Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts

Atmospheric deposition of persistent organic pollutants and chemicals of emerging concern at two sites in northern Sweden

Supplemental Information

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Table S1 - Instrument Detection Limits (IDLs) and Method Detection Limits (MDLs). NA indicates that the compound was not detected in the blanks and a MDL could not be established.

	IDL (pg on column)	MDL (pg per sample)
α-TBECH	0.91	NA
β-TBECH	0.91	NA
DPTE	0.29	NA
EHTBB	0.30	NA
BTBPE	0.38	64
HBB	0.39	773
DP *syn*	0.49	48
DP *anti*	0.26	40
trifluralin	0.32	NA
chlorothalonil	0.27	NA
PCB 28	0.19	142
PCB 52	0.31	285
PCB 101	0.23	278
PCB 118	0.52	52
PCB 138	0.23	195
PCB 153	0.20	262
α-HCH	0.25	98
γ-HCH	0.32	203
cis-chlordane	0.11	19
trans-chlordane	0.11	11
cis-nonachlor	0.32	NA
trans-nonachlor	0.25	17
heptachlor	0.18	NA
heptachlor-*exo*-epoxide	0.14	21
oxychlordane	0.73	99
BDE-47	Not determined	255
BDE-99	Not determined	206
BDE-100	Not determined	45
BDE-153	Not determined	319
BDE-154	Not determined	86

Table S2 - Masses and retention times for all compounds.

Compound	Mass 1	Mass 2	Retention Time
α-TBECH	264.9228	266.9208	17.38
β-TBECH	264.9228	266.9208	17.69
DPTE	329.7891	331.7870	28.84
EHTBB	420.6720	422.6699	34.28
BTBPE	356.8124	358.7928	39.07
$^{13}C_{12}$ BTBPE	362.8326	364.8129	39.05
HBB	549.5059	551.5039	29.32
$^{13}C_{6}$ HBB	555.5261	557.5240	29.31
DP *syn*	271.8102	273.8072	40.96
DP *anti*	271.8102	273.8072	41.75
trifluralin	264.1087	306.0702	10.33
d_{14} trifluralin	267.0420	315.1270	10.18
chlorothalonil	263.8816	265.8786	13.20
PCB 28	255.9613	257.9584	14.43
$^{13}C_{12}$ PCB 28	268.0016	269.9987	14.42
PCB 52	289.9224	291.9194	16.09
$^{13}C_{12}$ PCB 52	301.9627	303.9597	16.08
PCB 101	325.8804	327.8775	20.68
$^{13}C_{12}$ PCB 101	337.9207	339.9178	20.67
PCB 118	325.8804	327.8775	24.20
$^{13}C_{12}$ PCB 118	337.9207	339.9178	24.17
PCB 138	359.8415	361.8385	27.08
$^{13}C_{12}$ PCB 138	371.8818	373.8788	27.06
PCB 153	359.8415	361.8385	25.52
$^{13}C_{12}$ PCB 153	371.8818	373.8788	25.51
PCB 180	393.8025	395.7995	30.71
$^{13}C_{12}$ PCB 180	405.8428	407.8398	30.69
$^{13}C_{12}$ PCB 97	337.9207	339.9178	21.82
$^{13}C_{12}$ PCB 188	405.8428	407.8398	25.06
α-HCH	180.9379	182.9349	10.72
γ -HCH	180.9379	182.9349	11.96
$^{13}C_{6}$ lindane	186.9580	188.9550	11.95
cis-chlordane	372.8260	374.8230	20.92
trans-chlordane	372.8260	374.8230	20.08
cis-nonachlor	406.7870	408.7840	24.72
trans-nonachlor	406.7870	408.7840	21.21

$^{13}C_{10}$ *trans*-nonachlor	416.8206	418.8176	21.19
heptachlor	271.8102	273.8072	15.06
heptachlor-*exo*-epoxide	352.8442	354.8413	18.79
$^{13}C_{10}$ heptachlor-*exo*-epoxide	362.8778	364.8749	18.76
oxychlordane	386.8052	388.8023	18.85
BDE-47	483.7132	485.7113	15.62
$^{13}C_{12}$ BDE-47	495.7357	497.7513	15.62
BDE-99	403.7870	405.7850	17.60
$^{13}C_{12}$ BDE-99	415.8273	417.8429	17.60
BDE-100	403.7870	405.7850	17.16
$^{13}C_{12}$ BDE-100	415.8273	417.8429	17.16

Table S3a – Bulk deposition of compounds at the Abisko site in ng per sample, integrated over each two-month period. ND indicates that the compound was either not detected on the chromatogram or fell below the MDL/IDL before blank correction.

	2009 Oct-Nov	2010 Dec-Jan	2010 Feb-Mar	2010 Apr-May	2010 June-July	2010 Aug-Sept	2010 Oct-Nov
α-TBECH	ND	ND	ND	0.27	0.54	0.17	0.09
β-TBECH	ND	ND	ND	0.23	0.54	ND	0.09
DP *syn*	0.39	0.26	3.6	0.56	1.7	0.44	4.9
DP *anti*	0.22	0.087	1.0	0.26	0.54	0.10	0.84
trifluralin	0.23	ND	ND	0.061	ND	0.030	0.04
chlorothalonil	0.11	0.040	ND	ND	ND	0.044	ND
PCB 28	15	3.4	2.5	5.7	14	6.2	3.3
PCB 52	3.3	1.7	1.1	5.2	26	5.5	2.6
PCB 101	1.3	0.94	0.67	1.8	8.1	1.6	0.92
PCB 118	0.35	0.18	0.19	0.42	1.2	0.29	0.16
PCB 138	1.1	0.50	0.58	0.55	1.9	0.54	0.33
PCB 153	1.9	0.73	0.93	0.79	3.0	0.84	0.47
α-HCH	1.6	0.72	0.28	2.4	6.9	2.1	1.0
γ-HCH	4.3	2.2	1.1	11	41	9.1	6.1
cis-chlordane	0.063	0.058	0.032	0.030	0.18	0.041	0.02
trans-chlordane	0.050	0.051	0.044	0.042	0.23	0.052	0.03
cis-nonachlor	ND	ND	ND	ND	ND	ND	ND
trans-nonachlor	0.055	ND	ND	0.032	ND	0.037	ND
heptachlor	0.038	ND	ND	0.068	0.38	0.13	0.06
heptachlor-*exo*-epoxide	0.076	0.053	0.030	0.061	ND	0.044	ND
BDE-47	0.57	0.24	0.64	0.32	0.69	0.39	0.31
BDE-99	ND	ND	0.25	ND	0.30	0.16	0.33
BDE-100	ND	ND	0.14	ND	0.073	0.10	0.097

Table S3b – Bulk deposition of compounds at the Krycklan site in ng per sample, integrated over each two-month period. ND indicates that the compound was either not detected on the chromatogram or fell below the MDL/IDL before blank correction.

	2009 Oct-Nov	2010 Dec-Jan	2010 Feb-Mar	2010 April-May	2010 June-July	2010 Aug-Sept
α-TBECH	0.032	0.19	0.50	x	0.26	ND
β-TBECH	ND	0.16	0.28	x	0.22	ND
DP *syn*	ND	0.090	0.034	x	0.041	ND
DP *anti*	ND	0.067	0.13	x	0.078	ND
trifluralin	0.38	0.10	0.063	x	0.079	0.071
chlorothalonil	ND	ND	ND	x	0.037	ND
PCB 28	0.53	5.7	9.3	x	5.4	0.66
PCB 52	0.27	1.6	2.2	x	1.4	0.56
PCB 101	0.57	1.3	1.4	x	1.5	0.70
PCB 118	0.12	0.21	0.22	x	0.20	0.067
PCB 138	0.35	0.57	0.65	x	0.61	0.26
PCB 153	0.49	0.72	0.87	x	0.92	0.39
α-HCH	0.25	0.20	0.074	x	0.31	0.10
γ-HCH	0.57	1.5	0.97	x	2.4	0.30
cis-chlordane	0.044	0.027	0.044	x	0.029	ND
trans-chlordane	0.054	ND	0.029	x	0.023	0.011
cis-nonachlor	ND	0.008	0.008	x	ND	ND
trans-nonachlor	0.036	0.039	0.045	x	0.027	ND
heptachlor	ND	0.032	0.039	x	0.025	ND
heptachlor-*exo*-epoxide	0.16	0.057	0.082	x	0.085	0.031
BDE-47	1.8	3.2	1.1	x	1.4	0.96
BDE-99	ND	0.46	ND	x	ND	ND
BDE-100	ND	0.59	ND	x	ND	ND

Table S4 - Temperature and precipitation data for the Abisko and Krycklan sites.

	2009	2009-10	2010	2010	2010	2010	2010
	Oct. - Nov.	Dec. - Jan.	Feb. - Mar.	Apr. - May	June - July	Aug. - Sept.	Oct. – Nov.
Abisko mean temperature, ^{o}C	-2.5	-10.8	-11.5	1.8	9.1	7.6	-2.7
Abisko total precipitation (mm)	23	11	29	40	96	43	32
Krycklan mean temperature, ^{o}C	-0.2	-10.8	-9.7	5.4	13.8	9.9	
Krycklan total precipitation (mm)	111	88	95	61	168	146	

Details for calculating MDLs

With two independent measurements of blanks, the probability that a sample value (Y) is greater than the geometric mean of the two blank values (X) by a factor of k can be calculated in the following way:

$$Prob(Y/X > k) = Prob(Z > \ln(k) / sqrt(3log(cv^2+1)/2)$$

where Z is a standard normal random variable and cv is the coefficient of variance. Using 1.645 for Z (to correspond to a 95% probability) and a CV of 1, k was calculated to be 5.351. This was multiplied by the geometric mean of the two blank levels to set the method detection limits. For compounds not found in the blank, a positive response was judged to be a peak with signal-to-noise ratio >3:1 (>IDL).

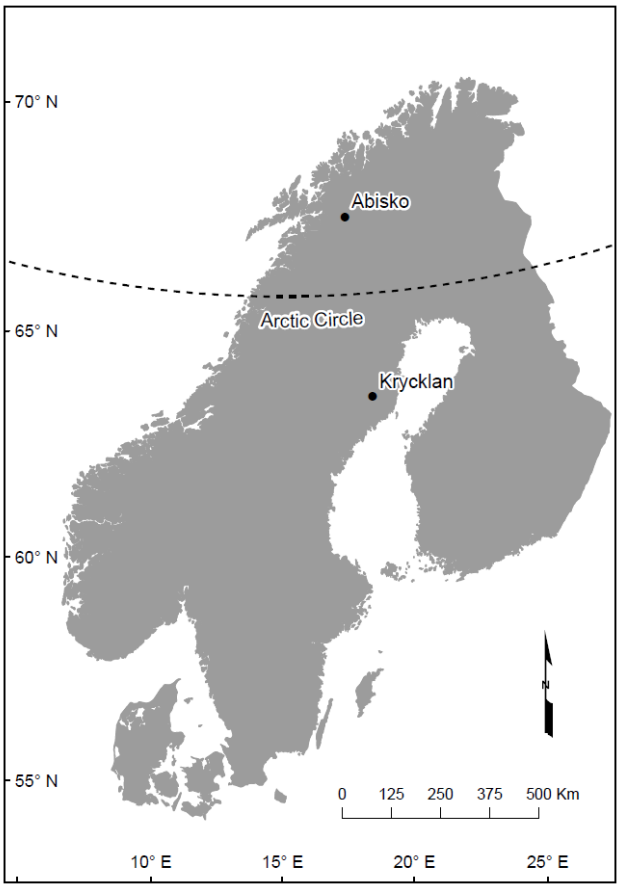

Figure S1 - Location of the two sampling sites

Figure S2 - A picture of the sampling sites Abisko (top) and Krycklan (bottom)

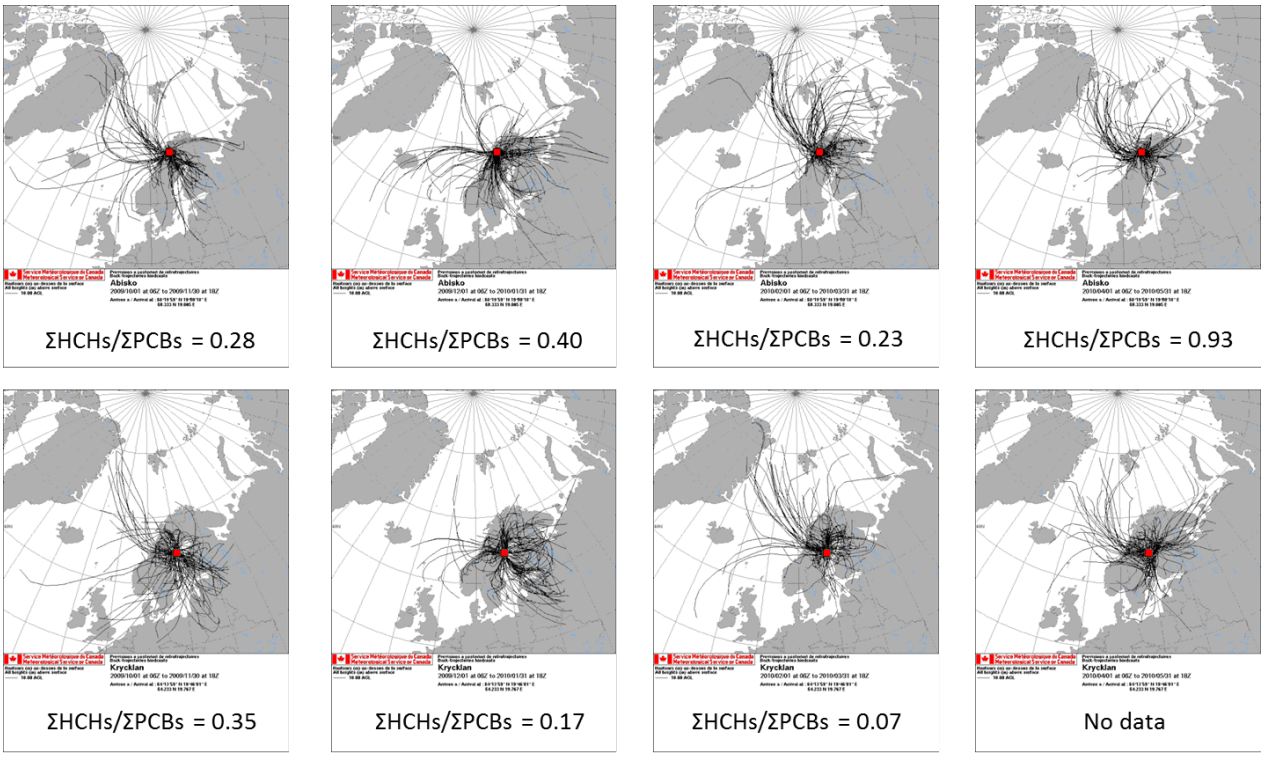

Figure S3a - Air parcel back trajectories at 10 m above ground level, computed 72 h backward from Abisko (top) and Krycklan (bottom). Trajectories were run at 0000, 0600, 1200 and 1800 UTC. The combined trajectories at 0600 and 1800 for two-month sampling periods are displayed, with ratios of ΣHCHs/ΣPCBs in deposition.

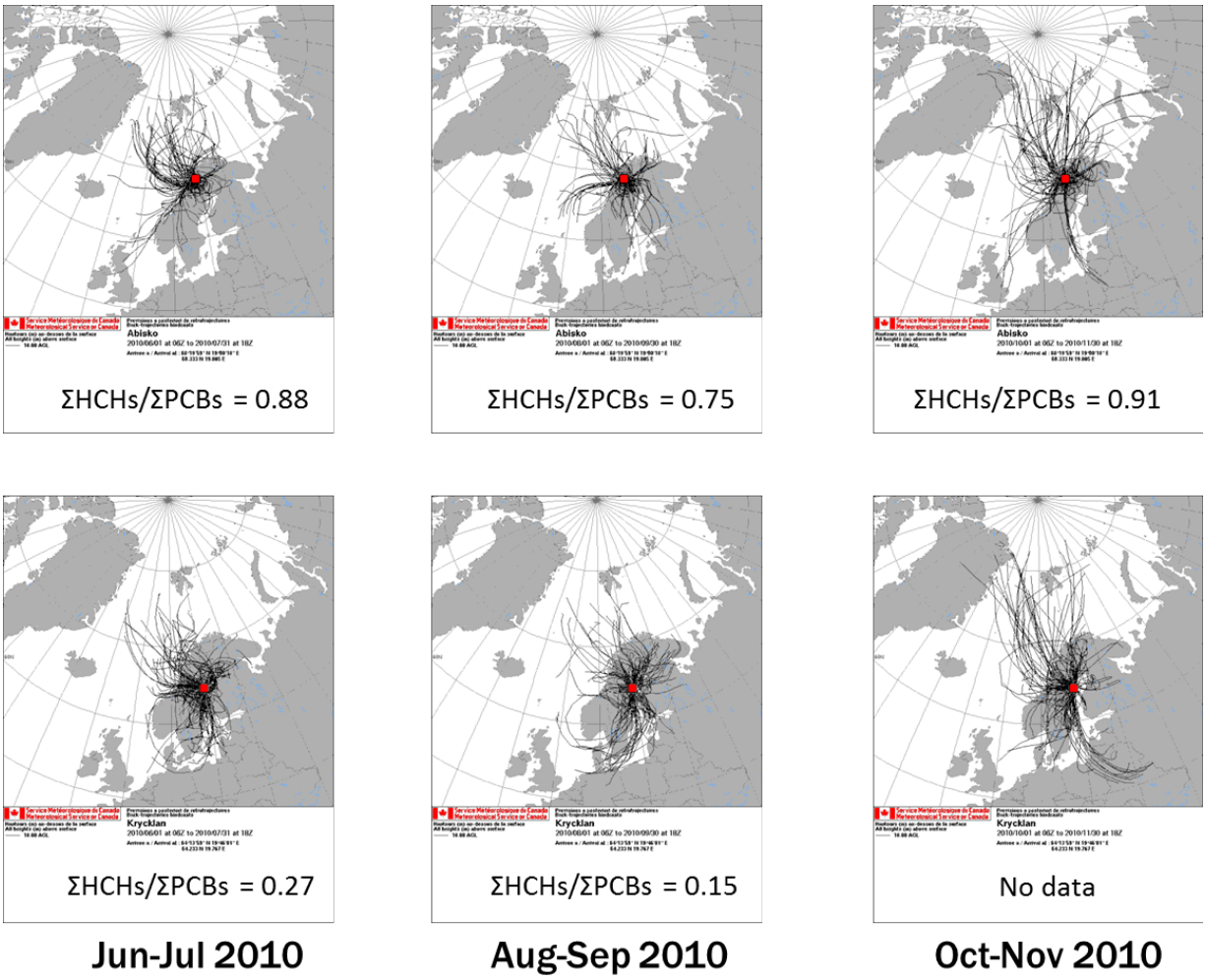

Figure S3b - Air parcel back trajectories, as in Figure S1A.