
E6	Elbe	22-Feb-2011	53.67	9.51	5	No data
E9	Elbe	22-Feb-2011	53.88	9.23	5	No data
NE3	Elbe estuary	24-Feb-2011	54.04	8.47	5	25.3
NS3	Weser	23-Feb-2011	53.98	8.35	5	24.6
W1	Weser	24-Feb-2011	53.54	8.57	5	5.3

Table S4. *m*/*z* values used for quantification and quality control of target compounds in ECNCI-(SIM)-mode, and spike test recoveries of air columns and water columns

	Retention time (min)	Q	Q1	Spike test recoveries of air columns (%)	Spike test recoveries of water columns (%)
trifluralin-d_{14}	12.66	349	319	82 ± 7	99 ± 10
trifluralin	12.88	335	305	80 ± 11	96 ± 9
α-HCH	13.36	255	71	59 ± 4	87 ± 7
^{13}C-HCB	13.72	294	290	Injection standard	Injection standard
HCB	13.72	284	249.9	43 ± 3	86 ± 6
γ-HCH	15.08	255	71	64 ± 5	91 ± 4
chlorpyrifos	22.74	313	315	86 ± 12	92 ± 11
dacthal	23.01	332	330	88 ± 8	101 ± 3
α-endosulfan	27.27	405.9	371.9	81 ± 5	98 ± 7
β-endosulfan	31.74	405.9	371.9	81 ± 6	108 ± 7
quintozene	15.38	265	263	87 ± 8	77 ± 5
pentachloroanisole	14.00	280	278	61 ± 5	83 ± 7
CB-207	48.34	463.7	461.7	Injection standard	Injection standard

Table S5. Mean absolute blank values of air, water, air filter and water filter samples in individual sampling cruise (pg)

F1, fraction 1; F2, fraction 2. TFL, trifluralin; ENDO-I, α-endosulfan; ENDO-II, β-endosulfan; CPF, chlorpyrifos; DCPA, dacthal; PCNB, qintozene; PeCA, pentachloroanisole; –, pentachloroanisole and qintozene were not detected in fraction 2

	HCB	α-HCH	γ-HCH	TFL	ENDO-I	ENDO-II	CPF	DCPA	PCNB	PeCA
Air samples										
H319 F1	386	0.3	31	2	2	1	18	1	4	31
H319 F2	205	22	26	3	0.3	3	40	9	–	–
H325 F1	92	0.3	0.3	3	10	2	3	1	0.3	21
H325 F2	50	15	41	0.3	0.3	24	0.3	0.3	–	–
H331 F1	143	0.3	74	6	3	7	0.3	19	19	50
H331 F2	101	70	105	8	9	3	13	12	–	–
Water samples										
H319 F1	204	13	12	5	5	6	10	2	0.2	15
H319 F2	47	78	22	4	14	6	37	2	–	–
H325 F1	145	19	23	11	4	4	19	3	0.2	26
H325 F2	49	35	28	3	2	5	21	3	–	–
H331 F1	130	26	10	6	3	4	11	1	9	5
H331 F2	43	50	25	6	3	3	24	2	–	–
Air filter samples										
H319 F1	96	6	4	0.6	0.6	0.8	4	0.4	2	7
H319 F2	41	72	15	2	1	1.7	12	1.4	–	–
H325 F1	544	9	3	0.4	0.8	0.9	5	0.6	1	6
H325 F2	40	12	8	1	1	0.9	15	1.3	–	–
H331 F1	119	7	3	0.3	0.8	0.9	2	0.9	1	4
H331 F2	40	6	4	1	0.7	0.7	8	1.2	–	–
Water filter samples										
H319 F1	23	0.4	0.2	0.1	0.03	0.2	0.2	0.1	0.3	2
H319 F2	41	15	12	1	1	1	16	0.8	–	–
H325 F1	14	0.4	0.2	0.1	0.05	0.1	0.2	0.04	0.2	2
H325 F2	36	12	6	2	1	1	12	1.3	–	–
H331 F1	1	1	0.5	0.1	0.1	0.3	0.7	0.1	0.4	0.5
H331 F2	37	14	4	1	1	1	10	1.2	–	–

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Table S6. Method detection limits (pg m^{-3} for air samples; pg L^{-1} for water samples) of air, water, air filter and water filter samples in individual sampling cruises

Mean sample volumes of 300 m^3 and 180 L were estimated for air and water samples. F1, fraction 1; F2, fraction 2. TFL, trifluralin; ENDO-I, α-endosulfan; ENDO-II, β-endosulfan; CPF, chlorpyrifos; DCPA, dacthal; PCNB, qintozene; PeCA, pentachloroanisole; –, pentachloroanisole and qintozene were not detected in fraction 2

	HCB	α-HCH	γ-HCH	TFL	ENDO-I	ENDO-II	CPF	DCPA	PCNB	PeCA
Air samples										
H319 F1	1.3	0.0010	0.10	0.0080	0.0080	0.0040	0.061	0.0040	0.012	0.10
H319 F2	0.68	0.21	0.19	0.010	0.0010	0.0090	0.13	0.029	–	–
H325 F1	0.31	0.0010	0.0010	0.011	0.032	0.0080	0.0090	0.0020	0.0010	0.071
H325 F2	0.17	0.18	0.27	0.0010	0.0010	0.079	0.0010	0.0010	–	–
H331 F1	0.48	0.0010	0.25	0.019	0.0090	0.023	0.0010	0.062	0.064	0.17
H331 F2	0.34	0.70	1.0	0.027	0.031	0.010	0.043	0.041	–	–
Water samples										
H319 F1	1.1	0.073	0.068	0.025	0.027	0.034	0.057	0.0090	0.0010	0.082
H319 F2	0.26	2.0	0.31	0.020	0.079	0.034	0.21	0.010	–	–
H325 F1	0.80	0.11	0.13	0.061	0.020	0.022	0.10	0.018	0.0010	0.15
H325 F2	0.27	0.37	0.23	0.019	0.013	0.027	0.12	0.017	–	–
H331 F1	0.72	0.14	0.053	0.032	0.019	0.022	0.059	0.0080	0.050	0.027
H331 F2	0.24	0.44	0.30	0.033	0.015	0.014	0.14	0.013	–	–
Air filter samples										
H319 F1	0.84	0.043	0.034	0.0050	0.0050	0.0040	0.018	0.0020	0.0090	0.043
H319 F2	0.15	1.0	0.062	0.011	0.0050	0.0080	0.11	0.010	–	–
H325 F1	3.9	0.053	0.025	0.0030	0.0080	0.0070	0.033	0.0040	0.0060	0.044
H325 F2	0.14	0.10	0.053	0.0080	0.011	0.0080	0.13	0.011	–	–
H331 F1	1.4	0.052	0.019	0.0020	0.012	0.013	0.013	0.014	0.0050	0.022
H331 F2	0.15	0.042	0.043	0.0050	0.0030	0.0050	0.041	0.0050	–	–
Water filter samples										
H319 F1	0.37	0.0040	0.0020	0.0010	0.00030	0.0010	0.0020	0.0010	0.0020	0.025
H319 F2	0.23	0.11	0.10	0.028	0.0080	0.015	0.10	0.0050	–	–
H325 F1	0.27	0.0050	0.0030	0.0010	0.0010	0.0010	0.0020	0.0010	0.0030	0.024
H325 F2	0.21	0.14	0.065	0.014	0.010	0.018	0.10	0.0090	–	–
H331 F1	0.015	0.015	0.0050	0.0010	0.0010	0.0030	0.0090	0.0010	0.0040	0.004
H331 F2	0.22	0.24	0.032	0.017	0.0070	0.018	0.091	0.011	–	–

Table S7. Method detection limits in pg L^{-1} for riverine and estuarine surface water samples (dissolved phase)

TFL, trifluralin; ENDO-I, α-endosulfan; ENDO-II, β-endosulfan; CPF, chlorpyrifos; DCPA, dacthal; PCNB, qintozene; PeCA, pentachloroanisole; –, pentachloroanisole and qintozene were not detected in fraction 2

	HCB	α-HCH	γ-HCH	TFL	ENDO-I	ENDO-II	CPF	DCPA	PCNB	PeCA
Fraction 1	4136	4.77	6.96	0.19	0.24	0.59	1.57	0.23	0.81	0.52
Fraction 2	3.61	3.53	5.91	0.64	2.51	6.37	7.69	1.82	–	–

Table S8. Gaseous concentrations of target compounds in air samples (pg m^{-3})

TFL, trifluralin; ENDO-I, α-endosulfan; ENDO-II, β-endosulfan; CPF, chlorpyrifos; DCPA, dacthal; PCNB, qintozene; PeCA, pentachloroanisole. –, not detected

	HCB	α-HCH	γ-HCH	TFL	ENDO-I	ENDO-II	CPF	DCPA	PCNB	PeCA
March										
H319 A1	36	1.7	0.11	0.30	0.53	–	0.24	–	0.034	2.1
H319 A2	10	0.20	–	1.0	1.8	0.037	4.6	0.17	0.026	0.77
H319 A3	46	0.47	4.4	0.28	0.59	–	6.2	–	0.038	2.8
H319 A4	20	0.41	–	2.4	3.2	–	3.0	0.28	0.026	1.6
H319 A5	38	0.57	0.35	2.3	3.5	–	2.8	0.24	0.030	2.1
H319 A6	7.1	0.29	0.62	0.48	3.6	–	–	–	–	0.30
Mean	23 ± 17	0.61 ± 0.55	1.4 ± 2.0	1.1 ± 1.0	2.2 ± 1.4	–	3.4 ± 2.2	0.23 ± 0.06	0.031 ± 0.0052	1.6 ± 0.9
May										
H325 A1	120	2.0	7.6	1.6	2.9	0.16	26	45	0.16	7.5
H325 A2	56	3.5	8.2	0.53	1.2	–	0.45	2.1	0.087	2.6
H325 A3	68	4.7	24	5.0	2.4	–	26	1.5	0.20	4.5
H325 A4	80	6.2	4.1	0.65	2.4	–	2.2	0.57	0.0076	2.3
H325 A5	59	6.1	2.9	0.40	1.8	–	4.8	0.52	0.053	2.5
H325 A6	64	8.8	5.4	0.91	2.3	–	18	1.1	1.0	5.0
H325 A7	180	3.1	10	1.6	2.8	0.092	45	2.7	0.55	14
Mean	89 ± 44	4.9 ± 2.3	8.9 ± 7.1	1.5 ± 1.6	2.3 ± 0.6	0.13 ± 0.05	17 ± 16	7.6 ± 16.5	0.29 ± 0.36	5.5 ± 4.1
July										
H331 A2	94	18	64	8.1	15	1.6	74	17	0.45	43
H331 A3	86	12	39	8.6	11	1.8	35	9.0	0.52	32
H331 A4	78	2.6	19	0.53	8.8	1.1	14	7.2	0.55	15
H331 A5	70	6.9	7.6	0.30	2.1	–	10	53	–	8.5
H331 A6	69	6.1	14	0.42	2.9	0.24	10	39	0.32	12
H331 A7	89	6.2	18	0.32	7.1	–	5.6	7.9	–	28
Mean	81 ± 10	8.7 ± 5.7	27 ± 21	3.0 ± 4.1	8 ± 5	1.2 ± 0.7	25 ± 26	22 ± 19	0.46 ± 0.10	23 ± 14

Table S9. Percentages (%) of particulate phase in air samples

TFL, trifluralin; ENDO-I, α-endosulfan; ENDO-II, β-endosulfan; CPF, chlorpyrifos; DCPA, dacthal; PCNB, qintozene; PeCA, pentachloroanisole. G, only gaseous phase was detected; P, only particulate phase was detected; –, neither the gas phase nor the particle phase was detected

	HCB	α-HCH	γ-HCH	TFL	ENDO-I	ENDO-II	CPF	DCPA	PCNB	PeCA
March										
H319 A1	G	G	G	55	74	P	G	P	G	G
H319 A2	G	G	G	2.2	16	22	3.0	6.5	G	G
H319 A3	G	G	G	50	73	P	3.2	P	G	1.7
H319 A4	0.8	G	G	3.1	5.7	–	G	3.2	G	G
H319 A5	G	G	G	G	G	–	G	G	G	G
H319 A6	26	G	G	8.3	11	–	–	–	–	41
May										
H325 A1	7.0	G	G	1.0	2.3	15	G	0.43	G	G
H325 A2	7.1	G	G	4.0	1.8	–	G	1.5	G	G
H325 A3	G	G	G	0.34	2.0	P	G	4.0	G	1.7
H325 A4	G	G	G	G	0.69	–	G	G	G	G
H325 A5	G	G	G	G	1.0	–	5.4	3.8	G	G
H325 A6	G	G	G	G	3.8	P	2.6	14	G	G
H325 A7	1.3	G	G	5.8	0.85	33	0.47	3.4	G	0.70
July										
H331 A2	G	G	G	G	0.31	12	5.3	1.0	G	G
H331 A3	0.18	G	1.2	0.63	0.74	12	11	3.2	G	0.34
H331 A4	0.21	G	G	1.2	0.32	13	0.71	2.2	G	G
H331 A5	G	G	G	G	0.61	–	0.45	0.64	–	G
H331 A6	G	G	G	G	0.65	17	0.80	0.87	G	G
H331 A7	1.0	G	G	12	13	P	G	14	–	0.55

Table S10. Details of target compounds' CC equations and ΔHex (kJ mol^{-1}), which originated from German Bight air samples

N, detectable sample numbers. **, correlation is significant at the 0.01 level. *, correlation is significant at the 0.05 level

	N	–ΔHex/R	B	R^2	ΔHex
HCB	18	–5889 ± 1759	–12 ± 6	0.36**	49 ± 15
α-HCH	18	–12294 ± 2283	7.5 ± 0.4	0.61**	102 ± 19
γ-HCH	16	–15716 ± 3164	20 ± 11	0.60**	131 ± 26
trifluralin	18	–2705 ± 3022	–28 ± 11	0.05	22 ± 25
α-endosulfan	18	–7323 ± 1665	–10 ± 6	0.50**	61 ± 14
chlorpyrifos	17	–9457 ± 3641	–2 ± 13	0.25*	79 ± 30
dacthal	16	–18553 ± 3685	29 ± 13	0.62**	154 ± 31
quintozene	15	–12733 ± 3235	6 ± 12	0.49**	106 ± 27
PeCA	18	–13228 ± 1728	11 ± 6	0.76**	110 ± 14

Table S11. Dissolved concentrations of target compounds in seawater samples (pg L^{-1})

TFL, trifluralin; ENDO-I, α-endosulfan; ENDO-II, β-endosulfan; CPF, chlorpyrifos; DCPA, dacthal; PCNB, qintozene; PeCA, pentachloroanisole. –, not detected

	HCB	α-HCH	γ-HCH	TFL	ENDO-I	ENDO-II	CPF	DCPA	PCNB	PeCA
March										
H319 W1	7.8	40	60	6.1	3.0	0.19	100	22	0.15	3.4
H319 W2	5.8	20	29	26	1.8	0.12	140	29	0.13	1.2
H319 W3	4.8	21	37	10	2.2	0.16	110	18	0.22	1.2
H319 W4	3.2	12	16	2.0	1.1	–	53	11	0.062	0.75
H319 W5	4.5	11	14	7.2	1.1	–	58	13	0.072	0.63
H319 W7	4.6	28	33	2.9	2.0	0.14	42	13	0.064	1.4
H319 W8	5.0	12	18	2.8	1.2	0.053	55	12	0.062	1.0
H319 W9	4.9	19	18	8.2	0.78	–	73	26	0.046	0.74
H319 W10	4.5	13	12	4.8	0.74	–	59	18	0.031	0.76
H319 W11	2.9	11	14	14	1.0	0.059	84	19	0.036	0.22
Mean	4.8 ± 1.4	18 ± 9	24 ± 15	8.4 ± 7.2	1.5 ± 0.7	0.12 ± 0.06	71 ± 31	17 ± 6	0.087 ± 0.060	1.1 ± 0.9
May										
H325 W1	36	25	45	2.9	0.84	0.36	81	27	0.056	3.7
H325 W2	13	30	54	2.6	1.0	0.46	85	30	0.065	2.1
H325 W3	7.6	11	22	2.2	0.48	0.12	72	17	0.038	1.0
H325 W4	22	150	64	2.8	1.0	0.36	100	34	–	1.9
H325 W5	22	38	51	2.8	0.90	0.31	110	30	0.059	1.8
H325 W6	3.9	20	30	3.3	0.63	0.10	81	26	0.032	1.0
H325 W7	4.9	29	30	9.3	0.89	–	140	42	0.034	0.76
H325 W8	3.3	19	14	1.6	0.50	–	68	25	–	0.86
H325 W9	3.3	19	15	1.1	0.51	–	80	25	0.011	0.88
H325 W10	3.8	24	32	0.8	0.55	–	52	22	0.022	1.1
H325 W11	8.8	38	57	0.9	0.78	0.10	78	36	0.025	1.3
H325 W12	11	31	59	2.6	0.73	0.11	89	38	0.040	1.6
Mean	12 ± 10	36 ± 35	39 ± 18	2.7 ± 2.2	0.73 ± 0.19	0.24 ± 0.15	86 ± 22	29 ± 7	0.035 ± 0.020	1.5 ± 0.8
July										
H331/10 W1	4.7	54	83	1.0	1.9	0.31	41	74	–	1.8
H331/10 W5	3.1	31	54	0.5	0.93	0.11	30	53	–	1.1
H331/10 W6	3.1	10	31	0.10	0.53	0.14	28	36	–	0.29
H331/10 W7	2.4	10	24	0.091	0.34	0.10	21	26	–	0.60
H331/10 W8	2.8	9.0	28	0.15	0.31	–	29	31	–	0.83
H331/10 W9	2.3	18	19	0.048	0.34	0.070	23	38	–	0.63
H331/10 W10	1.7	14	13	0.045	0.19	–	30	41	–	0.52
H331/10 W11	2.9	30	27	0.077	0.29	–	36	50	–	0.70
H331/10 W12	2.6	11	38	0.16	0.38	–	19	43	–	0.69
H331/10 W13	2.4	19	42	0.11	0.19	0.64	14	28	–	0.71
Mean	2.8 ± 0.8	21 ± 14	36 ± 20	0.23 ± 0.29	0.54 ± 0.54	0.23 ± 0.12	27 ± 8.0	42 ± 14	–	0.79 ± 0.82

Table S12. Percentages (%) of particulate phase in seawater samples

TFL, trifluralin; ENDO-I, α-endosulfan; ENDO-II, β-endosulfan; CPF, chlorpyrifos; DCPA, dacthal; PCNB, qintozene; PeCA, pentachloroanisole. D, only dissolved phase was detected; P, only particulate phase was detected; –, neither the dissolved phase nor the particle phase was detected

	HCB	α-HCH	γ-HCH	TFL	ENDO-I	ENDO-II	CPF	DCPA	PCNB	PeCA
March										
H319 W1	0.08	D	0.01	0.8	0.4	0.08	D	0.05	D	1.1
H319 W2	0.02	0.03	D	0.2	D	0.02	0.04	0.2	1.9	0.7
H319 W3	D	D	D	1.8	D	D	0.4	0.3	0.7	3.5
H319 W4	D	D	D	D	–	D	D	0.2	D	D
H319 W5	D	D	D	D	–	D	0.1	0.3	D	D
H319 W7	D	D	0.2	2.2	22	D	0.5	0.2	D	1.2
H319 W8	D	D	0.4	2.8	D	D	0.5	0.4	1.1	0.9
H319 W9	D	D	D	0.4	–	D	D	0.1	D	D
H319 W10	D	D	D	1.5	–	D	D	0.3	1.2	0.9
H319 W11	D	D	D	2.5	D	D	0.2	0.1	1.3	D
May										
H325 W1	D	D	0.2	D	D	D	D	0.1	8.8	1.8
H325 W2	D	D	D	D	0.3	D	D	0.1	4.0	D
H325 W3	D	D	D	D	D	D	D	0.01	3.3	D
H325 W4	D	D	D	D	D	D	P	D	–	D
H325 W5	D	D	D	D	D	D	0.1	0.03	2.0	D
H325 W6	D	D	0.2	D	0.7	D	D	0.1	20	0.3
H325 W7	1.5	D	0.3	1.0	P	1.5	0.4	0.1	16	0.6
H325 W8	D	D	D	D	P	D	0.5	0.1	P	D
H325 W9	D	D	D	D	–	D	0.1	D	D	D
H325 W10	D	D	D	D	–	D	0.01	D	14	D
H325 W11	D	D	0.6	D	1.1	D	D	0.2	15	D
H325 W12	1.4	D	D	0.02	D	1.4	D	0.001	5.7	P
July										
H331 W1	D	D	0.04	2.6	0.6	D	2.4	0.3	P	0.6
H331 W5	0.3	D	D	8.5	D	0.3	5.3	0.4	P	1.0
H331 W6	D	D	D	D	D	D	D	0.3	P	2.0
H331 W7	D	D	D	3.8	D	D	6.5	0.2	P	0.06
H331 W8	D	D	D	11	–	D	D	0.2	P	0.7
H331 W9	D	D	D	3.2	D	D	0.7	0.2	P	0.5
H331 W10	D	D	D	3.0	–	D	0.3	0.1	P	0.5
H331 W11	D	D	D	13	–	D	D	0.3	P	0.06
H331 W12	D	D	D	D	–	D	D	0.4	–	0.9
H331 W13	D	D	D	D	D	D	D	D	–	0.6

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Table S13. Pearson correlations between concentrations of pesticides in seawater and corresponding salinity

TFL, trifluralin; ENDO-I, α-endosulfan; ENDO-II, β-endosulfan; CPF, chlorpyrifos; DCPA, dacthal; PCNB, qintozene; PeCA, pentachloroanisole. ** Correlation is significant at the 0.01 level (2-tailed). * Correlation is significant at the 0.05 level (2-tailed)

	HCB	α-HCH	γ-HCH	TFL	ENDO-I	CPF	DCPA	PCNB	PeCA
March									
Pearson correlation Salinity	–0.650*	–0.913(**)	–0.898(**)	0.241	–0.893(**)	–0.067	0.039	–0.475	–0.853(**)
Sig. (2-tailed)	0.042	0.000	0.000	0.503	0.001	0.854	0.916	0.165	0.002
n	10	10	10	10	10	10	10	10	10
May									
Pearson correlation Salinity	–0.780**	–0.413	–0.820(**)	0.135	–0.611	–0.163	–0.176	–0.432	–0.643(*)
Sig. (2-tailed)	0.008	0.236	0.004	0.710	0.061	0.654	0.627	0.246	0.045
n	10	10	10	10	10	10	10	9	10
July									
Pearson correlation Salinity	–0.476	–0.412	–0.810(**)	–0.710(*)	–0.601	0.028	–0.318		–0.535
Sig. (2-tailed)	0.164	0.236	0.004	0.021	0.066	0.938	0.371		0.111
n	10	10	10	10	10	10	10	0	10

Table S14. Dissolved concentrations of target compounds in riverine and estuarine surface water samples (pg L^{-1})

TFL, trifluralin; ENDO-I, α-endosulfan; ENDO-II, β-endosulfan; CPF, chlorpyrifos; DCPA, dacthal; PCNB, qintozene; PeCA, pentachloroanisole. –, not detected

	HCB	α-HCH	γ-HCH	TFL	ENDO-I	ENDO-II	CPF	DCPA	PCNB	PeCA
E3	–	182	94	1.1	0.4	–	8	0.5	–	2.1
E6	–	189	17	2.7	–	–	56	2.8	–	2.1
E9	–	177	57	2.2	–	–	69	1.6	–	1.8
NE3	–	38	5	–	–	–	–	8.3	–	1.0
NS3	–	12	10	0.9	–	–	14	15.6	–	0.6
W1	–	16	156	1.1	1.2	–	30	–	–	4.6

Table S15. Fugacity ratios of pesticides in the German Bight in March, May and July

TFL, trifluralin; ENDO-I, α-endosulfan; ENDO-II, β-endosulfan; CPF, chlorpyrifos; DCPA, dacthal; PCNB, qintozene; PeCA, pentachloroanisole

Paired water and air samples		HCB	α-HCH	γ-HCH	TFL	ENDO-I	CPF	DCPA	PCNB	PeCA
March										
H319 W1	H319 A1	2.0	1.9	0.045	0.023	0.46	0.0038	0.00017	0.40	1.7
H319 W2	H319 A1	2.2	3.3	0.083	0.005	0.66	0.0020	0.00011	0.45	4.4
H319 W3	H319 A2	0.79	0.15	0.066	0.042	2.0	0.057	0.33	0.21	1.7
H319 W4	H319 A2	1.2	0.28	0.16	0.22	4.2	0.12	0.53	0.72	2.6
H319 W5	H319 A3	3.6	0.68	7.3	0.016	1.2	0.12	0.00025	0.86	11
H319 W7	H319 A4	2.0	0.26	0.080	0.39	4.3	0.12	0.82	0.74	3.2
H319 W8	H319 A4	1.6	0.58	0.14	0.38	6.3	0.077	0.82	0.73	4.4
H319 W9	H319 A5	2.6	0.46	0.43	0.12	9.8	0.043	0.30	1.1	6.7
H319 W10	H319 A5	3.0	0.69	0.65	0.20	11	0.057	0.44	1.6	6.8
H319 W11	H319 A6	0.84	0.40	0.97	0.014	8.3	0.0027	0.00017	0.40	3.3
	Mean	2.0 ± 0.9	0.87 ± 0.97	0.99 ± 2.24	0.14 ± 0.15	4.8 ± 3.8	0.060 ± 0.049	0.32 ± 0.33	0.72 ± 0.41	4.6 ± 2.8
May										
H325 W1	H325 A1	0.81	0.98	3.1	0.19	5.9	0.23	45	3.8	4.0
H325 W2	H325 A1	2.3	0.78	2.6	0.20	5.0	0.21	40	3.2	7.0
H325 W3	H325 A2	1.8	3.9	7.0	0.081	4.3	0.0045	3.4	3.0	5.1
H325 W4	H325 A2	0.64	0.30	2.4	0.066	2.1	0.0032	1.7	120	2.8
H325 W5	H325 A3	0.72	1.5	8.5	0.59	4.3	0.16	1.3	4.5	4.7
H325 W6	H325 A3	4.5	3.0	15	0.52	6.7	0.24	1.6	8.9	8.9
H325 W7	H325 A4	4.3	2.7	2.7	0.024	4.8	0.012	0.38	0.32	6.2
H325 W8	H325 A4	6.1	4.0	5.5	0.14	8.4	0.024	0.63	10	5.4
H325 W9	H325 A5	4.2	3.8	3.5	0.13	5.9	0.041	0.55	6.4	5.5
H325 W10	H325 A5	3.8	3.1	1.6	0.18	5.6	0.065	0.63	3.2	4.4
H325 W11	H325 A6	1.6	2.6	1.7	0.34	4.6	0.14	0.77	49	7.1
H325 W12	H325 A6	1.2	3.2	1.6	0.11	4.9	0.12	0.74	31	5.6
	Mean	2.7 ± 1.8	2.5 ± 1.3	4.6 ± 4.0	0.21 ± 0.18	5.2 ± 1.5	0.11 ± 0.09	8.1 ± 16.2	20 ± 34	5.6 ± 1.6

Table S15. (*Cont.*)

Paired water and air samples		HCB	α-HCH	γ-HCH	TFL	ENDO-I	CPF	DCPA	PCNB	PeCA
July										
H331 W5	H331 A3	2.9	2.7	8.4	3.5	10	0.26	1.8	7.6	22
H331 W6	H331 A3	3.1	8.5	15	18	19	0.29	2.8	8.1	90
H331 W7	H331 A4	3.8	1.9	9.6	1.3	25	0.18	3.7	10	24
H331 W8	H331 A4	3.4	2.2	8.4	0.81	28	0.13	3.2	10	17
H331 W9	H331 A5	3.7	3.0	5.0	1.4	6.2	0.12	20	0.89	14
H331 W10	H331 A5	5.4	3.9	7.9	1.6	12	0.10	20	1.0	19
H331 W11	H331 A6	3.1	1.6	6.5	1.3	10	0.081	11	6.4	18
H331 W12	H331 A6	3.0	4.0	4.4	0.58	7.1	0.13	11	5.5	16
H331 W13	H331 A7	4.2	2.3	5.0	0.61	34	0.10	3,3	0.76	35
	Mean	3.6 ± 0.8	3.4 ± 2.1	7.8 ± 3.2	3.3 ± 5.7	17 ± 10	0.15 ± 0.08	8.6 ± 7.4	5.6 ± 3.9	28 ± 24

Table S16. Air-seawater gas exchange fluxes (ng m^{-2} day^{-1}) of pesticides in the German Bight in March, May and July

TFL, trifluralin; ENDO-I, α-endosulfan; ENDO-II, β-endosulfan; CPF, chlorpyrifos; DCPA, dacthal; PCNB, qintozene; PeCA, pentachloroanisole

Paired water and air samples		HCB	α-HCH	γ-HCH	TFL	ENDO-I	CPF	DCPA	PCNB	PeCA
March										
H319 W1	H319 A1	–11	–1.7	1.8	6.9	0.44	46	0.47	0.039	–0.68
H319 W2	H319 A1	–8.1	–1.9	0.74	24	0.14	63	0.54	0.024	–0.97
H319 W3	H319 A2	1.7	0.98	1.20	13	–0.69	57	0.29	0.082	–0.26
H319 W4	H319 A2	–0.89	0.36	0.39	1.6	–0.87	21	0.10	0.0066	–0.33
H319 W5	H319 A3	–9.1	0.10	–1.8	4.3	–0.045	16	0.18	0.0024	–1.1
H319 W7	H319 A4	–1.1	0.29	0.30	0.36	–0.48	4.0	0.015	0.0017	–0.24
H319 W8	H319 A4	–0.62	0.069	0.15	0.30	–0.45	5.3	0.014	0.0016	–0.23
H319 W9	H319 A5	–8.3	0.39	0.27	5.9	–1.5	29	0.32	–0.0009	–0.96
H319 W10	H319 A5	–9.6	0.16	0.11	3.2	–1.6	23	0.18	–0.0063	–1.0
H319 W11	H319 A6	0.14	0.12	0.0044	3.7	–0.68	14	0.16	0.0029	–0.050
	Mean	–4.7	–0.11	0.32	6.3	–0.58	28	0.23	0.015	–0.58
	s.d.	5.0	0.92	0.95	7.2	0.66	21	0.18	0.027	0.40
May										
H325 W1	H325 A1	2.5	0.0069	–1.1	0.65	–0.41	12	–9.2	–0.020	–1.1
H325 W2	H325 A1	–5.6	0.11	–0.94	0.53	–0.37	12	–8.6	–0.018	–1.1
H325 W3	H325 A2	–2.9	–0.64	–1.7	0.71	–0.18	17	–0.36	–0.012	–0.47
H325 W4	H325 A2	6.3	2.9	–1.7	1.5	–0.18	37	–0.29	–0.027	–0.54
H325 W5	H325 A3	3.2	–0.38	–5.4	0.45	–0.38	24	–0.082	–0.035	–0.82
H325 W6	H325 A3	–12	–1.2	–8.6	1.0	–0.67	24	–0.2	–0.064	–1.4
H325 W7	H325 A4	–10	–1.2	–0.77	4.2	–0.48	40	0.27	0.0044	–0.53
H325 W8	H325 A4	–3.1	–0.65	–0.48	0.20	–0.22	7.1	0.046	–0.0008	–0.22
H325 W9	H325 A5	–1.2	–0.49	–0.23	0.086	–0.11	5.7	0.046	–0.0033	–0.17
H325 W10	H325 A5	–8.0	–1.4	–0.37	0.34	–0.42	17	0.099	–0.011	–0.60
H325 W11	H325 A6	–4.5	–1.9	–0.76	0.35	–0.53	28	0.11	–0.31	–1.4
H325 W12	H325 A6	–4.1	–3.0	–1.0	2.2	–0.79	49	0.18	–0.45	–1.9
	Mean	–3.3	–0.65	–1.9	1.0	–0.40	23	–1.5	–0.079	–0.86
	s.d.	5.5	1.4	2.5	1.2	0.21	14	3.5	0.14	0.54
July										
H331 W5	H331 A3	–20	–12	–50	–2.3	–9.1	27	–3.2	–0.29	–21
H331 W6	H331 A3	–22	–15	–53	–3.3	–9.7	21	–4.9	–0.31	–23
H331 W7	H331 A4	–22	–8.9	–31	–3.4	–6.9	20	–4.2	–0.33	–9.8
H331 W8	H331 A4	–16	–7.4	–25	–2.5	–5.6	27	–3.3	–0.27	–7.8
H331 W9	H331 A5	–17	–0.21	–13	–0.12	–4.9	28	–37	0.0032	–5.0
H331 W10	H331 A5	–14	–0.5	–11	–0.094	–3.9	27	–30	0.00027	–4.0
H331 W11	H331 A6	–13	–2.2	–4.0	0.0089	–1.0	46	–25	–0.16	–6.9
H331 W12	H331 A6	–9.3	–3.2	–2.7	0.11	–0.76	19	–21	–0.12	–5.3
H331 W13	H331 A7	–5.6	–1.5	–4.5	0.016	–0.84	8.8	–2.4	0.0044	–9.1
	Mean	–1.5	–5.6	–21	–1.3	–4.8	25	–14	–0.16	–10
	s.d.	5.6	5.2	19	1.5	3.4	9.9	14	0.14	6.9

Table S17. Physical-chemical properties of target compounds at 298 K

Henry's law constants (HLC), the enthalpy of water–air exchange (ΔH_{WA}) and vapour pressures are not salinity-corrected. TFL, trifluralin; ENDO-I, α-endosulfan; ENDO-II, β-endosulfan; CPF, chlorpyrifos; DCPA, dacthal; PCNB, qintozene; PeCA, pentachloroanisole. N.A., not available

	HCB	α-HCH	γ-HCH	TFL	ENDO-I	ENDO-II	CPF	DCPA	PCNB	PeCA
HLC, 298 K (Pa m^{-3} mol^{-1})	35[1]	0.3[2]	0.27[2]	11.2[3]	0.82[2]	0.045[4]	3.6[2]	0.221[5]	4.42[5]	2.91[6]
ΔH_{WA} (Pa m^{-3} mol^{-1})	57.7[1]	45.9[2]	27.2[2]	29.8[3]	N.A.	34.6[4]	64.9[2]	N.A.	N.A.	N.A.
log K_{OW}	5.64[4]	3.94[7]	3.83[7]	4.83[8]	4.94[4]	4.78[4]	4.96[5]	4.4[9]	4.64[5]	5.66[6]
log K_{OA}	7.21[4]	7.464[7]	7.74[7]	7.716[5]	8.49[4]	8.64[5]	8.882[5]	8.330[5]	7.383[5]	7.986[5]
P L (Pa)	0.094[4]	0.245[7]	0.0757[7]	0.01[5]	0.0044[4]	0.0040[4]	0.004[5]	0.00644[5]	0.00362[5]	0.0458[5]
SL (mol m^{-3})	0.0014[4]	0.333[7]	0.247[7]	0.0006[5]	0.0063[4]	0.089[4]	0.001[5]	0.0015[5]	0.0015[5]	0.0013[5]

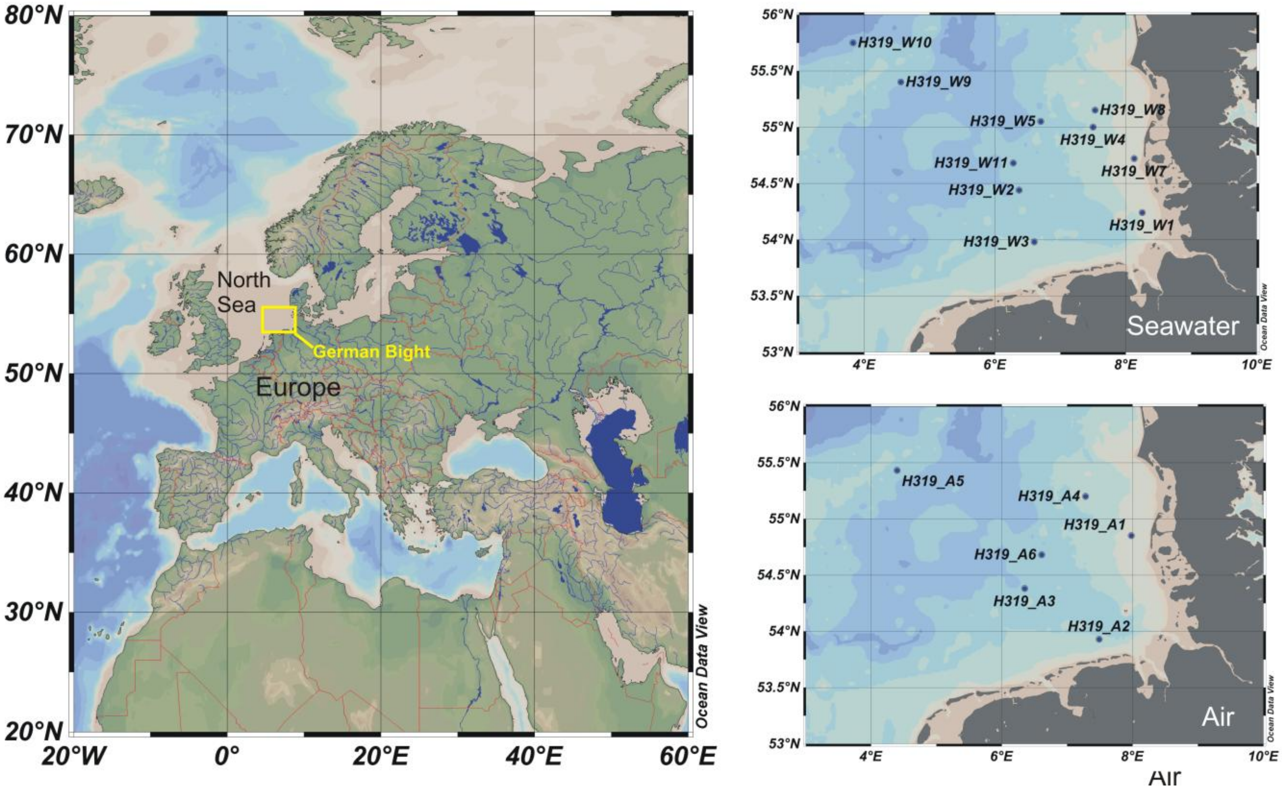
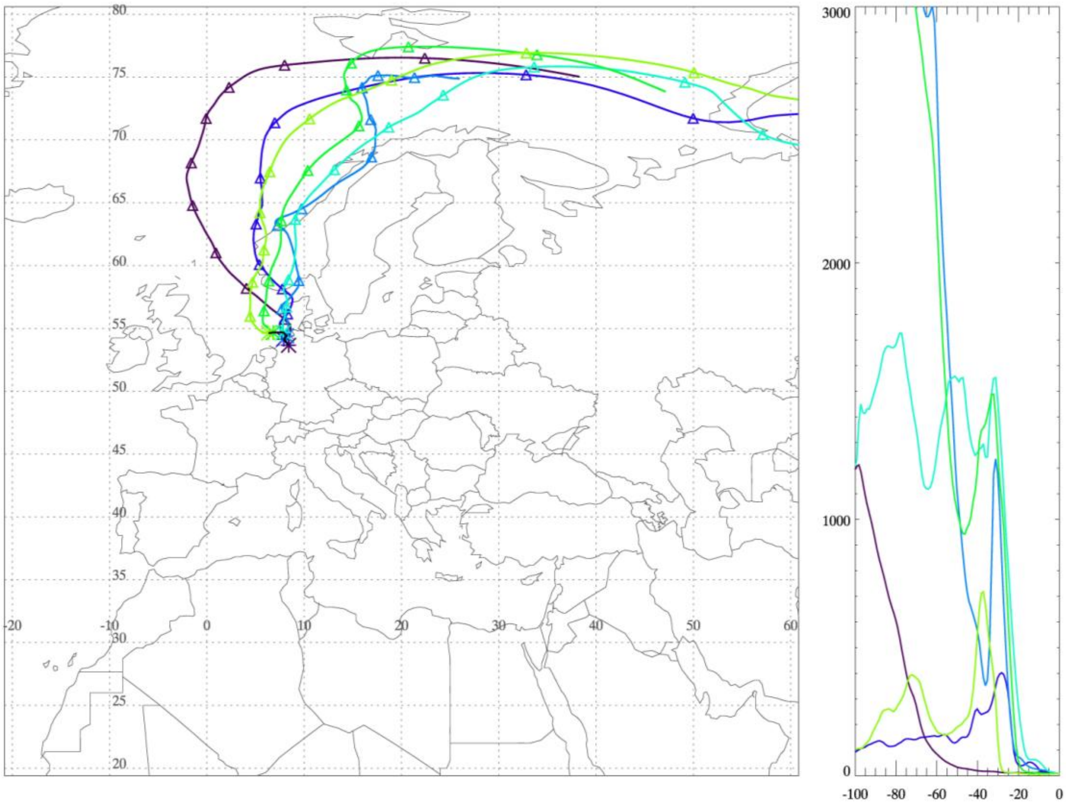


Fig. S1. Maps of air and seawater sampling sites in March 2010. Maps of sampling sites in May and July 2010 were not provided here because the distributions of sampling sites were similar as those in March 2010.

H319_A1



H319_A2

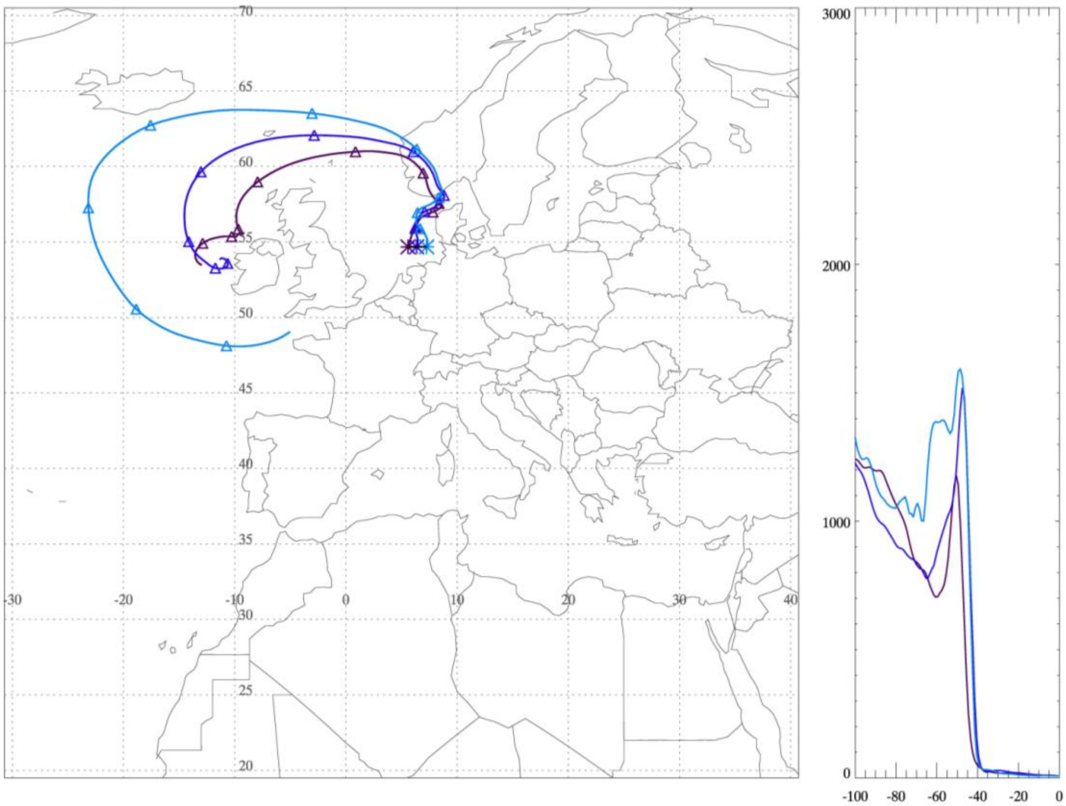
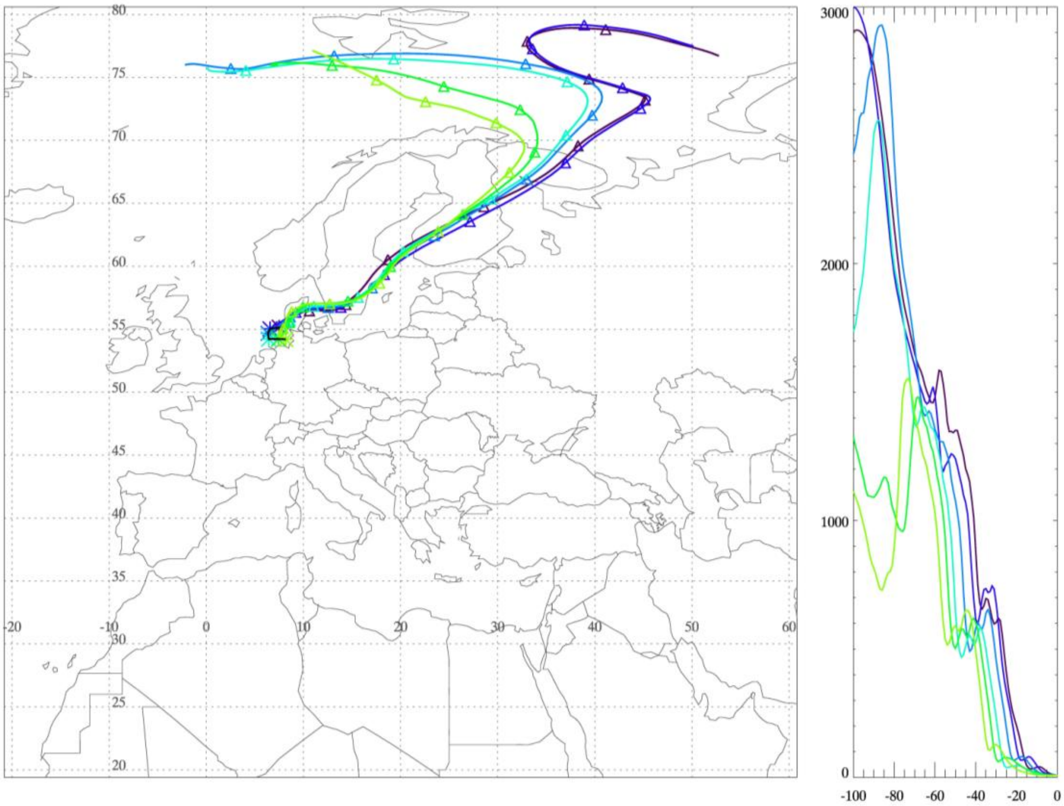


Fig. S2. One hundred and twenty-hour air mass back trajectories (4-h steps) and altitudinal profiles of the air mass parcels for the cruises H319, H325 and H331. The black line indicates the cruise leg.

H319_A3



H319_A4

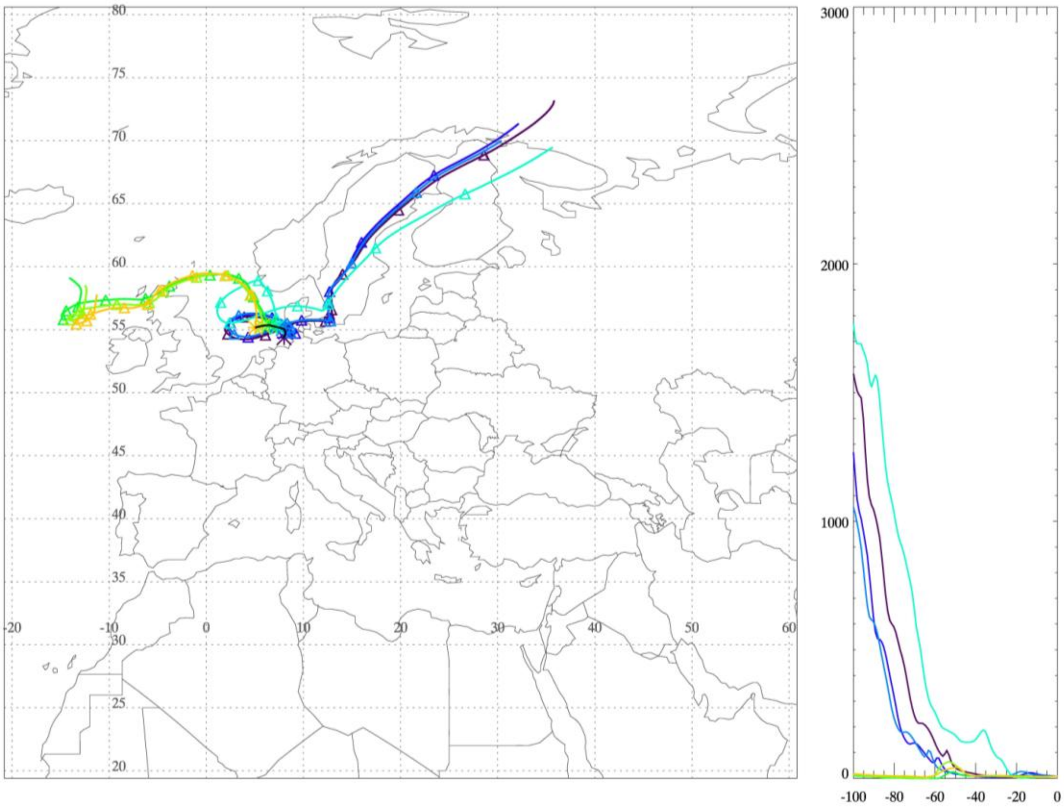
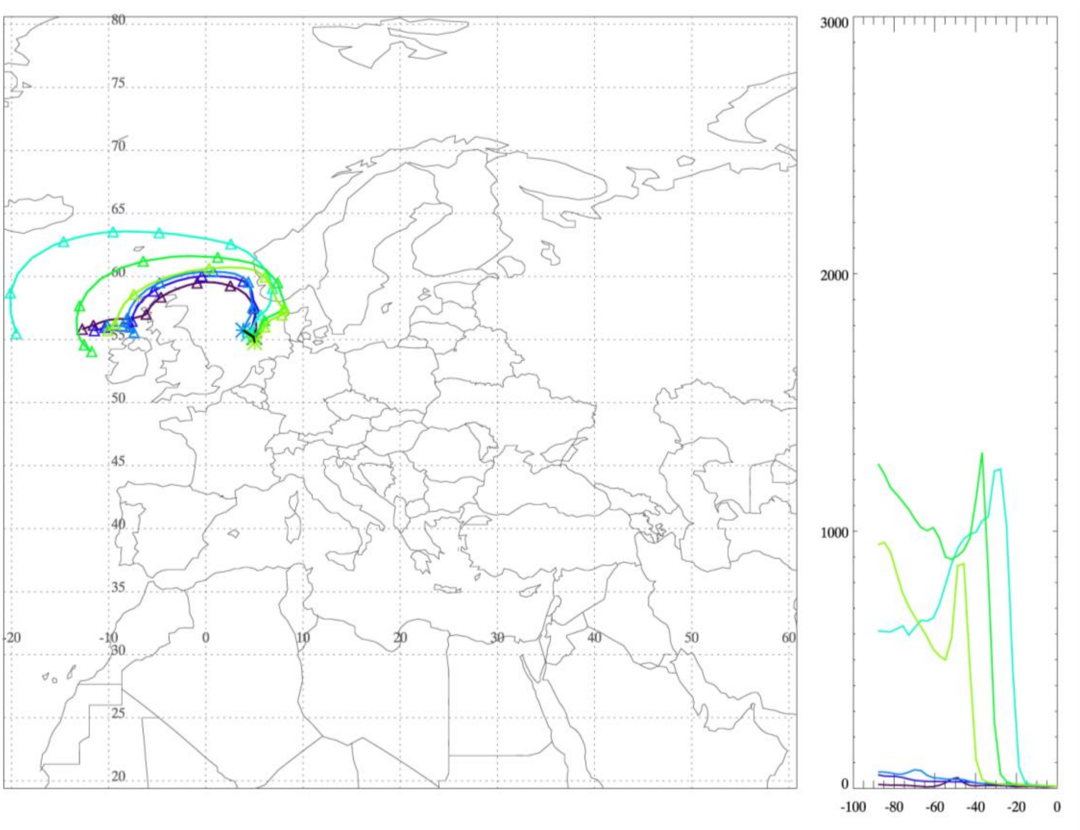


Fig. S2. (*Cont.*)

H319_A5



H319_A6

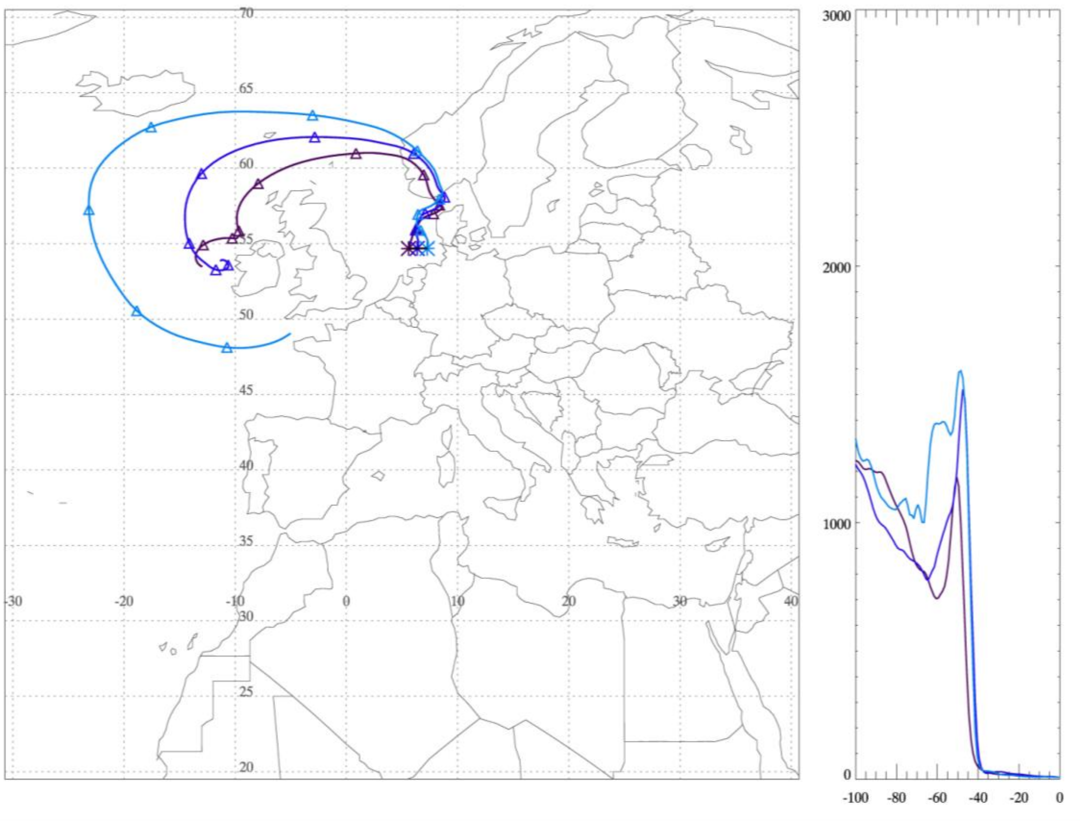
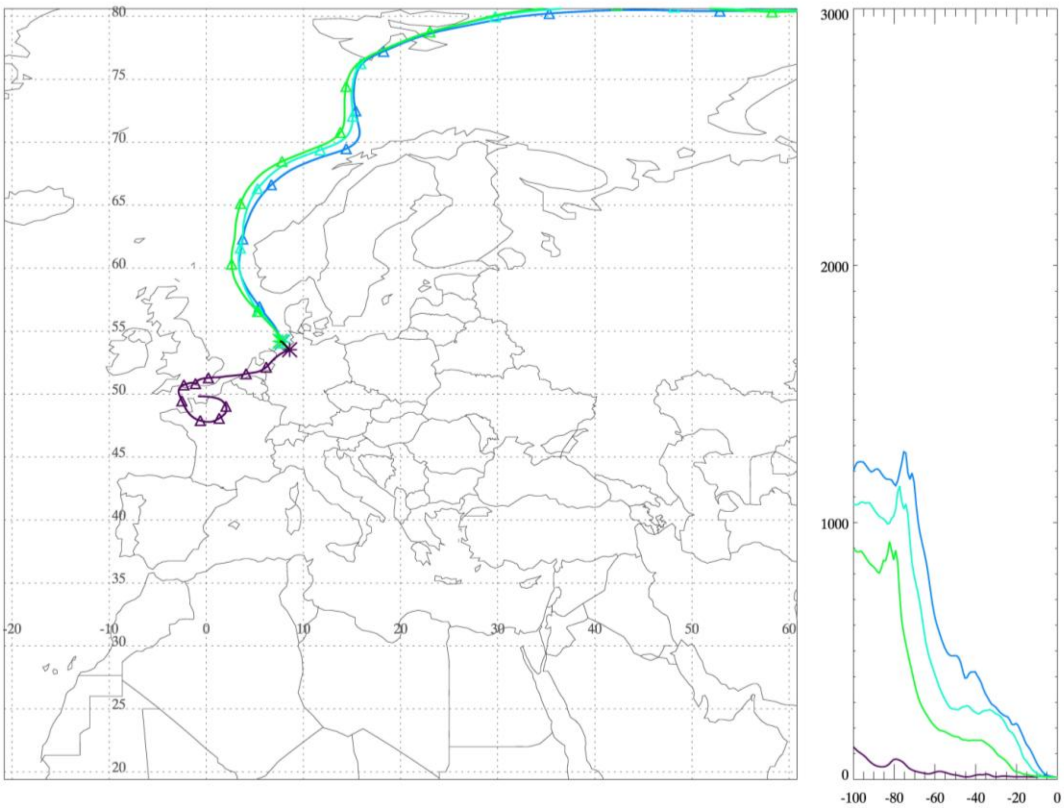


Fig. S2. (*Cont.*)

H325_A1



H325_A2

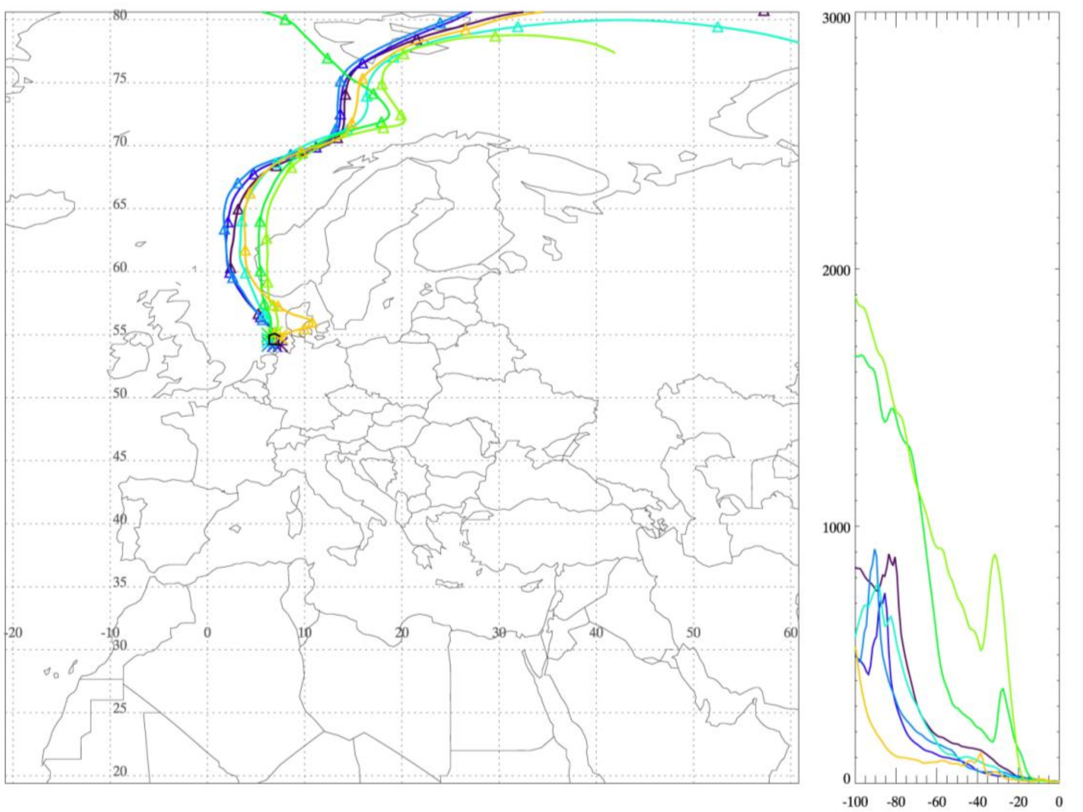
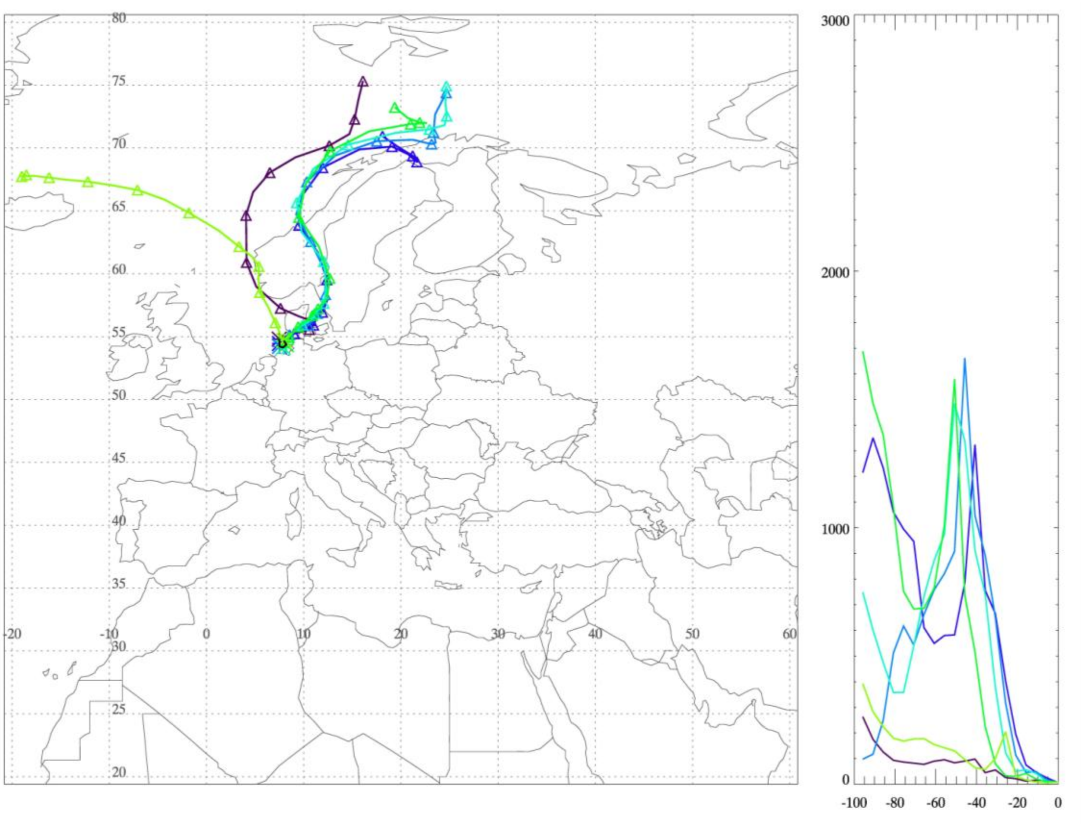


Fig. S2. (*Cont.*)

H325_A3



H325_A4

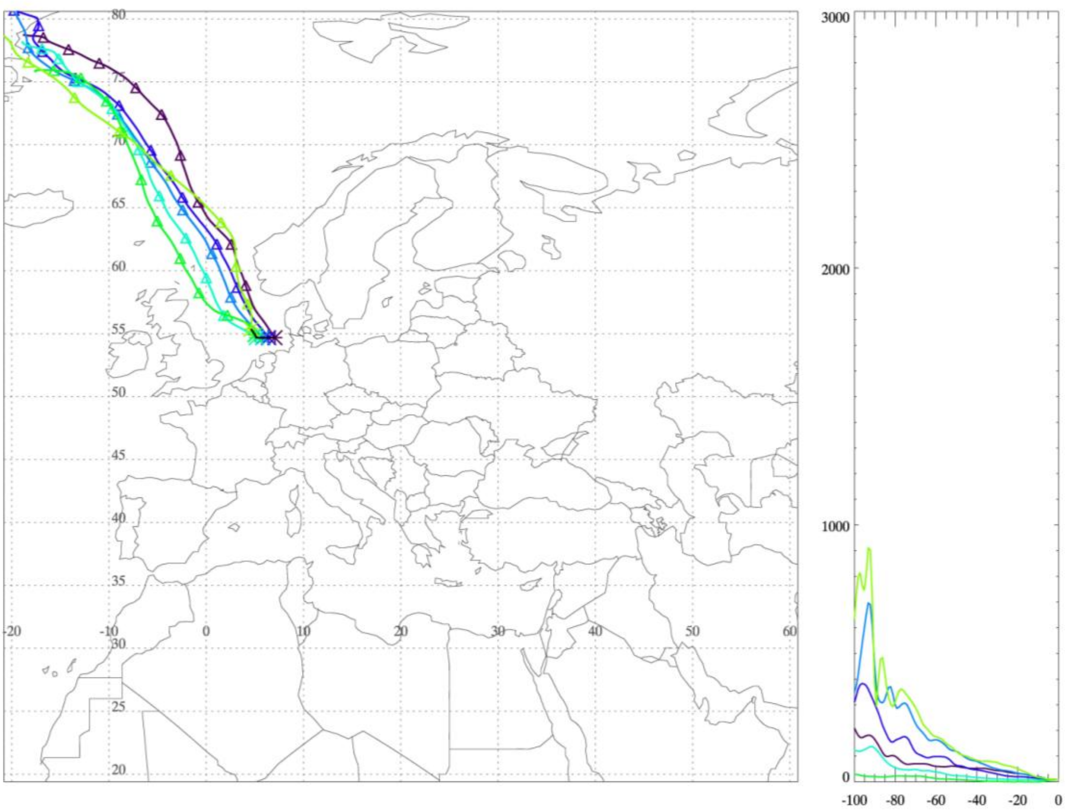
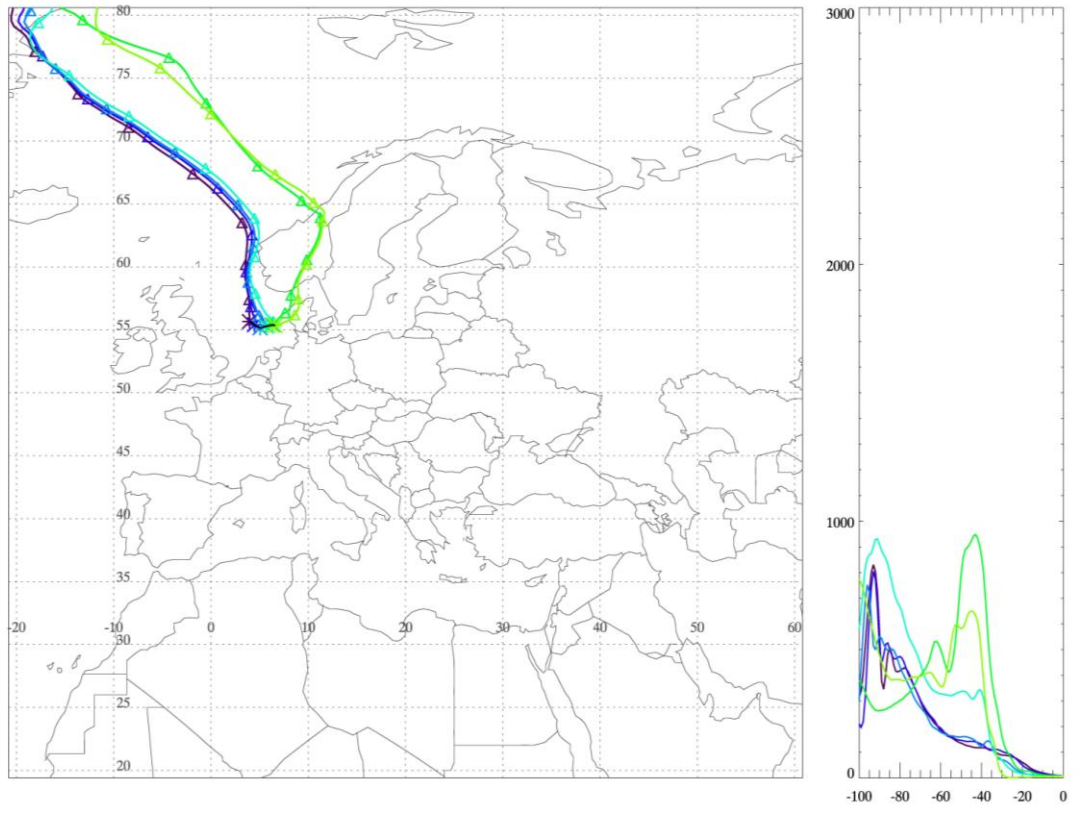


Fig. S2. (*Cont.*)

H325_A5



H325_A6

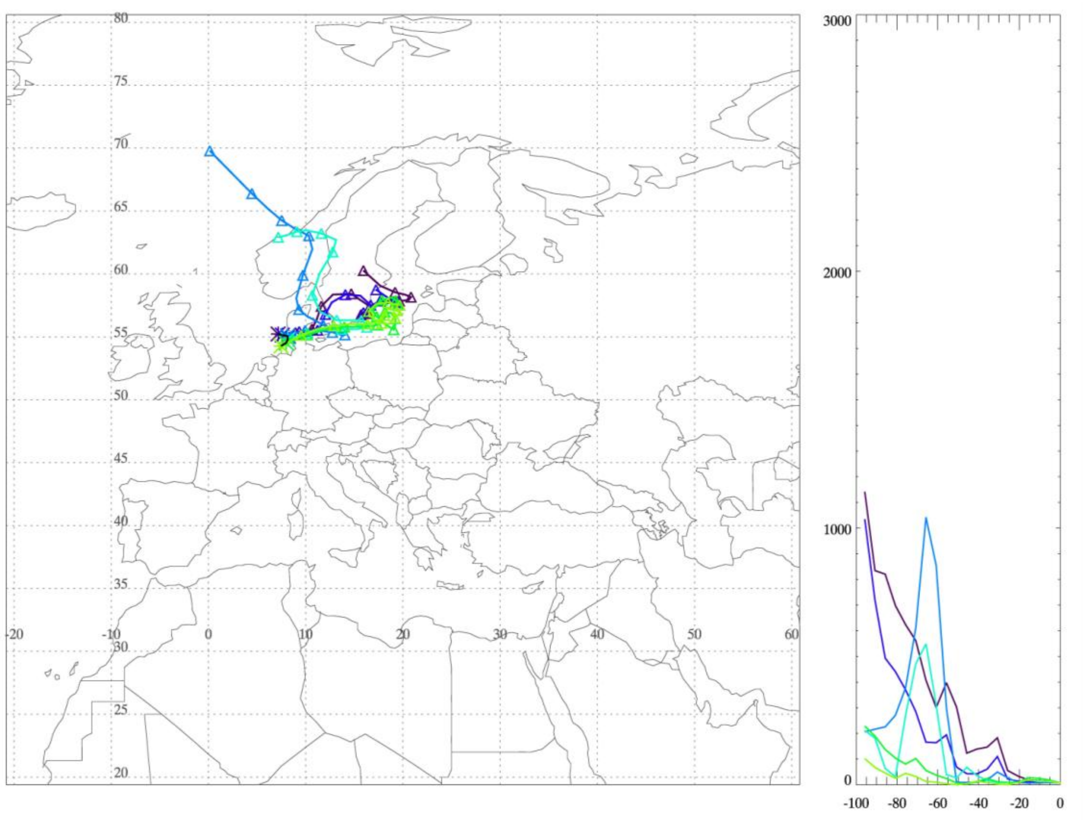
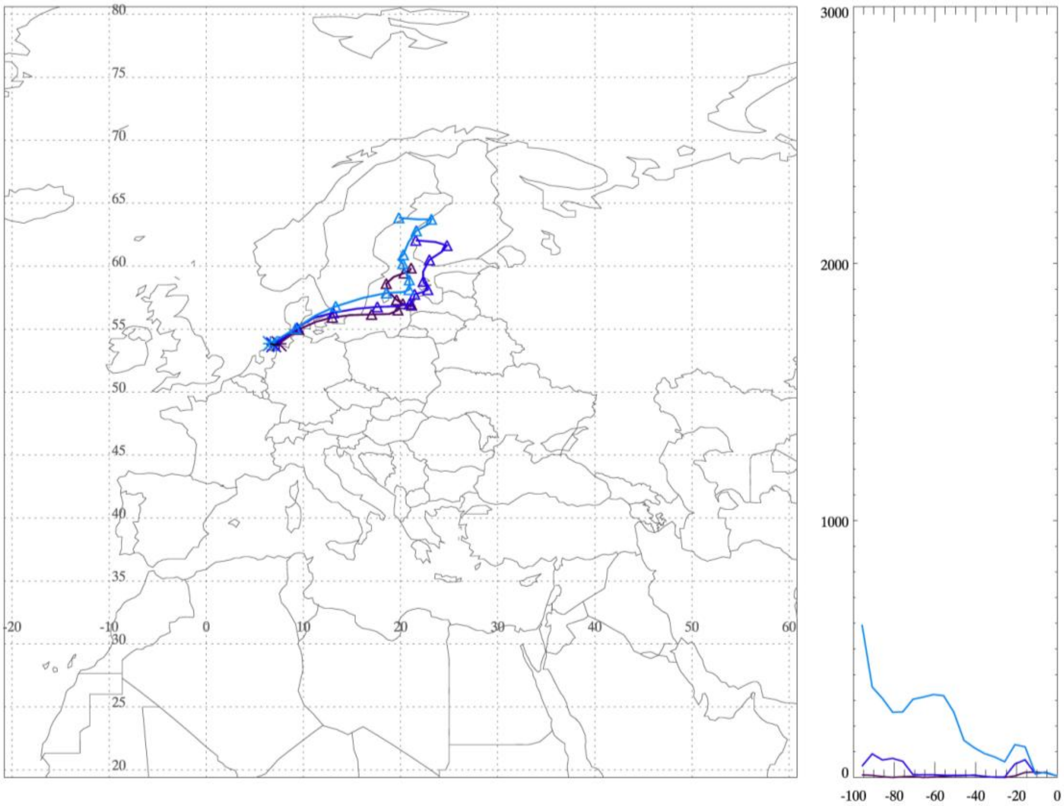


Fig. S2. (*Cont.*)

H325_A7



H331_A1

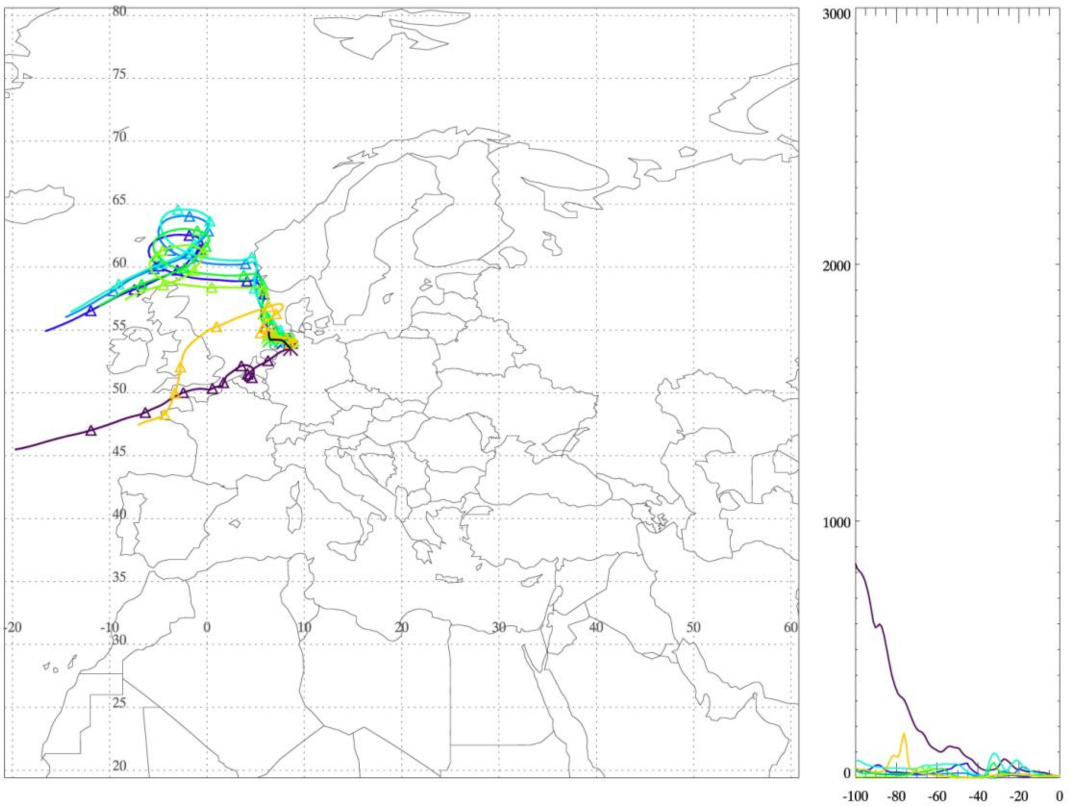
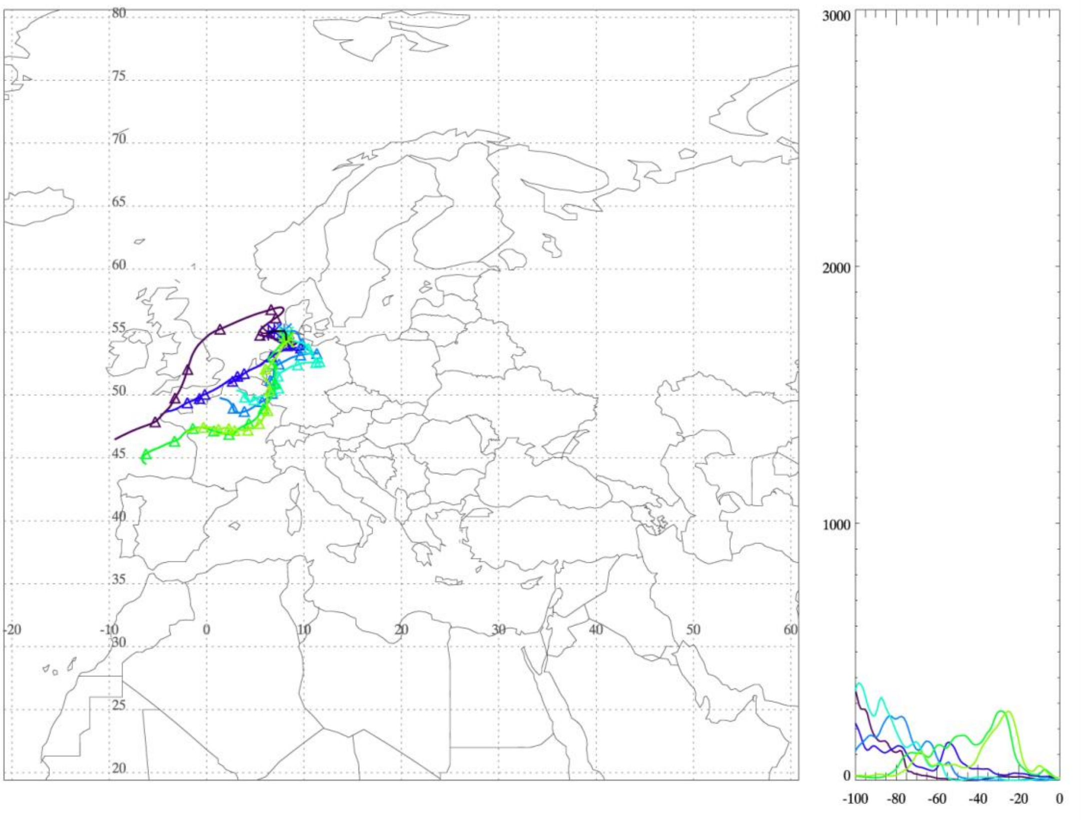


Fig. S2. (*Cont.*)

H331_A2



H331_A3

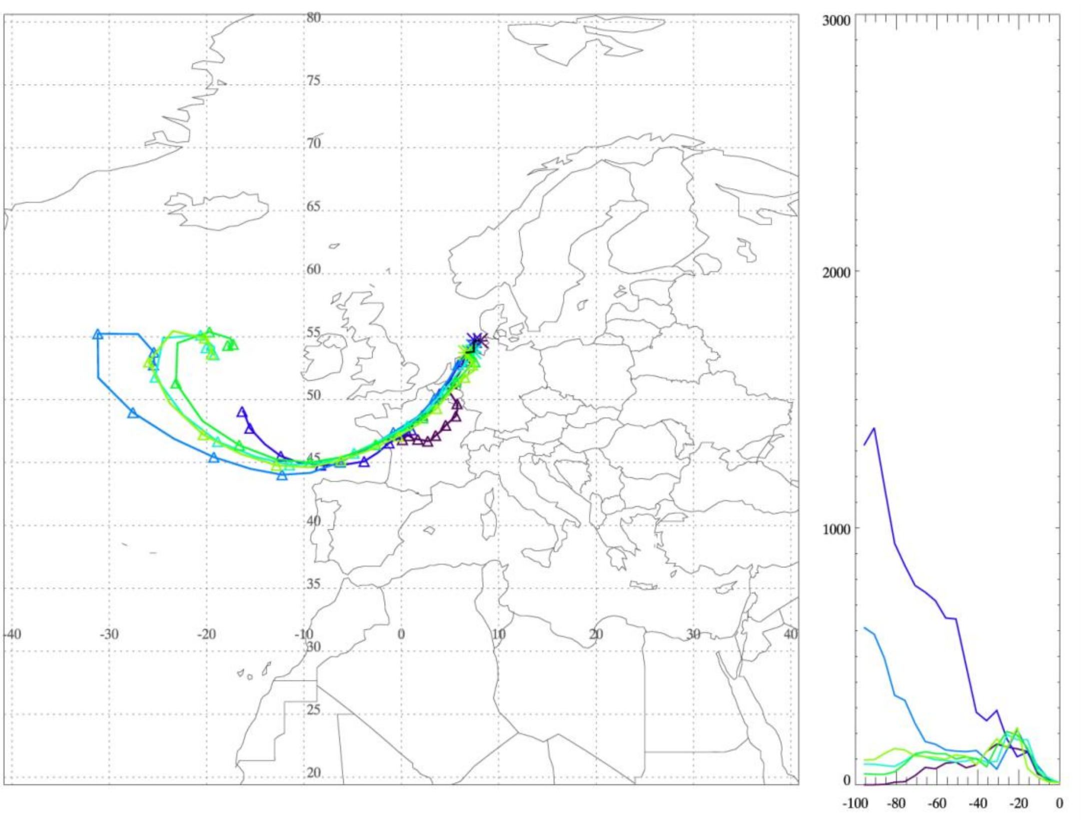
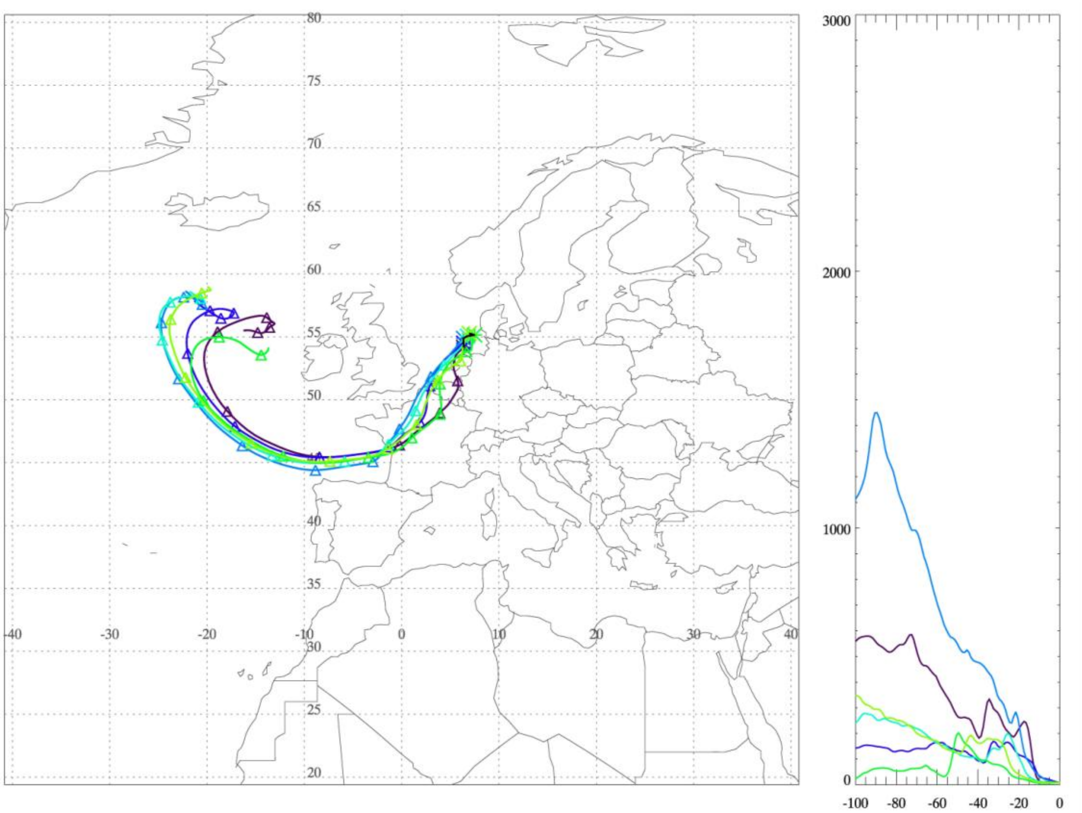


Fig. S2. (*Cont.*)

H331_A4



H331_A5

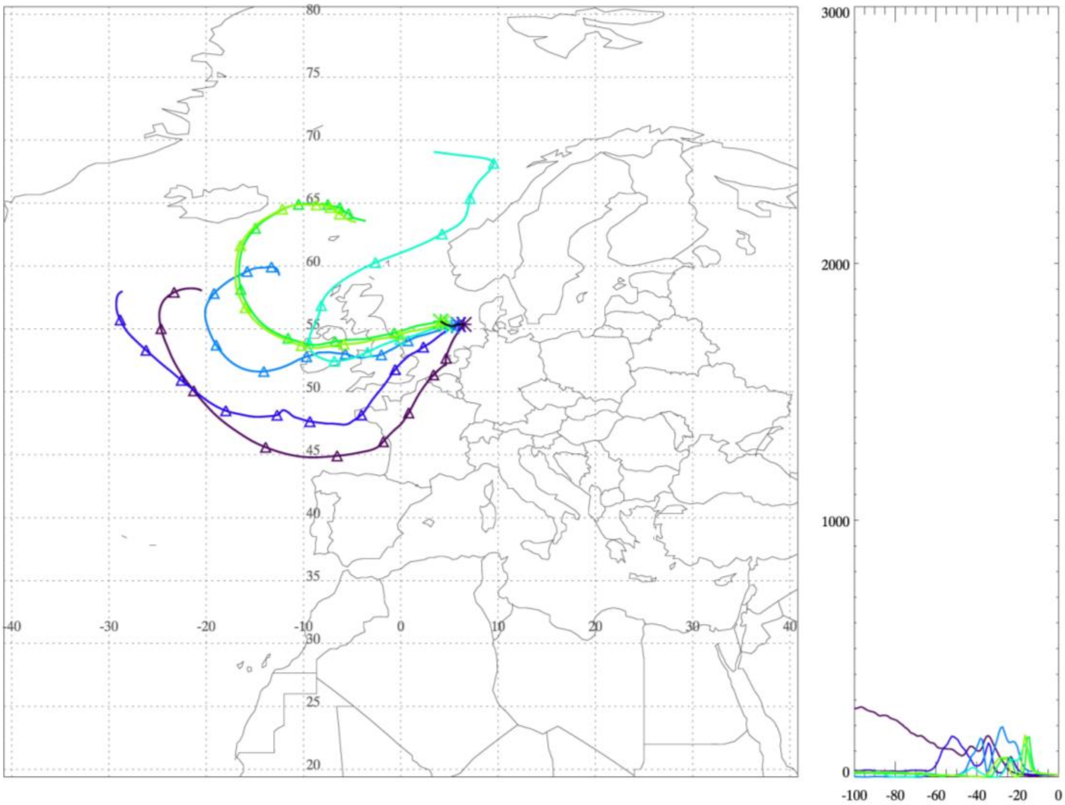
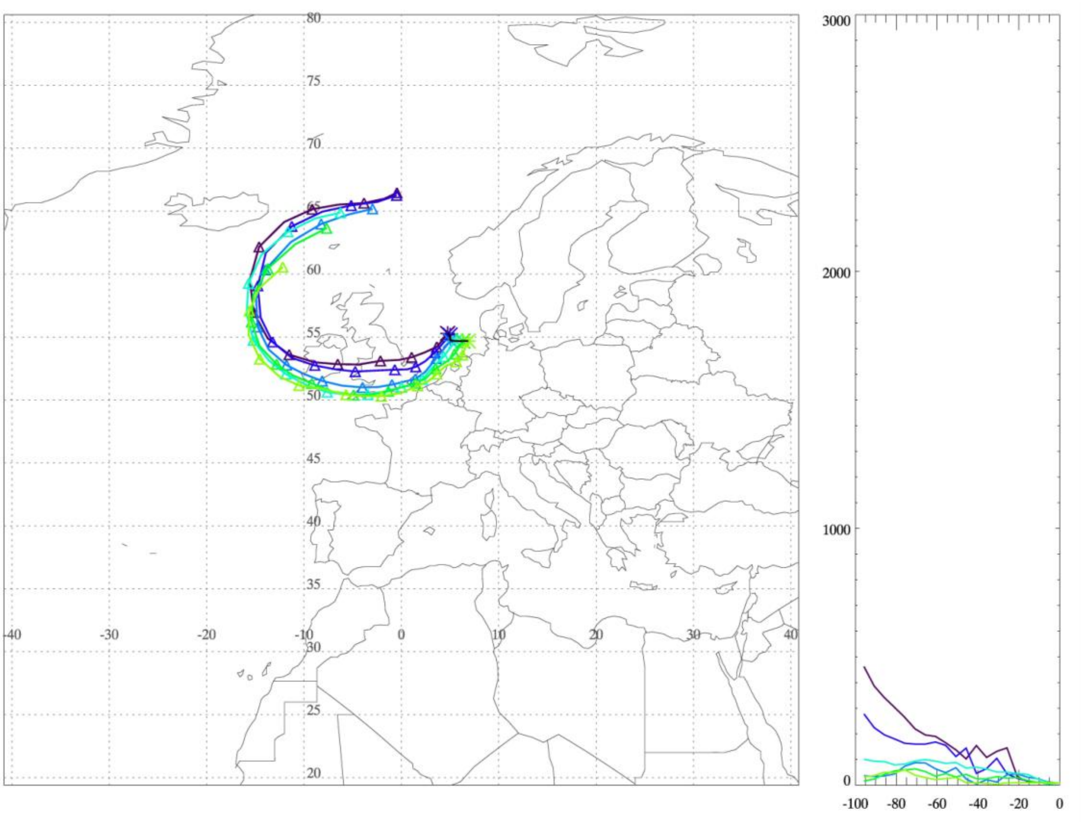


Fig. S2. (*Cont.*)

H331_A6



H331_A7

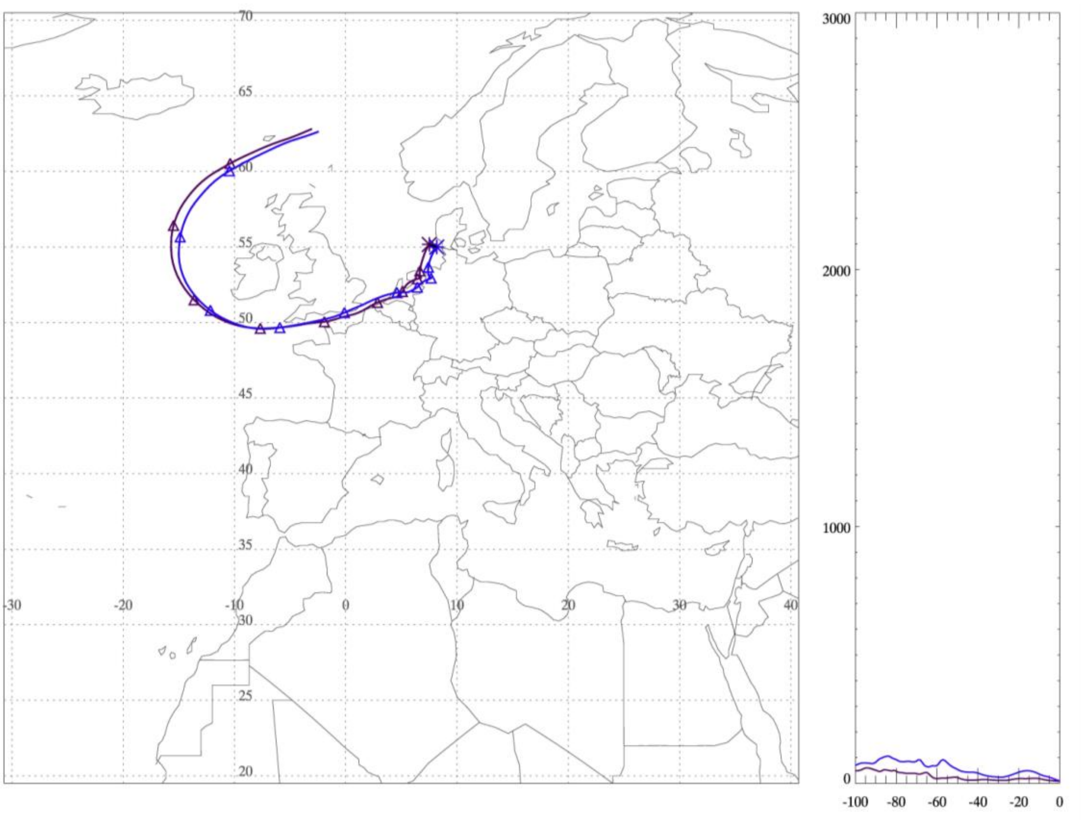


Fig. S2. (*Cont.*)

Calculation of the fugacity ratios, air–seawater gas exchange flux

Fugacity ratio (*FR*) f_a/f_w for the paired air and water samples (see Table S15) was calculated according to

$$FR = \frac{f_a}{f_w} = \frac{C_a \mathrm{R} T_a}{C_w H(t, sal)} \quad \text{(S1)}$$

where f_a and f_w are the fugacities in air and water, C_a and C_w are gaseous (pg m^{-3}) and dissolved concentration (pg L^{-1}), T_a is air temperature (K), R is universal gas constant (8.31 Pa m^3 K^{-1} mol^{-1}) and $H(T, sal)$ (Pa m^3 mol^{-1}) is the water temperature salinity-corrected. *FR*s > 1 were treated as net deposition and *FR*s < 1 as net volatilization. *FR*s = 1 indicated air-water equilibrium. Considering relations established for ~200 compounds investigated, the average slope of the temperature dependence line was found to correspond to an increase in Henry's law constants (HLCs) by a factor of 1.88 per 10°C rise in temperature.[3] So for dacthal, quintozene and pentachloroanisole, which only have HLCs in non-saline water at 298 K (see Table S17), we assumed HLC increase a factor of 1.88 per 10°C rise in temperature. HLCs in saline water as a function of temperature are only available for α-HCH, γ-HCH, α-endosulfan and chlorpyrifos.[2] Water temperature-corrected HLCs are available for HCB[1] and trifluralin.[3] For HCB, trifluralin, dacthal, quintozene and pentachloroanisole, the dimensionless Henry's Law constant was corrected by the salinity[10]:

$$H'_{salt,T} = H' \times 10^{\mathrm{K_S} C_S} \quad \text{(S2)}$$

$\mathrm{K_S}$ is the Setschenow constant (L mol^{-1}), which was calculated according to[11]:

$$\mathrm{K_S} = 0.04 \log K_{OW} + 0.114 \quad \text{(c)}$$

The error associated with the fugacity was propagated from the estimated relative standard deviations of the water and air concentrations (±20 %) and HLC (estimated to be ±30 % for α-HCH, γ-HCH, chlorpyrifos and α-endosulfan, ±50 % for HCB and trifluralin) and air temperature during sampling (±10 %) resulting in total *FR* uncertainties of ±36 % for α-HCH, γ-HCH, chlorpyrifos and α-endosulfan, ±42 % for HCB and trifluralin. Since HLCs temperature dependence line of dacthal quintozene and pentachloroanisole were unavailable, we assumed an uncertainty of a factor of at least three for the fugacity ratio.

The air–seawater gas exchange flux (F_{aw}, pg m^{-2} day^{-1}) was calculated based on the modified version of the Whitman two–film resistance model[12,13]:

$$F_{aw} = k_{ol} \left[C_w - \frac{C_a \mathrm{R} T_a}{C_w H(t, sal)} \right] \quad \text{(S4)}$$

where k_{ol} (m h^{-1}) is the air-water gas exchange mass transfer coefficient(MTC), compromising the resistances to mass transfer in both water (k_w, m h^{-1}) and air (k_a, m h^{-1}) and is defined by:

$$\frac{1}{k_{ol}} = \frac{1}{k_w} + \frac{\mathrm{R} T_a}{k_a H(t, sal)} \quad \text{(S5)}$$

where[14,15]:

$$k_a = (0.2U_{10} + 0.3) \times \left(\frac{D_{i,air}}{D_{H_2O,air}} \right)^{0.61} \times 36 \quad (S6)$$

$$k_w = (0.45U_{10}^{\ 1.64}) \times \left(\frac{Sc_1}{Sc_{CO_2}} \right)^{-0.5} \times 0.01 \quad (S7)$$

D_{air} is the diffusity in air, U_{10} is the wind speed at 10-m height above sea level (m s^{-1}), and *Sc* is the Schmidt number which was taken from Schwarzenbach et al.[10] for CO_2. D_{air} was calculated using the method described by Fuller et al.[15] and *Sc* for the pesticides was calculated using the method described by Hayduk and Laudi.[16] A positive F_{aw} value indicates a net flux from the water to the atmosphere. The overall uncertainty was calcultated to be ±57 % for α-HCH, γ-HCH, chlorpyrifos and α-endosulfan, 70% for HCB and trifluralin based on an uncertainty of 40 % for k_{ol}.[17,18] An uncertainty of at least ±500 % was estimated for dacthal, quintozene and pentachloraonisole, since the uncertainties of both HLC and k_{ol} for these compounds are not known.

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