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

Electronic Supplementary Information (ESI)

Evaluating the PAS-SIM Model Using a Passive Air Sampler Calibration Study for Pesticides

ANDRÉS RAMÍREZ RESTREPO[1,2], STEPHEN J. HAYWARD[1,3], JAMES M. ARMITAGE[1*], FRANK WANIA[1]

[1]*Department of Physical and Environmental Sciences, University of Toronto Scarborough, 1265 Military Trail, Toronto, Ontario, Canada, M1C 1A4,* [2]*Grupo GDCON, Facultad de Ingeniería, Sede de Investigaciones Universitarias (SIU), Universidad de Antioquia, Calle 70 No 52 -21, Medellín, Colombia,* [3]*Department of Chemical Engineering and Applied Chemistry, University of Toronto, 200 College St W, Toronto, Ontario, Canada, M5S 3E5*

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S1: Sample extraction and quantification

The LV-AAS and XAD-PAS samples were analyzed by gas chromatography (Agilent 6890 GC) using an Agilent 5973 mass-selective (MS) detector in both negative chemical ionization (NCI) mode and electron ionization (EI) mode and a DB-5MS column (J&W Scientific; 60 m x 0.25 mm i.d., 0.10 µm film thickness). NCI mode was employed for analyzing chlorthalonil, endosulfan, DCPA (Dimethyl tetrachloroterephthalate, Dacthal), trifluralin, pendimethalin, hexachlorobenzene (HCB), α- and γ-hexachlorocyclohexane (HCH), trans- and cis-chlordane, and trans-nonachlor; EI mode was used for analyzing disulfoton, atrazine, alachlor, and metolachlor.[1, 2] The GC temperature program was based on Gouin et al.[3]: 90 ºC for 1 min, 15 ºC min^{-1} to 240 ºC, 6 ºC min^{-1} to 270 ºC, then 25 ºC min^{-1} to 290 ºC and held for 6 min. The inlet, transfer line, ion source, and quadrupole temperatures were 265, 250, 150, and 106 ºC, respectively. The detector was operated in selective ion monitoring (SIM) mode to enhance sensitivity. SIM ions used to quantify target pesticides include the following: hexachlorobenzene (284, 286), trifluralin (335, 336), DCPA (332, 330), HCHs (255, 257), chlorthalonil (266, 264), trans- and cis chlordane (410, 412), trans-nonachlor (444, 446), pendimethalin (281, 282), endosulfan I and II (406, 404), and endosulfan sulfate (386, 388).[3]

Quality assurance protocols for the extraction of XAD-PAS samples have been previously established[4] and were followed during these extractions. All LV-AAS and XAD-PAS samples were spiked with 10 µL of 100 $\mu g \cdot L^{-1}$ each of d^{14}-trifluralin and d^{10}-chlorpyrifos, extracted in a Soxhlet apparatus for 24 hours using dichloromethane, followed by rotoevaporation, solvent exchange into iso-octane, and final nitrogen blow-down to a volume of 1mL. Mirex (10 µL of 10 $ng \cdot \mu L^{-1}$) was added as an internal standard to all samples prior to analysis. Method recoveries of the two spiked compounds in the LV-AAS samples ranged from 95–115% and therefore these data were not recovery corrected.[2] Method recoveries of the two spiked compounds in the XAD-PAS ranged from 58-127% (average = 90%, median = 90%) (see ESI Table S2 below). Due to the wider variation in recoveries, the amounts of pesticides detected were thus corrected for recovery using the average recovery for d^{14}-trifluralin and d^{10}-chlorpyrifos (see ESI Table S2 and S3 below). Laboratory blanks (n = 8) and field blanks (n = 3 for XAD-PAS, n = 8 for LV-AAS) were consistently below the limit of quantitation (LOQ) of 2.5 $pg \cdot \mu L^{-1}$ (NCI mode) and 9.8 $pg \cdot \mu L^{-1}$ (EI mode), where the LOQ was defined as five times the instrument detection limit (IDL), the amount at which the signal-to-noise ratio equals 3.[1]

S2: Table S1. Solute Descriptors and chemical property values used for the PAS-SIM modeling[5-11]

Compound	CAS	MW	ρ (g/mL)	MV	log K_{SA}	ΔU_{SA} J mol^{-1}	log K_{QA}	ΔU_{QA} J mol^{-1}	E	S	A	B	L	V
Alachlor	15972-60-8	269.8	1.133	238.1	8.09	-45168	8.40	-89777	1.170	1.190	0.050	1.170	8.410	2.140
Atrazine	1912-24-9	215.7	1.230	175.4	7.64	-45666	7.93	-106327	1.220	1.290	0.170	1.010	7.783	1.620
cis-Chlordane	5103-71-9	409.8	1.610	254.5	7.98	-42779	8.58	-92885	2.100	1.470	0.000	0.450	8.730	2.194
trans-Chlordane	5103-71-9	409.8	1.610	254.5	8.29	-43773	8.55	-92885	2.060	1.250	0.000	0.530	9.110	2.194
Chlorthalonil	1897-45-6	265.9	1.800	147.7	7.17	-36268	7.17	-103732	1.640	2.100	-0.290	0.480	7.646	1.515
DCPA	1861-32-1	332.0	1.700	195.3	8.14	-44416	8.61	-99849	**1.245**	**1.737**	**0.000**	**0.614**	8.540	1.918
Disulfoton	298-04-4	274.4	1.144	239.9	7.69	-43042	7.14	-84090	**1.247**	**0.738**	**0.000**	**0.902**	7.960	2.048
Endosulfan I	959-98-8	406.9	1.745	233.2	7.80	-42067	7.91	-108287	2.230	0.980	0.000	0.870	8.563	2.148
Endosulfan II	33213-65-9	406.9	1.745	233.2	8.79	-50444	9.86	-108287	2.440	0.950	0.350	1.200	9.734	2.148
Endosulfan SO_4	1031-07-8	423.0	1.940	218.0	9.08	-46544	10.67	-145564	**1.785**	**2.211**	**0.000**	**1.232**	10.000	2.206
HCB	118-74-1	284.8	2.044	139.3	7.16	-41105	6.16	-86718	1.490	0.990	0.000	0.000	7.390	1.451
α-HCH	319-84-6	290.8	1.870	155.5	7.12	-41030	6.18	-87043	1.450	0.730	0.000	0.710	7.317	1.580
γ-HCH	58-89-9	290.8	1.850	157.2	7.23	-41384	6.51	-88228	1.450	0.910	0.000	0.680	7.467	1.580
Metolachlor	51218-45-2	283.8	1.120	253.4	8.46	-46636	8.73	-88418	1.150	1.010	0.070	1.380	8.863	2.281
trans-Nonachlor	39765-80-5	444.2	1.860	238.8	9.26	-46555	9.70	-101585	**2.210**	**1.451**	**0.002**	**0.516**	**10.428**	**2.250**
Pendimethalin	40487-42-1	281.3	1.190	236.4	8.42	-45828	9.06	-91356	**1.423**	**1.594**	**0.050**	**0.570**	8.950	2.151
Trifluralin	1582-09-8	335.3	1.294	259.1	7.34	-40605	6.45	-85288	1.060	0.400	-0.100	1.350	7.475	2.264

where MW is molecular weight (g/mol), ρ is density, MV is molar volume (cm^3/mol), K_{SA} is the sampler-air partition coefficient, ΔU_{SA} is the internal energy of phase change (for sampler-air partitioning), K_{QA} is the aerosol-air partition coefficient, ΔU_{QA} is the internal energy of phase change (for aerosol-air partitioning) and E, S, A, B, L and V are the solute descriptors required for the ppLFER calculations, as discussed in Hayward et al.[10] The solute descriptors in **bold** text were estimated using ABSOLV ACD/ADME Suite v. 5.0.8

S3: Step-by-step derivation of NRE

The residual is a term used in analytical chemistry to describe the absolute error between an expected and a reference value.

$$Residual = x - \mu \tag{A}$$

At certain values, the residual value becomes a standard deviation (σ).

$$\sigma = x_{\sigma} - \mu \tag{B}$$

For the PAS-SIM model, the air-side boundary layer thickness upon which the calculations are based have three different values (see Methods). Using a 10 mm layer as a reference and 7.5 mm and 15 mm as dispersion values may be a reasonable first approximation for a mean value (μ) and the values that give σ (x_{σ}). We may then write:

$$\sigma_{+} = m_{SIM_{7.5}} - m_{SIM_{10}} \tag{C}$$

$$\sigma_{-} = m_{SIM_{10}} - m_{SIM_{15}} \tag{D}$$

$$\sigma = \frac{\sigma_{+} + \sigma_{-}}{2} = \frac{m_{SIM_{7.5}} - m_{SIM_{10}} + m_{SIM_{10}} - m_{SIM_{15}}}{2} = \frac{m_{SIM_{7.5}} - m_{SIM_{15}}}{2} \tag{E}$$

where m_{SIM_x} is the mass predicted by the PAS-SIM model with x being the layer thickness (7.5, 10 or 15 mm). With an estimate of the magnitude of the standard deviation we can normalize the residual obtained when comparing the model and the experimental results:

$$NRE = \frac{x - \mu}{\sigma} = \frac{2\left(m_{PAS} - m_{SIM_{10}}\right)}{m_{SIM_{7.5}} - m_{SIM_{15}}} \tag{F}$$

This normalized residual error (NRE) can be used at any point to define the agreement between the model output and the experimental values. Even if just a point exceeds the proposed acceptable deviation of ±2σ given by the 7.5 mm and 15 mm layers, the agreement may be put in doubt. That's why endosulfan II was considered to have systematic bias even with an average NRE of 1.96. For the same reason, it is possible to describe pendimethalin and trifluralin as cases where no agreement exists between model output and the empirical XAD-PAS data. The average

NRE of all the points just reflects the general behavior and gives an indication of the performance but the point-by-point NRE is the ultimate criterion of agreement.

S4: Table S2. Amounts of pesticides detected in XAD-PAS samplers from CARE (Egbert, Ontario) deployed in March 2006 (N.D. not detected)

Compound	**Sampler amounts (ng per sampler)**									
	April 27 2006		**June 30 2006**		**September 1 2006**		**October 27 2006**		**February 27 2007**	
Alachlor	N.D.	N.D.	21.97	16.59	25.89	24.91	36.03	25.43	38.18	38.43
Atrazine	N.D.	N.D.	43.04	35.18	39.19	33.29	52.82	35.48	54.03	53.79
cis-Chlordane	N.D.	N.D.	0.34	0.22	0.49	0.36	0.84	0.47	1.08	0.92
trans-Chlordane	N.D.	N.D.	0.38	0.25	0.43	0.37	0.73	0.42	0.94	0.89
Chlorthalonil	6.81	6.93	73.51	68.99	264.15	243.90	342.56	249.68	364.66	369.74
DCPA	0.28	0.06	1.45	1.00	1.82	0.53	1.99	1.22	2.25	2.19
Disulfoton	N.D.	N.D.	3.66	1.91	3.46	2.09	5.00	2.49	4.93	4.18
Endosulfan I	0.16	0.09	5.28	4.50	8.59	8.21	12.20	8.47	12.86	12.72
Endosulfan II	N.D.	N.D.	1.54	0.95	2.48	1.10	2.42	2.11	3.10	2.70
Endosulfan sulfate	N.D.	N.D.	0.60	0.17	0.52	0.16	0.67	0.20	0.66	0.45
HCB	1.30	1.13	4.31	3.61	3.68	2.93	4.79	3.01	6.35	6.24
α-HCH	0.58	0.32	3.14	2.55	2.31	2.19	3.73	2.55	4.33	4.44
γ-HCH	0.25	0.09	1.92	1.19	1.97	1.72	2.56	1.97	2.60	2.25
Metolachlor	N.D.	N.D.	25.40	27.33	32.71	34.58	48.97	32.45	50.36	51.65
trans-Nonachlor	N.D.	N.D.	0.38	0.21	0.34	0.17	0.57	0.30	0.66	0.62
Pendimethalin	2.56	2.34	7.03	5.77	3.28	2.52	2.27	1.08	2.03	1.63
Trifluralin	2.26	1.97	4.96	3.87	2.66	1.48	2.86	1.46	2.70	2.24
Recovery of labeled spike compounds (%)										
d^{14}-Trifluralin	85%	102%	127%	124%	58%	80%	90%	68%	91%	102%
d^{10}-Chloropyrifos	95%	95%	119%	116%	63%	73%	78%	62%	80%	91%
Average % recovery	90%	99%	123%	120%	61%	77%	84%	65%	86%	97%

S5: Table S3. Amounts of pesticides detected in XAD-PAS samplers from CARE (Egbert, Ontario) corrected for recovery of spiked compounds (N.D. not detected)

Compound	Sampler amounts (ng per sampler)									
	April 27 2006		June 30 2006		September 1 2006		October 27 2006		February 27 2007	
Alachlor	N.D.	N.D.	17.86	13.83	42.44	32.35	42.89	39.12	44.40	39.62
Atrazine	N.D.	N.D.	34.99	29.32	64.25	43.23	62.88	54.58	62.83	55.45
cis-Chlordane	N.D.	N.D.	0.28	0.18	0.80	0.47	1.00	0.72	1.26	0.95
trans-Chlordane	N.D.	N.D.	0.31	0.21	0.70	0.48	0.87	0.65	1.09	0.92
Chlorthalonil	7.57	7.00	59.76	57.49	433.03	316.75	407.81	384.12	424.02	381.18
DCPA	0.31	0.06	1.18	0.83	2.98	0.69	2.37	1.88	2.62	2.26
Disulfoton	N.D.	N.D.	2.98	1.59	5.67	2.71	5.95	3.83	5.73	4.31
Endosulfan I	0.18	0.09	4.29	3.75	14.08	10.66	14.52	13.03	14.95	13.11
Endosulfan II	N.D.	N.D.	1.25	0.79	4.07	1.43	2.88	3.25	3.60	2.78
Endosulfan sulfate	N.D.	N.D.	0.49	0.14	0.85	0.21	0.80	0.31	0.77	0.46
HCB	1.44	1.14	3.50	3.01	6.03	3.81	5.70	4.63	7.38	6.43
α-HCH	0.64	0.32	2.55	2.13	3.79	2.84	4.44	3.92	5.03	4.58
γ-HCH	0.28	0.09	1.56	0.99	3.23	2.23	3.05	3.03	3.02	2.32
Metolachlor	N.D.	N.D.	20.65	22.78	53.62	44.91	58.30	49.92	58.56	53.25
trans-Nonachlor	N.D.	N.D.	0.31	0.18	0.56	0.22	0.68	0.46	0.77	0.64
Pendimethalin	2.84	2.36	5.72	4.81	5.38	3.27	2.70	1.66	2.36	1.68
Trifluralin	2.51	1.99	4.03	3.23	4.36	1.92	3.40	2.25	3.14	2.31

S6: Table S4. Average amounts of pesticides detected in XAD-PAS at CARE (Egbert, Ontario), corrected for recovery of spiked compounds (N.D. not detected)

Compound	**Sampler amount (ng per sampler ± range)**				
	April 27/06	**June 30/06**	**Sep 1/06**	**Oct 27/06**	**Feb 27/07**
Alachlor	N.D.	15.8 ± 2.02	37.7 ± 5.1	41.0 ± 1.9	42.2 ± 2.4
Atrazine	N.D.	32.2 ± 2.84	54.2 ± 5.2	58.7 ± 4.2	59.5 ± 3.7
cis-Chlordane	N.D.	0.23 ± 0.04	0.64 ± 0.17	0.86 ± 0.14	1.11 ± 0.15
trans-Chlordane	N.D.	0.26 ± 0.05	0.59 ± 0.12	0.76 ± 0.11	1.01 ± 0.09
Chlorthalonil	7.30 ± 0.27	58.6 ± 2.1	378 ± 48	396 ± 22	405 ± 28
DCPA	0.19 ± 0.13	1.01 ± 0.17	1.85 ± 1.2	2.12 ± 0.25	2.45 ± 0.18
Disulfoton	N.D.	2.28 ± 0.69	4.22 ± 1.5	4.89 ± 1.1	5.04 ± 0.72
Endosulfan I	0.13 ± 0.04	4.02 ± 0.27	12.5 ± 1.7	13.8 ± 0.75	14.1 ± 0.93
Endosulfan II	N.D.	1.02 ± 0.23	2.77 ± 1.3	3.06 ± 0.18	3.21 ± 0.41
Endosulfan sulfate	N.D.	0.32 ± 0.17	0.54 ± 0.33	0.55 ± 0.25	0.62 ± 0.15
HCB	1.30 ± 0.15	3.26 ± 0.25	4.96 ± 1.1	5.17 ± 0.53	6.94 ± 0.48
α-HCH	0.49 ± 0.16	2.34 ± 0.21	3.34 ± 0.47	4.18 ± 0.26	4.83 ± 0.23
γ-HCH	0.18 ± 0.10	1.28 ± 0.28	2.75 ± 0.50	3.04 ± 0.01	2.69 ± 0.35
Metolachlor	N.D.	21.7 ± 1.06	49.6 ± 4.4	54.1 ± 4.2	56.2 ± 2.7
trans-Nonachlor	N.D.	0.24 ± 0.07	0.39 ± 0.17	0.57 ± 0.11	0.70 ± 0.07
Pendimethalin	2.61 ± 0.23	5.26 ± 0.45	4.36 ± 1.1	2.18 ± 0.52	2.03 ± 0.34
Trifluralin	2.25 ± 0.26	3.63 ± 0.40	3.17 ± 1.2	2.83 ± 0.57	2.74 ± 0.42

S7: Table S5. Calibrated PSR_E for XAD-PAS using Method 1[a]

Compound	**Passive Sampler Rate ($m^3\ d^{-1}$)**					
	Deployment period from March 1, 2006 to					**Average**
	April 27, 2006	**June 30, 2006**	**Sep 1, 2006**	**Oct 27, 2006**	**Feb 27, 2007**	
Alachlor	-	0.75	0.66	0.65	0.58	0.66 ± 0.07
Atrazine	-	0.79	0.73	0.72	0.63	0.72 ± 0.06
cis-Chlordane	-	0.54	0.52	0.44	0.41	0.48 ± 0.06
trans-Chlordane	-	0.53	0.58	0.58	0.53	0.56 ± 0.03
Chlorthalonil	1.83	2.54	2.45	2.42	2.09	2.27 ± 0.30
DCPA	-	0.57	0.52	0.42	0.37	0.47 ± 0.09
Disulfoton	-	0.67	0.75	0.69	0.62	0.68 ± 0.05
Endosulfan I	0.88	1.03	0.91	0.88	0.77	0.89 ± 0.09
Endosulfan II	-	0.72	0.71	0.67	0.59	0.67 ± 0.06
Endosulfan sulfate	-	0.31	0.31	0.32	0.3	0.31 ± 0.01
HCB	0.75	0.99	0.96	0.92	0.78	0.88 ± 0.10
α-HCH	1.06	1.42	1.22	1.09	0.95	1.15 ± 0.18
γ-HCH	0.74	1.17	1.01	0.9	0.85	0.93 ± 0.16
Metolachlor	-	0.77	0.76	0.74	0.67	0.74 ± 0.04
trans-Nonachlor	-	0.46	0.46	0.43	0.38	0.43 ± 0.04
Pendimethalin	-	1.15	*-0.63*	*-0.32*	*-0.26*	0.95 ± 0.34[b]
Trifluralin	1.13	0.56	*-0.35*	*-0.28*	*-0.22*	
					Overall Average:	0.80 ± 0.47[c]

[a] Using cumulative amount detected in XAD-PAS and cumulative average air concentration in LV-AAS. A full description can be found in the manuscript text.

[b] Sampling rate is determined from April and June values for both trifluralin and pendimethalin. Numbers in brackets are not used to calculate this average due to losses of these compounds from the XAD-PAS.

[c] Calculated from all sampling rates for all chemicals in all sampling periods.

S8: Table S6. Calibrated PSR_{E} determined as the slope of the regression of a plot of the amount of pesticide (ng/sampler) sequestered in an XAD-PAS against $C_{\mathrm{LV\text{-}AAS}}$ x t (Method 2)

Compound	**$\mathrm{PSR_E}$ ($\mathrm{m^3\ d^{-1}}$)**	**r^2**
Alachlor	0.63 ± 0.02	0.945
Atrazine	0.70 ± 0.03	0.856
cis-Chlordane	0.43 ± 0.02	0.964
trans-Chlordane	0.55 ± 0.01	0.944
Chlorthalonil	2.29 ± 0.09	0.989
DCPA	0.42 ± 0.03	0.814
Disulfoton	0.67 ± 0.03	0.871
Endosulfan I	0.84 ± 0.04	0.982
Endosulfan II	0.65 ± 0.03	0.903
Endosulfan sulfate	0.31 ± 0.01	0.898
HCB	0.86 ± 0.04	0.945
α-HCH	1.06 ± 0.07	0.929
γ-HCH	0.91 ± 0.04	0.985
Metolachlor	0.72 ± 0.02	0.913
trans-Nonachlor	0.41 ± 0.02	0.908
Pendimethalin	not calculated	
Trifluralin	not calculated	
Overall Average:	0.75 ± 0.46	

S9: Table S7. Calibrated PSR_E for XAD-PAS using Method 3[a]

Compound	Passive Sampler Rate (m^3 d^{-1})						S/W
	Deployment period[b] from March 1, 2006 to					Average	
	April 27, 2006	June 30, 2006	Sep 1, 2006	Oct 27, 2006	Feb 27, 2007		
Alachlor	-	0.71	0.60	0.53	-	0.61 ± 0.09	1.25
Atrazine	-	0.75	0.66	0.56	-	0.66 ± 0.10	1.26
cis-Chlordane	-	0.52	0.5	0.32	0.35	0.42 ± 0.10	1.52
trans-Chlordane	-	0.50	0.63	0.54	0.48	0.54 ± 0.07	1.11
Chlorthalonil	1.83	2.59	2.41	1.57	1.08	1.90 ± 0.62	1.67
DCPA	-	0.44	0.47	0.18	0.32	0.35 ± 0.13	1.81
Disulfoton	-	0.64	0.84	0.46	-	0.65 ± 0.19	1.61
Endosulfan I	0.88	0.99	0.86	0.65	0.53	0.78 ± 0.19	1.34
Endosulfan II	-	0.71	0.71	0.41	0.66	0.62 ± 0.15	1.33
Endosulfan SO_4	-	0.30	0.31	-	0.41	0.34 ± 0.06	0.74
HCB	0.75	1.25	0.90	0.43	0.52	0.77 ± 0.33	1.9
α-HCH	1.06	1.51	0.91	0.79	0.69	0.99 ± 0.32	1.43
γ-HCH	0.74	1.25	0.82	0.46	1.10	0.88 ± 0.31	1.35
Metolachlor	-	0.73	0.74	0.57	-	0.68 ± 0.10	1.30
trans-Nonachlor	-	0.44	0.45	0.39	0.28	0.39 ± 0.08	1.32
Pendimethalin	-	0.55	*(-0.38)*	-	-	0.66 ± 0.43[c]	0.38
Trifluralin	1.13	0.30	*(-0.18)*	*(-0.30)*	*(-0.11)*		
					Overall Average:	0.75 ± 0.47[d]	

S/W: ratio of the PSR_E for summer and winter months. R_{Summer}/R_{Winter}.

R_{Summer} = average of R determined in April-August periods.

R_{Winter} = average of R determined in March-April and September 2006-February 2007 periods.

[a] Using amount detected in XAD-PAS, and average air concentration in LV-AAS, for each sampling period respectively. A full description can be found in the manuscript text.

[b] Method 3 defines XAD-PAS "deployment intervals" by calculating the amount of pesticides captured during each two month interval (see text for full description). PAS retrieved at the end of each interval were still originally deployed in March 2006.

[c] Sampling rate is determined from April and June values for both trifluralin and pendimethalin. Numbers in brackets are not used to calculate this average due to losses of these compounds from the XAD-PAS.

[d] Calculated from all sampling rates for all chemicals in all sampling periods.

Literature Cited

1. Hayward, S. J.; Gouin, T.; Wania, F., Comparison of four active and passive sampling techniques for pesticides in air. *Environmental science & technology* **2010,** *44*, (9), 3410-6.
2. Hayward, S. J.; Gouin, T.; Wania, F., Levels and seasonal variability of pesticides in the rural atmosphere of Southern Ontario. *Journal of agricultural and food chemistry* **2010,** *58*, (2), 1077-84.
3. Gouin, T.; Wania, F.; Ruepert, C.; E. Castillo, L., Field Testing Passive Air Samplers for Current Use Pesticides in a Tropical Environment. *Environmental science & technology* **2008,** *42*, (17), 6625-6630.
4. Wania, F.; Shen, L.; Lei, Y. D.; Teixeira, C.; Muir, D. C. G., Development and Calibration of a Resin-Based Passive Sampling System for Monitoring Persistent Organic Pollutants in the Atmosphere. *Environmental science & technology* **2003,** *37*, (7), 1352-1359.
5. Abraham, M. H.; Enomoto, K.; Clarke, E. D.; Sexton, G., Hydrogen bond basicity of the chlorogroup; hexachlorocyclohexanes as strong hydrogen bond bases. *The Journal of organic chemistry* **2002,** *67*, (14), 4782-6.
6. Abraham, M. H.; Enomoto, K.; Clarke, E. D.; Roses, M.; Rafols, C.; Fuguet, E., Henry's Law constants or air to water partition coefficients for 1,3,5-triazines by an LFER method. *Journal of environmental monitoring : JEM* **2007,** *9*, (3), 234-9.
7. Arp, H. P. H.; Schwarzenbach, R. P.; Goss, K.-U., Ambient Gas/Particle Partitioning. 2: The Influence of Particle Source and Temperature on Sorption to Dry Terrestrial Aerosols. *Environmental science & technology* **2008,** *42*, (16), 5951-5957.
8. Tülp, H. C.; Goss, K.-U.; Schwarzenbach, R. P.; Fenner, K., Experimental Determination of LSER Parameters for a Set of 76 Diverse Pesticides and Pharmaceuticals. *Environmental science & technology* **2008,** *42*, (6), 2034-2040.
9. Sprunger, L. M.; Achi, S. S.; Acree Jr, W. E.; Abraham, M. H., Development of correlations for describing solute transfer into acyclic alcohol solvents based on the Abraham model and fragment-specific equation coefficients. *Fluid Phase Equilibria* **2010,** *288*, (1–2), 139-144.
10. Hayward, S. J.; Lei, Y. D.; Wania, F., Sorption of a diverse set of organic chemical vapors onto XAD-2 resin: Measurement, prediction and implications for air sampling. *Atmospheric Environment* **2011,** *45*, (2), 296-302.
11. EU Reference Laboratories for Residues of Pesticides EURL DataPool. http://www.eurl-pesticides-datapool.eu/