Assessment of pesticides volatilization potential based on their molecular properties using the TyPol tool

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Supporting information

Table S1

Pesticides applied and analysed in the five French experimental sites (Alsace, Bretagne, Centre-Val de Loire, Lorraine, Nouvelle Aquitaine) and applied amounts during the studied cropping periods. In red and bold: pesticides detected in the air; in green: pesticides applied but not detected in the air; in black: pesticides not analysed; "nd": no data.

Table S2

Main physico-chemical properties of the 178 pesticides considered in TyPol clustering for emission potentials: water solubility (Sw), octanol-water partition coefficient (log Kow), vapor pressure (P_{vap}), adsorption coefficient normalized to soil organic carbon content (Koc), typical degradation half-life in soil (DT50) (from PPDB, 2018). Pesticides detected in the air of the five French experimental sites (Alsace, Bretagne, Centre-Val de Loire, Lorraine, Nouvelle Aquitaine) are in red and bold and highlighted in grey, those that were applied but not detected are indicated in green.

Table S3
Application periods of the measured pesticides in the five French experimental sites (Alsace, Bretagne, Centre-Val de Loire, Lorraine, Nouvelle Aquitaine)

Table S4
TyPol clustering of the 178 pesticides using the 40 molecular descriptors and five parameters (vapor pressure P_{vap}, water solubility Sw, octanol-water partition coefficient log Kow, adsorption coefficient normalized to soil organic carbon content Koc, and degradation half-life in soil DT50) for global emission potential. Pesticides detected in the air of the five experimental sites (Alsace, Bretagne, Centre-Val de Loire, Lorraine, Nouvelle Aquitaine) are indicated in red and bold, pesticides applied but not detected in air are indicated in green. The values of molecular descriptors and parameters are the median values for the cluster. MCI: Molecular connectivity index, HOMO: Highest occupied molecular orbital, LUMO: Lowest unoccupied molecular orbital.

Table S5
TyPol clustering of the 178 pesticides using the 40 molecular descriptors and four parameters (vapor pressure P_{vap}, water solubility Sw, adsorption coefficient normalized to soil organic carbon content Koc, and degradation half-life in soil DT50) for soil emission potential. Pesticides detected in the air of the five experimental sites (Alsace, Bretagne, Centre-Val de Loire, Lorraine, Nouvelle Aquitaine) are indicated in red and bold, pesticides applied but not detected in air are indicated in green. The values of molecular descriptors and parameters are the median values for the cluster. MCI: Molecular connectivity index, HOMO: Highest occupied molecular orbital, LUMO: Lowest unoccupied molecular orbital.

Table S6
TyPol clustering of the 178 pesticides using the 40 molecular descriptors and three parameters (vapor pressure P_{vap}, water solubility Sw, and octanol-water partition coefficient log Kow) for plant emission potential. Pesticides detected in the air of the five experimental sites (Alsace, Bretagne, Centre-Val de Loire, Lorraine, Nouvelle Aquitaine) are indicated in red and bold, pesticides applied but not detected in air are indicated in green. The values of molecular descriptors and parameters are the median values for the cluster. MCI: Molecular connectivity index, HOMO: Highest occupied molecular orbital, LUMO: Lowest unoccupied molecular orbital.

Fig. S1. Meteorological data (daily precipitations (mm) ■, daily mean temperature (°C) —, daily mean wind speed (m s^{-1}) —) measured in the five experimental sites: (a) Alsace, (b) Lorraine, (c) Bretagne, (d) Centre-Val de Loire, (e) Nouvelle Aquitaine.

Fig. S2. Dynamics of pesticide concentrations measured in the air of the five experimental sites: Alsace (a), Lorraine (b), Bretagne (c), Centre-Val de Loire (d) and Nouvelle Aquitaine (e).

Fig. S3. TyPol barplots for the heights of the dendrograms obtained for global (a), soil (b) and plant (c) potential emission to air analyses.

Fig. S4. Range of variation (box-and-whisker plots) of the values of the five parameters considered into TyPol (water solubility Sw, octanol water partition coefficient log Kow, vapor pressure P_{vap}, adsorption coefficient normalized to soil carbon organic content Koc, and degradation half-life in soil DT50) and of some relevant molecular descriptors (molar mass, polarizability, total energy) for each cluster after analysis of the 178 pesticides for global emission potential to air. Dotted lines represent the limits between volatile (log P_{vap} > -1) and non-volatile compounds (log P_{vap} < -1) (FOCUS, 2008); mobile (log Koc < 2.7) and non-mobile compounds (log Koc > 2.7) (Mc Call et al., 1980); persistent (log DT50 > 1.78) and non-persistent compounds in soil (log DT50 < 1.78) (Regulation (EC) No 1107/2009, 2009). Table summarizes the number of pesticides in each cluster and the number of applied, detected and not detected pesticides.

Fig. S5. Range of variation (box-and-whisker plots) of the values of the four parameters considered into TyPol (water solubility Sw, vapor pressure P_{vap}, adsorption coefficient normalized to soil carbon organic content Koc, and pesticide degradation half-life in soil DT50) and of some relevant molecular descriptors (molar mass, polarizability, total energy) for each cluster after analysis of the 178 pesticides for soil emission potential to air. Dotted lines represent the limits between volatile (log P_{vap} > -1) and non-volatile compounds (log P_{vap} < -1) after emission from soil (FOCUS, 2008); mobile (log Koc < 2.7) and non-mobile compounds (log Koc > 2.7) (Mc Call et al., 1980); persistent (log DT50 > 1.78) and non-persistent compounds in soil (log DT50 < 1.78) (Regulation (EC) No 1107/2009, 2009). Table summarizes the number of pesticides in each cluster and the number of applied, detected and not detected pesticides.

Fig. S6. Range of variation (box-and-whisker plots) of the values of the three parameters considered into TyPol (water solubility Sw, octanol water partition coefficient log Kow, and vapor pressure P_{vap}) and of some relevant molecular descriptors (molar mass, polarizability, total energy) for each cluster after analysis of the 178 pesticides for plant emission potential to air. Dotted line represents the limit between volatile (log P_{vap} > -2) and non-volatile compounds (log P_{vap} < -2) following emission from plant (FOCUS, 2008). Table summarizes the number of pesticides in each cluster and the number of applied, detected and not detected pesticides.

Table S1
Pesticides applied and analysed in the five French experimental sites (Alsace, Bretagne, Centre-Val de Loire, Lorraine, Nouvelle Aquitaine) and applied amounts during the studied cropping periods. In red and bold: pesticides detected in the air; in green: pesticides applied but not detected in the air; in black: pesticides not analysed; "nd": no data.

Alsace		**Bretagne**		**Centre-Val de Loire**		**Lorraine**		**Nouvelle Aquitaine**	
Pesticide	**Applied amount (kg)**	**Pesticide**	**Applied amount (kg)**	**Pesticide**	**Applied amount (kg)**	**Pesticide**	**Applied amount (kg)**	**Pesticide**	**Applied amount (kg)**
Azoxystrobin	nd	Aclonifen	nd	1-naphthylacetic acid	nd	Boscalid	9	Beta-cyfluthrin	nd
Benoxacor	nd	Azoxystrobin	nd	6-benzyladenine	nd	**Chlorothalonil**	**17.5**	**Boscalid**	**2.1**
Beta-cyfluthrin	nd	Boscalid	nd	Abamectin	nd	Cypermethrin	0.1	**Chlorpyrifos-methyl**	**4.5**
Bromoxynil octanoate	nd	**Bromoxynil**	**2.6**	Acetamiprid	nd	**Cyprodinyl**	**3.5**	**Cymoxanil**	**1.7**
Carfentrazone-ethyl	nd	**octanoate**		Aclonifen	34.2	Dicamba	0.1	Difenoconazole	nd
Chlorothalonil	**21**	**Chlorothalonil**	**21.1**	Azoxystrobin	nd	**Dimethenamid-P**	**32.5**	**Dimethenamid-P**	**0.9**
Clomazone	**0.8**	Clodinafop-propargyl	nd	Beflubutamid	nd	Epoxiconazole	1.5	**Dimethomorph**	**6.5**
Clopyralid	nd	**Clomazone**	**0.36**	Benoxacor	0.77	**Fenpropidin**	**8.5**	**Fenbuconazole**	**0.065**
Cypermethrin	nd	**Cyprodinil**	**0.6**	Bixafen	nd	Mesotrione	0.1	**Folpet**	**0.123**
Cyproconazole	nd	**Diflufenican**	**0.04**	Boscalid	5.3	Metconazole	2.5	**Kresoxim-methyl**	**0.0037**
Dicamba	nd	**Dimethenamid-P**	**47.1**	Captan	291	Nicosulfuron	0.1	**Propyzamide**	**0.47**
Dimethenamid-P	**47**	Epoxiconazole	nd	Chlorantraniliprole	nd	**Pendimethalin**	**22**	**Quinoxyfen**	**1.8**
Epoxiconazole	nd	**Pendimethalin**	**27.1**	Chlormequat chloride	45	Propiconazole	3	**Spiroxamine**	**10.5**
Ethofumesate	**21.5**	**Propiconazole**	**1.6**	**Chlorothalonil**	**17.2**	Prosulfuron	0.1	**Tebuconazole**	**19**
Fenpropimorph	**28**	**Prosulfocarb**	**0.8**	Chlorpyrifos	2.71	Pyraclostrobin	2.5	**Tetraconazole**	**0.052**
Fluroxypyr	nd	**S-metolachlor**	**6.2**	Clopyralid	0.58	Tebuconazole	5	**Trifloxystrobin**	**2.1**
Isoxadifen-ethyl	nd	Tebuconazole	nd	Cloquintocet-mexyl	nd	Trifloxystrobin	1		
Lambda-cyhalothrin	nd	**Tri-allate**	**3.5**	Cyproconazole	2.21				
Lenacil	nd	Trifloxystrobin	nd	**Cyprodinil**	**0.15**				
Mesosulfuron-methyl	nd			Deltamethrin	nd				
Mesotrione	nd			Difenoconazole	2.97				
Metaldehyde	nd			Diflufenican	16.9				
Metamitron	nd			Dimethenamid-P	13.3				
Nicosulfuron	nd			Dimoxystrobin	nd				
Pendimethalin	**17**			Dithianon	103				
Phenmedipham	nd			Dodine	87.7				
Pinoxaden	nd			Epoxiconazole	2.43				
Prochloraz	nd			Ethephon	2.01				
Propiconazole	nd			Fenoxycarb	nd				
Prosulfuron	nd			Flonicamid	6.58				
S-metolachlor	**55**			Florasulam	nd				
Tebuconazole	nd			Fludioxonil	nd				
Tembotrione	nd			Flufenacet	20.0				
Thiophanate-methyl	nd			Fluopyram	nd				
				Flurochloridone	nd				

Tribenuron-methyl	nd			Fluroxypyr	nd				
Triflusulfuron-methyl	nd			Fluoxastrobin	nd				
Trinexapac-ethyl	nd			Flurtamone	nd				
Tritosulfuron	nd			Fluxapyroxad	nd				
				Glufosinate ammonium	nd				
				Glyphosate	230				
				Iodosulfuron-methyl-sodium	nd				
				Isoproturon	nd				
				Kresoxim-methyl	0.75				
				Lambda-cyhalothrin	1.69				
				Mancozeb	260				
				Mefenpyr-diethyl	nd				
				Mesosulfuron-methyl-sodium	nd				
				Mesotrione	nd				
				Metaldehyde	5.68				
				Metamitron	1.54				
				Metazachlor	13.3				
				Metconazole	4.85				
				Metrafenone	nd				
				Metsulfuron-methyl	nd				
				Penconazole	0.83				
				Pendimethalin	**14.16**				
				Picoxystrobin	nd				
				Pinoxaden	nd				
				Prohexadione calcium	nd				
				Propiconazole	nd				
				Propyzamide	25.84				
				Prothioconazole	nd				
				Pyraclostrobin	5.99				
				Pyrimethanil	3.33				
				Pyroxsulam	nd				
				Quinmerac	nd				
				Quizalofop-P-ethyl	nd				
				S-metolachlor	**15.41**				
				Spirotetramat	nd				
				Spiroxamine	**3.48**				
				Tau-fluvalinate	nd				
				Tebuconazole	5.97				
				Thiacloprid	2.46				

				Thifensulfuron methyl Thiophanate-methyl Thiram **Tri-allate** Tribenuron-methyl Trifloxystrobin	nd 28.81 242 **76.68** nd 7.309				

Table S2

Main physico-chemical properties of the 178 pesticides considered in TyPol clustering for emission potentials: water solubility (Sw), octanol-water partition coefficient (log Kow), vapor pressure (P_{vap}), adsorption coefficient normalized to soil organic carbon content (Koc), typical degradation half-life in soil (DT50) (from PPDB, 2018). Pesticides detected in the air of the five French experimental sites (Alsace, Bretagne, Centre-Val de Loire, Lorraine, Nouvelle Aquitaine) are in red and bold and highlighted in grey, those that were applied but not detected are indicated in green.

Pesticide	CAS number	Sw ($mg\ L^{-1}$)	log Kow (-)	P_{vap} (mPa)	Koc ($L\ kg^{-1}$)	DT50 (d)
1-naphthylacetic acid	86-87-3	16.8	-0.02	1.27	84.8	42.0
2,4-D	94-75-7	24300	-0.82	0.009	39.3	4.4
2,4-DB	94-82-6	4385	1.22	$9.0\ 10^{-4}$	224	2.9
6-benzyladenine	1214-39-7	64.5	2.16	$6.0\ 10^{-4}$	896	1.1
Abamectin	71751-41-2	1.21	4.40	$3.7\ 10^{-3}$	5638	28.7
Acetamiprid	135410-20-7	2950	0.80	$1.7\ 10^{-4}$	200	1.6
Acetochlor	34256-82-1	282	4.14	0.022	156	14.0
Aclonifen	74070-46-5	1.4	4.37	0.016	7126	117
Alachlor	15972-60-8	240	3.09	2.9	335	14.0
Aldrin	309-00-2	0.027	6.50	8.6	17500	28.0
Ametoctradin	865318-97-4	0.15	4.40	$2.1\ 10^{-7}$	7713	1.8
Amitrole	61-82-5	264000	-0.97	0.033	87	7.4
Azoxystrobin	131860-33-8	6.7	2.50	$1.1\ 10^{-7}$	589	7.8
Beflubutamid	113614-08-7	3.29	4.28	0.011	1171	29.6
Benalaxyl-M	98243-83-5	33	3.68	0.059	7175	80.0
Benoxacor	98730-04-2	20	2.69	0.589	109	50.0
Bentazone	25057-89-0	7110	-0.46	0.170	55.3	20.0
Beta-cyfluthrin	1820573-27-0	0.0012	5.90	$5.6\ 10^{-5}$	64300	13.0
Bifenthrin	82657-04-3	0.001	6.60	0.018	236610	26.0
Bixafen	581809-46-3	0.49	3.30	$4.6\ 10^{-5}$	3869	500
Boscalid	**188425-85-6**	**4.6**	**2.96**	**$7.2\ 10^{-4}$**	**772**	**484**
Bromoxynil	1689-84-5	38000	0.27	1.04	302	0.63
Bromoxynil octanoate	**1689-99-2**	**0.05**	**6.20**	**0.024**	**24439**	**1.7**
Bupirimate	41483-43-6	13.06	3.68	0.057	1882	79.0
Butralin	33629-47-9	0.308	4.93	0.769	46400	22.0
Captan	133-06-2	5.2	2.50	$4.2\ 10^{-3}$	200	0.8
Carbaryl	63-25-2	9.1	2.36	0.042	300	16.0
Carbetamide	16118-49-3	3270	1.78	$3.0\ 10^{-4}$	88.6	12.4
Carfentrazone-ethyl	128639-02-1	29.3	3.70	0.007	866	1.0
Chlorantraniliprole	500008-45-7	0.88	2.86	$6.3\ 10^{-9}$	362	597
Chlordane	57-74-9	0.1	2.78	1.31	20000	365
Chlormequat chloride	999-81-5	886000	-3.47	0.001	132	27.4
Chlorothalonil	**1897-45-6**	**0.81**	**2.94**	**0.076**	**1960**	**6.4**
Chlorotoluron	15545-48-9	74	2.50	0.005	196	45.0
Chlorpropham	101-21-3	110	3.76	24	470	13.1
Chlorpyrifos	2921-88-2	1.05	4.70	1.43	5510	386
Chlorpyrifos-methyl	**5598-13-0**	**2.74**	**4.00**	**3.0**	**4645**	**12.0**
Clodinafop-propargyl	105512-06-9	4	3.90	0.0032	1466	0.8
Clomazone	**81777-89-1**	**1210**	**2.54**	**27.0**	**300**	**22.6**
Clopyralid	1702-17-6	7850	-2.63	1.36	5	23.2
Cyazofamid	120116-88-3	0.107	3.20	0.0133	1338	10.0
Cycloxydym	101205-02-1	53	1.36	0.010	59	0.65
Cyflufenamid	180409-60-3	0.52	4.70	0.0354	1590	33.8
Cyfluthrin	68359-37-5	0.0066	6.00	$3.0\ 10^{-4}$	124000	33.0
Cymoxanil	57966-95-7	780	0.67	0.150	43.6	0.7
Cypermethrin	52315-07-8	0.009	5.55	0.0068	308000	22.1
Cyproconazole	94361-06-5	93	3.09	0.026	364	142
Cyprodinil	**121552-61-2**	**13**	**4.00**	**0.509**	**2277**	**37.0**
Deltamethrin	52918-63-5	0.0002	4.60	$1.2\ 10^{-5}$	10240000	58.2
Dicamba	1918-00-9	249996	-1.88	1.67	12.4	4.0
Dichlorprop-P	15165-67-0	672	0.67	0.056	44	12.0
Dichlorvos	62-73-7	18000	1.90	2100	50	2.0
Dicloran	99-30-9	6.4	2.80	0.261	812	401
Dieldrin	60-57-1	0.14	3.70	0.024	12000	1400

Pesticide	CAS number	Sw ($mg\ L^{-1}$)	log Kow (-)	P_{vap} (mPa)	Koc ($L\ kg^{-1}$)	DT50 (d)
Difenoconazole	119446-68-3	15	4.36	$3.3\ 10^{-5}$	3760	130
Diflufenican	**83164-33-4**	**0.05**	**4.20**	**0.0042**	**5500**	**94.5**
Dimethenamid	87674-68-8	1200	2.20	0.370	69	13.0
Dimethenamid-P	**163515-14-8**	**1499**	**1.89**	**2.51**	**227**	**11.0**
Dimethoate	60-51-5	25900	0.75	0.247	28.3	2.5
Dimethomorph	**110488-70-5**	**28.95**	**2.68**	**$9.7\ 10^{-4}$**	**419**	**72.7**
Dimoxystrobin	149961-52-4	4.3	3.59	$6.0\ 10^{-6}$	486	210
Dithianon	3347-22-6	0.22	3.20	$1.07\ 10^{-7}$	3627	10.5
Diuron	330-54-1	35.6	2.87	0.0011	680	147
Dodine	2439-10-3	930	1.25	0.0055	4236500	4.7
Endrin	72-20-8	0.24	3.20	$2.0\ 10^{-7}$	10000	4300
Epoxiconazole	133855-98-8	7.1	3.30	$3.5\ 10^{-4}$	894	354
Ethephon	16672-87-0	100000	-1.89	1.00	2540	13.1
Ethion	563-12-2	2	5.07	0.200	10000	90.0
Ethofumesate	**26225-79-6**	**50**	**2.70**	**0.360**	**118**	**21.6**
Etofenprox	80844-07-1	0.0225	6.90	$8.1\ 10^{-4}$	17757	11.0
Fenarimol	60168-88-9	13.7	3.69	0.065	734	250
Fenbuconazole	**114369-43-6**	**2.47**	**3.79**	**$3.4\ 10^{-4}$**	**4425**	**60.0**
Fenpropidin	**67306-00-7**	**530**	**2.60**	**17.0**	**3808**	**90.0**
Fenpropimorph	**67564-91-4**	**4.32**	**4.50**	**3.90**	**4382**	**35.0**
Fipronil	120068-37-3	3.78	3.75	0.002	727	142
Flazasulfuron	104040-78-0	2100	-0.06	0.0133	46.2	41.2
Flonicamid	158062-67-0	5200	-0.24	$9.4\ 10^{-4}$	1.6	3.1
Florasulam	145701-23-1	6360	-1.22	0.01	22	1.85
Fluazinam	79622-59-6	0.135	4.03	7.5	16430	11.0
Fludioxonil	131341-86-1	1.8	4.12	$3.9\ 10^{-4}$	145600	164
Flufenacet	142459-58-3	51	3.50	0.090	401	19.7
Flumetralin	62924-70-3	0.01	5.53	0.720	10000	727
Flumioxazin	103361-09-7	0.786	2.55	0.319	889	21.9
Fluopicolide	239110-15-7	2.8	2.90	$3.0\ 10^{-4}$	321.1	271
Fluopyram	658066-35-4	16	3.30	0.0012	278.9	309
Fluoxastrobin	361377-29-9	2.56	2.86	$5.6\ 10^{-7}$	848	58.8
Flurochloridone	61213-25-0	21.9	3.36	0.270	700	53.0
Fluroxypyr	69377-81-7	6500	0.04	$3.8\ 10^{-6}$	68	13.1
Flurtamone	96525-23-4	10.7	3.24	$7.0\ 10^{-7}$	257.3	10.7
Folpet	**133-07-3**	**0.8**	**3.02**	**0.021**	**304**	**4.7**
Fosetyl-aluminium	39148-24-8	111300	-2.10	$1.0\ 10^{-4}$	0.10	0.02
Glufosinate	51276-47-2	500000	-4.01	0.031	600	7.4
Glyphosate	1071-83-6	10500	-3.20	0.0131	1420	15.0
Heptachlor	76-44-8	0.056	5.44	53.2	24000	285
Imidacloprid	138261-41-3	610	0.57	$4.0\ 10^{-7}$	225	191
Indoxacarb	173584-44-6	0.2	4.65	$9.8\ 10^{-6}$	4480	113
Iodosulfuron-methyl-sodium	144550-36-7	25000	-0.70	$2.6\ 10^{-6}$	45	2.7
Isoproturon	34123-59-6	70.2	2.50	0.0055	122	12.0
Isoxaben	82558-50-7	0.93	3.94	$5.5\ 10^{-4}$	909	105
Kresoxim-methyl	**143390-89-0**	**2**	**3.40**	**0.0023**	**308**	**16.0**
Lambda-cyhalothrin	91465-08-6	0.005	5.50	$2.0\ 10^{-4}$	283707	175
Lenacil	2164-08-0	2.9	1.69	$1.7\ 10^{-6}$	165	49.7
Lindane	58-89-9	8.52	3.50	4.40	1270	980
Malathion	121-75-5	148	2.75	3.09	1800	0.17
Mancozeb	8018-01-7	6.2	1.33	0.013	998	0.10
Mandipropamid	374726-62-2	4.2	3.20	$9.4\ 10^{-4}$	847	49.1
Maneb	12427-38-2	178	-0.45	0.014	2000	1.0
Mecoprop	7085-19-0	249996	-0.19	1.60	47	8.2
Mefenpyr-diethyl	135590-91-9	20	3.83	0.0063	634	17.5
Meptyldinocap	131-72-6	0.248	6.55	0.0079	958245	12.0
Mesosulfuron-methyl	208465-21-8	483	-0.48	$1.1\ 10^{-5}$	92	43.5
Mesotrione	104206-82-8	1500	0.11	0.0057	122	19.6
Metalaxyl-M	70630-17-0	26000	1.71	3.29	78.9	6.5
Metaldehyde	108-62-3	188	0.12	6600	240	5.1
Metamitron	41394-05-2	1770	0.85	$7.4\ 10^{-4}$	77.7	30.0
Metazachlor	67129-08-2	450	2.49	0.093	54	8.6

Pesticide	CAS number	Sw ($mg\ L^{-1}$)	log Kow (-)	P_{vap} (mPa)	Koc ($L\ kg^{-1}$)	DT50 (d)
Metconazole	125116-23-6	30.4	3.85	$2.1\ 10^{-5}$	1116	142
Metiram	9006-42-2	2	1.76	$1.0\ 10^{-5}$	903000	1.3
Metolachlor	51218-45-2	530	3.40	1.70	120	90.0
Metrafenone	220899-03-6	0.492	4.30	0.153	7061	201
Metribuzin	21087-64-9	5932	1.70	0.121	43	9.3
Metsulfuron-methyl	74223-64-6	172	-1.87	$3.9\ 10^{-8}$	12	10.0
Mirex	2385-85-5	0.085	5.28	0.075	5794	300
Myclobutanil	88671-89-0	132	2.89	0.198	517	560
Napropamide	15299-99-7	74	3.30	0.022	839	70.0
Nicosulfuron	111991-09-4	7500	0.61	$8.0\ 10^{-7}$	30	26.0
Oryzalin	19044-88-3	1.13	3.73	$1.1\ 10^{-7}$	949	44.8
Oxadiazon	19666-30-9	0.57	5.33	0.670	3200	502
Oxyfluorfen	42874-03-3	0.116	4.86	0.026	7566	35.0
Penconazole	66246-88-6	73	3.72	0.366	2205	117
Pendimethalin	**40487-42-1**	**0.33**	**5.40**	**3.34**	**17900**	**182**
Pentachlorophenol	87-86-5	1000	3.32	16000	30	63
Permethrin	52645-53-1	0.2	6.1	0.007	100000	13
Phenmedipham	13684-63-4	1.8	2.70	$7.0\ 10^{-7}$	1780	12.0
Phosmet	732-11-6	15.2	2.96	0.065	3530	3.2
Picoxystrobin	117428-22-5	3.1	3.60	0.0055	965	24.4
Pinoxaden	243973-20-8	200	3.20	$2.0\ 10^{-4}$	349	0.50
Piperonyl butoxide	51-03-6	14.3	4.75	0.02	89125	13.0
Pirimicarb	23103-98-2	3100	1.70	0.43	388	86
Prochloraz	67747-09-5	26.5	3.50	0.150	500	120
Prohexadione-calcium	127277-53-6	786	-2.90	0.0133	204.5	0.70
Propaquizafop	111479-05-1	0.63	4.78	$4.4\ 10^{-7}$	2220	2.1
Propiconazole	**60207-90-1**	**150**	**3.72**	**0.056**	**1086**	**71.8**
Propyzamide	**23950-58-5**	**9.0**	**3.27**	**0.058**	**840**	**50.5**
Proquinazid	189278-12-4	0.93	5.50	0.090	12870	45.0
Prosulfocarb	**52888-80-9**	**13.2**	**4.48**	**0.790**	**1693**	**11.9**
Prosulfuron	94125-34-5	4000	1.50	0.0035	14.2	62.1
Pyraclostrobin	175013-18-0	1.9	3.99	$2.6\ 10^{-5}$	9300	41.9
Pyraflufen-ethyl	129630-19-9	0.082	3.49	$4.3\ 10^{-6}$	1949	0.32
Pyrimethanil	53112-28-0	110	2.84	1.10	356	50.9
Pyroxsulam	422556-08-9	3200	-1.01	$1.0\ 10^{-4}$	33.2	3.3
Quinmerac	90717-03-6	107000	-1.41	$1.0\ 10^{-7}$	86	30.0
Quinoxyfen	**124495-18-7**	**0.047**	**4.66**	**0.012**	**22929**	**308**
Quizalofop-P-ethyl	100646-51-3	0.61	4.61	$1.1\ 10^{-4}$	1816	2.0
S-metolachlor	**87392-12-9**	**480**	**3.05**	**3.70**	**226.1**	**15.0**
Spirotetramat	203313-25-1	29.89	2.51	$5.6\ 10^{-6}$	289	0.19
Spiroxamine	**118134-30-8**	**405**	**2.89**	**3.5**	**14567**	**25.0**
Tau-fluvalinate	102851-06-9	0.00103	7.02	$9.0\ 10^{-8}$	135000	4.0
Tebuconazole	**107534-96-3**	**36**	**3.70**	**0.0013**	**769**	**63.0**
Tebuthiuron	34014-18-1	2500	1.79	0.270	80	400
Tembotrione	335104-84-2	71000	-1.09	$1.1\ 10^{-5}$	66	14.5
Terbuthylazine	5915-41-3	6.6	3.40	0.150	231	72.0
Terbutryn	886-50-0	25	3.66	0.129	2430	74.0
Tetraconazole	**112281-77-3**	**156.6**	**3.56**	**0.180**	**1152**	**61.0**
Thiacloprid	111988-49-9	184	1.26	$3.0\ 10^{-7}$	615	0.88
Thiamethoxam	153719-23-4	4100	-0.13	$6.9\ 10^{-6}$	56.2	50.0
Thifensulfuron-methyl	79277-27-3	54.1	-1.65	$5.2\ 10^{-6}$	28.3	1.4
Thiophanate-methyl	23564-05-8	18.5	1.45	0.009	220	0.50
Thiram	137-26-8	18	1.84	0.02	9629	4.89
Tolylfluanid	731-27-1	0.9	3.90	0.200	1728	1.8
Toxaphene	8001-35-2	0.000323	3.51	11.7	1	2701
Triadimenol	55219-65-3	72	3.18	$5.0\ 10^{-4}$	750	250
Tri-allate	**2303-17-5**	**4.1**	**4.06**	**12.0**	**3030**	**82.0**
Tribenuron-methyl	101200-48-0	2483	0.42	$5.9\ 10^{-6}$	35	9.1
Triclopyr	55335-06-3	8100	4.62	0.200	27	18.8
Trifloxystrobin	**141517-21-7**	**0.61**	**4.50**	**0.0034**	**2290**	**0.34**
Trifluralin	1582-09-8	0.221	5.27	9.5	15800	181
Zoxamid	156052-68-5	0.681	3.76	0.008	1000	30.0

Table S3
Application periods of the measured pesticides in the five French experimental sites (Alsace, Bretagne, Centre-Val de Loire, Lorraine, Nouvelle Aquitaine)

Site	Measured pesticide	Application period
Alsace	Chlorothalonil	18 April to 2 May 2017
	Clomazone	2 to 9 May 2017
	Dimethenamid-P	10 to 17 April 2017, 2 to 9 May 2017
	Ethofumesate	3 to 17 April 2017, 24 April to 2 May 2017
	Fenpropimorph	22 to 29 May 2017, 3 to 10 July 2017
	Pendimethalin	24 April to 9 May 2017
	S-metolachlor	20 to 27 March 2017, 24 April to 9 May 2017
Bretagne	Bromoxynil octanoate	17 to 24 May 2017, 31 May to 6 June 2017
	Chlorothalonil	5 April to 17 May 2017
	Clomazone	15 to 29 March 2017, 19 to 26 April 2017, 10 to 17 May 2017, 14 to 21 June 2017
	Cyprodinil	5 to 12 April 2017
	Diflufenican	14 to 21 March 2017
	Dimethenamid-P	26 April to 17 May 2017
	Pendimethalin	26 April to 17 May 2017
	Propiconazole	5 to 19 April 2017, 26 April to 2 May 2017
	Prosulfocarb	14 to 21 March 2017
	S-metolachlor	3 to 17 May 2017, 14 to 21 June 2017
	Tri-allate	19 to 26 April 2017
Centre-Val de Loire	Chlorothalonil	10 to 17 April 2017
	Cyprodinil	13 March to 2 April 2017
	Pendimethalin	13 to 20 March 2017
	S-metolachlor	24 to 30 April 2017
	Spiroxamine	17 to 30 April 2017
	Tri-allate	3 to 9 October 2016
Lorraine	Chlorothalonil	27 March to 2 April 2017, 17 to 30 April 2017, 15 to 21 May 2017
	Cyprodinil	27 March to 2 April 2017, 24 to 30 April 2017
	Dimethenamid-P	27 March to 9 April 2017, 8 to 14 May 2017
	Fenpropidin	27 March to 2 April 2017, 24 to 30 April 2017
	Pendimethalin	27 March to 9 April 2017
Nouvelle Aquitaine	Boscalid	11 July to 7 August 2016
	Chlorpyrifos-methyl	27 June to 3 July 2016, 11 to 17 July 2016
	Dimethenamid-P	9 to 15 May 2016
	Dimethomorph	20 June to 17 July 2016
	Fenbuconazole	27 June to 3 July 2016
	Folpet	16 May to 19 June 2016, 27 June to 10 July 2016, 8 to 14 August 2016
	Kresoxim-methyl	13 to 26 June 2016, 11 July to 7 August 2016
	Propyzamide	18 to 24 January 2016
	Quinoxyfen	27 June to 24 July 2016
	Spiroxamine	16 to 29 May 2016, 6 to 19 June 2016, 27 June to 10 July 2016
	Tebuconazole	23 May to 19 June 2016, 27 June to 7 August 2016
	Tetraconazole	4 to 10 July 2016
	Trifloxystrobin	20 June to 10 July 2016, 18 to 24 July 2016

Table S4

TyPol clustering of the 178 pesticides using the 40 molecular descriptors and five parameters (vapor pressure P_{vap}, water solubility Sw, octanol-water partition coefficient log Kow, adsorption coefficient normalized to soil organic carbon content Koc, and degradation half-life in soil DT50) for global emission potential. Pesticides detected in the air of the five experimental sites (Alsace, Bretagne, Centre-Val de Loire, Lorraine, Nouvelle Aquitaine) are indicated in red and bold, pesticides applied but not detected in air are indicated in green. The values of molecular descriptors and parameters are the median values for the cluster. MCI: Molecular connectivity index, HOMO: Highest occupied molecular orbital, LUMO: Lowest unoccupied molecular orbital.

	Cluster 1	Cluster 2	Cluster 3	Cluster 4	Cluster 5	Cluster 6
Pesticides	Aclonifen Ametoctradin Beta-cyfluthrin Bifenthrin **Bromoxynil octanoate** Butralin Chlorpyrifos Cyfluthrin Cypermethrin Deltamethrin Dimoxystrobin Dithianon Etofenprox Fludioxonil Flumetralin Isoxaben Lambda-cyhalothrin Meptyldinocap Metiram Oryzalin Oxadiazon Oxyfluorfen **Pendimethalin** Permethrin Phenmedipham Piperonyl butoxide Propaquizafop Proquinazid Pyraclostrobin Pyraflufen-ethyl **Quinoxyfen** Quizalofop-p-ethyl Tau-fluvalinate	1-naphthylacetic acid 2,4-DB Acetamiprid Acetochlor Alachlor Benoxacor Captan Carbaryl Carbetamide Chlorpropham Chlortoluron **Clomazone** Cycloxydym Cymoxanil Cyproconazole Dichlorprop-P Dimethenamid **Dimethenamid-P** **Ethofumesate** **Fenpropidin** Flurochloridone Fluroxypyr **Folpet** Imidacloprid Isoproturon Malathion Maneb Metamitron Metazachlor Metolachlor Metribuzin Myclobutanil Penconazole	Abamectin Flazasulfuron Florasulam Fosetyl-aluminium Iodosulfuron-methyl-sodium Mesosulfuron-methyl Mesotrione Metsulfuron-methyl Nicosulfuron Prosulfuron Pyroxsulam Tembotrione Thifensulfuron-methyl Tribenuron-methyl	6-benzyladenine Azoxystrobin Beflubutamid Benalaxyl-M Bixafen **Boscalid** Bupirimate Carfentrazone-ethyl Chlorantraniliprole **Chlorothalonil** **Chlorpyrifos-methyl** Clodinafop-propargyl Cyazofamid Cyflufenamid **Cyprodinil** Dicloran Difenoconazole **Diflufenican** **Dimethomorph** Diuron Dodine Epoxiconazole Ethion Fenarimol **Fenbuconazole** **Fenpropimorph** Fipronil Fluazinam Flufenacet Flumioxazin Fluopicolide Fluopyram Fluoxastrobin	2,4-D Amitrole Bentazone Bromoxynil Chlormequat chloride Clopyralid Dicamba Dichlorvos Dimethoate Ethephon Flonicamid Glufosinate Glyphosate Mecoprop Metalaxyl-M Metaldehyde Pentachlorophenol Prohexadione-calcium	Aldrin Chlordane Dieldrin Endrin Heptachlore Lindane Mirex Toxaphene

	Trifloxystrobin Trifluralin	Phosmet Pirimicarb Prochloraz **Propiconazole** Pyrimethanil Quinmerac **S-metolachlor** **Spiroxamine** Tebuthiuron **Tetraconazole** Thiacloprid Thiamethoxam Thiophanate-methyl Triclopyr		Flurtamone Indoxacarb **Kresoxim-methyl** Lenacil Mancozeb Mandipropamid Mefenpyr-diethyl Metconazole Metrafenone Napropamide Picoxystrobin Pinoxaden **Propyzamide** **Prosulfocarb** Spirotetramat **Tebuconazole** Terbuthylazine Terbutryn Thiram Tolylfluanid Triadimenol **Tri-allate** Zoxamid		
Number of atoms	43	31	41.5	38.5	19.5	25
Number of non-hydrogen atoms	24	17	27	23	12	18
Number of hydrogen atoms	18	14	15.5	16	7.5	7
Number of carbon atoms	16	12	14	16.5	6.5	10
Number of nitrogen atoms	2	1	5	2	1	0
Number of oxygen atoms	3	2	6	2	3	0
Number of chlorine atoms	0	1	0	1	0	6.5
Number of fluorine atoms	0	0	0	0	0	0
Number of halogen atoms	2	1	0	2	1	6.5
Number of phosphorus atoms	0	0	0	0	0	0
Number of sulfur atoms	0	0	1	0	0	0
Number of bonds	45	31	43	40	19	26.5
Number of non-hydrogen bonds	25	17	28	24.5	12	20.5
Number of double bonds	2	1	4	1	1	1
Number of triple bonds	0	0	0	0	0	0
Number of multiple bonds	14	7	15.5	12	5.5	1
Number of rotatable bonds	7	3	6	5	2	0
Number of aromatic bonds	12	6	12	11	5.5	0
Sum of conventional bond order	33	22	37.5	31.5	15	22

Number of rings	2	2	2	2	1	3.5
Number of circuits	3	2	2	2	1	8
Molecular weight (g mol^{-1})	364.4	269.8	408.9	336.8	217.8	380.9
Connolly molecular surface area ($Å^2$)	303.8	226.5	311.0	291.9	174.9	231.3
MCI order 0	17.78	12.96	20.22	16.49	9.30	13.53
MCI order 1	11.56	8.02	12.67	11.16	5.31	8.25
MCI order 2	10.65	6.94	12.19	10.09	5.30	9.06
MCI order 3	7.99	5.54	9.02	8.02	3.75	9.48
MCI order 4	6.29	4.47	7.32	6.22	2.60	7.82
MCI order 5	5.03	3.33	5.57	4.72	1.68	6.20
Valence MCI order 0	14.80	11.10	15.66	13.56	8.08	13.88
Valence MCI order 1	8.27	6.13	9.11	7.62	4.35	8.44
Valence MCI order 2	5.99	4.73	7.06	5.92	3.42	9.10
Valence MCI order 3	3.96	3.29	4.83	4.08	2.06	9.60
Valence MCI order 4	2.59	2.17	3.47	2.57	1.21	7.60
Valence MCI order 5	1.66	1.35	2.22	1.67	0.67	5.92
Polarizability ($Å^3$)	36.440	26.124	36.301	34.515	19.284	32.556
Dipole moment (D)	3.865	3.282	5.525	3.472	3.272	1.600
HOMO energy (eV)	-9.195	-9.313	-10.116	-9.321	-9.783	-9.932
LUMO energy (eV)	-0.584	-0.486	-1.324	-0.531	-0.287	-0.343
Total energy (eV)	-4670.74	-3237.42	-5502.93	-4048.69	-2706.61	-4205.81
P_{vap} (mPa)	$8.13\ 10^{-4}$	0.121	$3.32\ 10^{-5}$	$5.88\ 10^{-3}$	0.497	2.41
Sw (mg L^{-1})	0.25	240	2819	6.30	25087	0.075
log Kow (-)	4.78	2.49	-0.59	3.45	-0.64	3.60
Koc (L kg^{-1})	15800	224	34.1	930	66.1	10954
DT50 (d)	26	16	12.25	50.1	6.95	672.5

Table S5

TyPol clustering of the 178 pesticides using the 40 molecular descriptors and 4 four parameters (vapor pressure P_{vap}, water solubility Sw, adsorption coefficient normalized to soil organic carbon content Koc, and degradation half-life in soil DT50) for soil emission potential. Pesticides detected in the air of the five experimental sites (Alsace, Bretagne, Centre-Val de Loire, Lorraine, Nouvelle Aquitaine) are indicated in red and bold, pesticides applied but not detected in air are indicated in green. The values of molecular descriptors and parameters are the median values for the cluster. MCI: Molecular connectivity index, HOMO: Highest occupied molecular orbital, LUMO: Lowest unoccupied molecular orbital.

	Cluster 1	**Cluster 2**	**Cluster 3**	**Cluster 4**	**Cluster 5**	**Cluster 6**	**Cluster 7**	**Cluster 8**	**Cluster 9**
Pesticides	6-benzyladenine Azoxystrobin Beflubutamid Benalaxyl-M Bupirimate Captan Carfentrazone-ethyl Clodinafop-propargyl Cyflufenamid Difenoconazole **Dimethomorph** Epoxiconazole Ethion Fenarimol **Fenbuconazole** **Fenpropimorph** Fipronil Fluazinam Flumioxazin Fluopicolide Fluopyram Fluoxastrobin Flurtamone **Folpet** Imidacloprid Indoxacarb **Kresoxim-methyl** Mandipropamid Mefenpyr-diethyl Metconazole	1-naphthylacetic acid Carbaryl **Chlorothalonil** Chlorpropham **Chlorpyrifos-methyl** Chlortoluron Cymoxanil **Cyprodinil** Dieldrin Diuron Glyphosate Isoproturon Lindane Myclobutanil Prohexadione-calcium **Propyzamide** **Prosulfocarb** Pyrimethanil Tebuthiuron Terbuthylazine Terbutryn **Tri-allate**	Flazasulfuron Florasulam Fosetyl-aluminium Iodosulfuron-methyl-sodium Mesosulfuron-methyl Nicosulfuron Pinoxaden Prosulfuron Pyroxsulam Tembotrione Tribenuron-methyl	2,4-DB Acetamiprid Acetochlor Alachlor Aldrin Benoxacor Carbetamide Chlordane Cycloxydym Cyproconazole Dichlorprop-P **Ethofumesate** **Fenpropidin** Flufenacet Flurochloridone Fluroxypyr Heptachlore Malathion Mesotrione Metaldehyde Metamitron Metazachlor Metolachlor Penconazole Pirimicarb Prochloraz **Propiconazole** Quinmerac **S-metolachlor** **Spiroxamine** **Tetraconazole** Thiamethoxam	Ametoctradin Beta-cyfluthrin Bifenthrin Chlorantraniliprole Cyfluthrin Cypermethrin Deltamethrin Dithianon Etofenprox Lambda-cyhalothrin Meptyldinocap Metiram Oryzalin Phenmedipham Tau-fluvalinate	Aclonifen Bixafen **Boscalid** **Bromoxynil octanoate** Butralin Chlorpyrifos Cyazofamid Dicloran **Diflufenican** Dimoxystrobin Dodine Fludioxonil Flumetralin Isoxaben Lenacil Mancozeb Maneb Metrafenone Oxadiazon Oxyfluorfen **Pendimethalin** Proquinazid **Quinoxyfen** Thiram Trifluralin	2,4-D Amitrole Bentazone Bromoxynil Chlormequat chloride **Clomazone** Clopyralid Dicamba Dichlorvos Dimethenamid **Dimethenamid-P** Dimethoate Ethephon Flonicamid Glufosinate Mecoprop Metalaxyl-M Metribuzin Pentachlorophenol Triclopyr	Abamectin Mirex	Endrin Toxaphene

	Metsulfuron-methyl Napropamide Permethrin Phosmet Picoxystrobin Piperonyl butoxide Propaquizafop Pyraclostrobin Pyraflufen-ethyl Quizalofop-p-ethyl Spirotetramat **Tebuconazole** Thiacloprid Thifensulfuron-methyl Thiophanate-methyl Tolylfluanid Triadimenol **Trifloxystrobin** Zoxamid								
Number of atoms	41	27	44	34.5	47	36	21	78	26.5
Number of non-hydrogen atoms	24	15	28	18	28	20	13	42	18.5
Number of hydrogen atoms	17	11.5	16	15.5	19	12	9	36	8
Number of carbon atoms	17	10	15	12.5	22	14	7.5	29	11
Number of nitrogen atoms	2	1.5	5	1	2	2	1	0	0
Number of oxygen atoms	3	1	6	2	3	2	2.5	7	0.5
Number of chlorine atoms	1	0.5	0	1	0	0	1	6	7
Number of fluorine atoms	0	0	0	0	0	0	0	0	0
Number of halogen atoms	1	0.5	1	1	2	1	1	6	7
Number of phosphorus	0	0	0	0	0	0	0	0	0

atoms									
Number of sulfur atoms	0	0	1	0	0	0	0	0	0
Number of bonds	43	27	45	34.5	49	37	20.5	83	29
Number of non-hydrogen bonds	26	15	29	19	30	20	13	47	21
Number of double bonds	2	1	3	1	2	2	1	3	1
Number of triple bonds	0	0	0	0	0	0	0	0	0
Number of multiple bonds	13	7	16	7	15	10	6.5	3	1
Number of rotatable bonds	6	2	6	4.5	7	4	2.5	4	0
Number of aromatic bonds	12	6	12	6	12	6	6	0	0
Sum of conventional bond order	33	19	38	22.75	39	27.5	17	50	22
Number of rings	2	1	2	2	3	2	1	6	3.5
Number of circuits	2	1	2	2	3	2	1	21.5	9
Molecular weight (g mol^{-1})	355.4	229.0	410.5	284.0	416.3	326.4	225.1	709.4	396.4
Connolly molecular surface area ($Å^2$)	302.2	204.0	322.6	241.5	316.9	269.6	181.7	477.9	235.9
MCI order 0	17.69	11.45	20.89	13.61	20.31	15.45	10.25	30.84	13.73
MCI order 1	11.72	6.99	12.83	8.69	13.32	9.58	6.08	19.50	8.50
MCI order 2	10.63	6.44	12.52	7.71	12.31	8.94	5.53	20.06	9.08
MCI order 3	8.47	4.76	9.17	6.11	9.39	6.66	4.26	19.75	9.07
MCI order 4	6.70	3.62	7.37	4.95	7.59	5.79	2.85	17.04	8.17
MCI order 5	5.13	2.24	5.59	3.69	5.90	4.66	2.04	14.16	6.40
Valence MCI order 0	14.12	9.80	15.87	12.06	16.94	13.02	8.76	28.41	14.37
Valence MCI order 1	8.08	5.15	9.23	6.89	9.56	6.92	4.53	16.58	8.52
Valence MCI order 2	6.14	3.93	7.13	5.10	7.41	5.56	3.69	16.28	9.06
Valence MCI order 3	4.08	2.32	4.92	3.44	5.05	3.51	2.21	15.90	8.97
Valence MCI	2.62	1.56	3.61	2.47	3.30	2.32	1.34	13.23	7.97

order 4									
Valence MCI order 5	1.76	0.92	2.31	1.47	2.23	1.52	0.75	10.61	6.10
Polarizability ($Å^3$)	35.744	24.014	37.397	30.000	45.368	32.806	20.163	67.782	33.070
Dipole moment (D)	3.648	3.159	5.347	3.065	3.945	3.945	2.774	2.582	2.235
HOMO energy (eV)	-9.334	-9.231	-9.630	-9.552	-9.195	-9.152	-9.716	-10.214	-9.860
LUMO energy (eV)	-0.584	-0.181	-1.323	-0.448	-0.486	-1.001	-0.296	-0.209	-0.363
Total energy (eV)	-4734.1	-2775.9	-5524.0	-3462.8	-4965.8	-3877.0	-2792.0	-8693.9	-4293.0
P_{vap} (mPa)	$2.00\ 10^{-3}$	0.15	$1.00\ 10^{-4}$	0.16	$1.24\ 10^{-5}$	0.016	0.61	0.016	$1.53\ 10^{-3}$
Sw (mg L^{-1})	5.20	20.5	4000	260	0.022	0.93	20914	0.011	$8.79\ 10^{-3}$
Koc (L kg^{-1})	894	593	35	233	124000	7061	52.6	5715	100
DT50 (d)	24.4	43.5	9.10	26.5	13	117	8.73	164	3500

Table S6

TyPol clustering of the 178 pesticides using the 40 molecular descriptors and three parameters (vapor pressure P_{vap}, water solubility Sw, and octanol-water partition coefficient log Kow) for plant emission potential. Pesticides detected in the air of the five experimental sites (Alsace, Bretagne, Centre-Val de Loire, Lorraine, Nouvelle

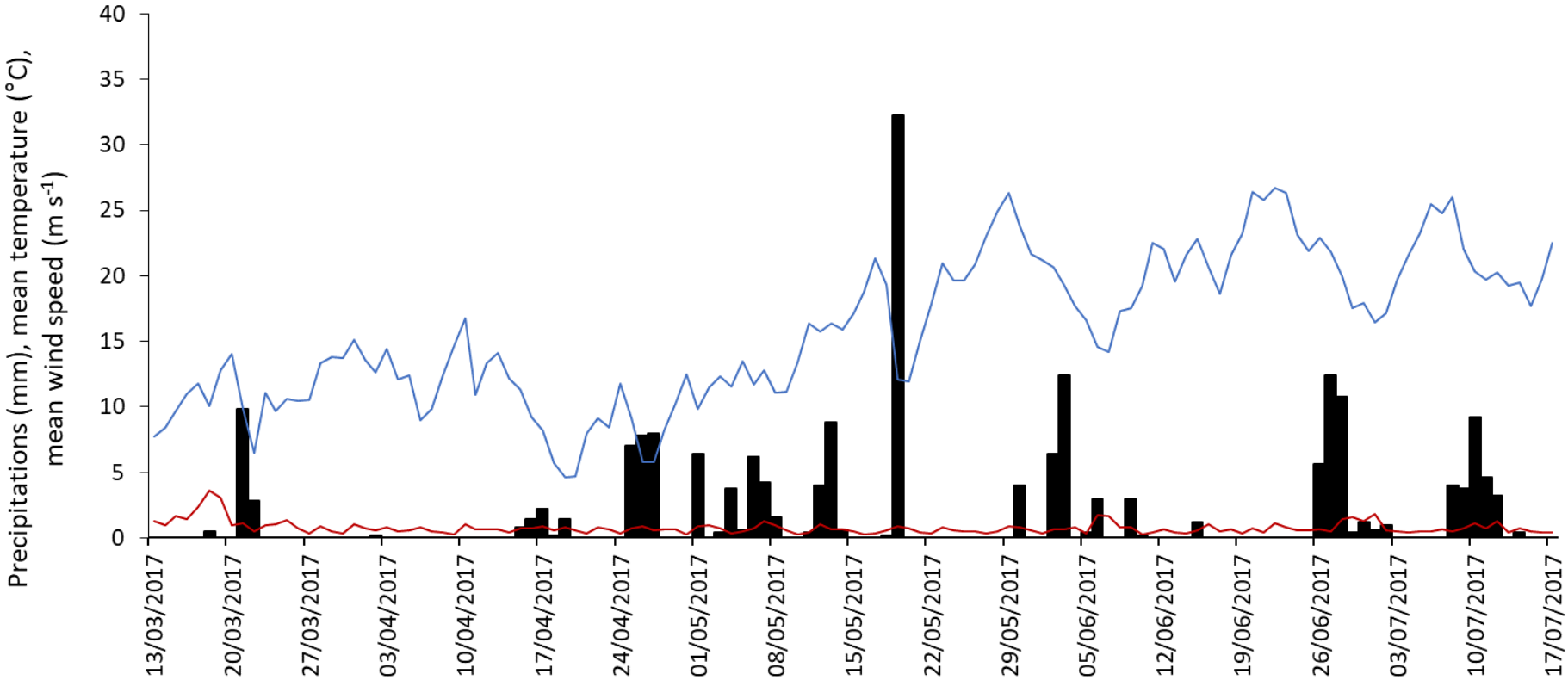
Aquitaine) are indicated in red and bold, pesticides applied but not detected in air are indicated in green. The values of molecular descriptors and parameters are the median values for the cluster. MCI: Molecular connectivity index, HOMO: Highest occupied molecular orbital, LUMO: Lowest unoccupied molecular orbital.

	Cluster 1	Cluster 2	Cluster 3	Cluster 4	Cluster 5	Cluster 6	Cluster 7	Cluster 8	Cluster 9	Cluster 10
Pesticides	Azoxystrobin Bixafen Chlorantraniliprole Chlordane Cyflufenamid Dieldrin Difenoconazole **Diflufenican** Endrin Fluoxastrobin Indoxacarb Mirex Propaquizafop Pyraclostrobin Pyraflufen-ethyl Quizalofop-p-ethyl	Acetochlor Alachlor Benoxacor Bupirimate Captan Carbaryl **Chlorothalonil** Chlorpropham **Chlorpyrifos-methyl** Chlortoluron **Cyprodinil** Dicloran Diuron **Ethofumesate** Flurochloridone Isoproturon Lindane Malathion Mancozeb Metiram Metolachlor Phosmet **Propyzamide** **Prosulfocarb** Pyrimethanil **S-metolachlor** Terbuthylazine Terbutryn Thiophanate-methyl Thiram **Tri-allate** Triclopyr	Flazasulfuron Florasulam Iodosulfuron-methyl-sodium Mesosulfuron-methyl Metsulfuron-methyl Nicosulfuron Prosulfuron Pyroxsulam Tembotrione Thifensulfuron-methyl Tribenuron-methyl	1-naphthylacetic acid 2,4-DB Acetamiprid Carbetamide **Clomazone** Cycloxydym Cymoxanil Dichlorprop-P Dichlorvos Dimethenamid **Dimethenamid-P** Dimethoate Dodine **Fenpropidin** Fluroxypyr Imidacloprid Maneb Mesotrione Metalaxyl-M Metaldehyde Metamitron Metazachlor Metribuzin Pentachlorophenol Pirimicarb **Spiroxamine** Tebuthiuron Thiacloprid Thiamethoxam	Beta-cyfluthrin Bifenthrin Cyfluthrin Deltamethrin Etofenprox Lambda-cyhalothrin Tau-fluvalinate	Aclonifen Aldrin Ametoctradin Beflubutamid Clodinafop-propargyl Cyazofamid Cypermethrin Dimoxystrobin Dithianon **Fenpropimorph** Fipronil Fluazinam Fludioxonil Flumetralin Flumioxazin Flurtamone **Folpet** Heptachlore Isoxaben **Kresoxim-methyl** Lenacil Metrafenone Oryzalin Permethrin Phenmedipham Piperonyl butoxide **Quinoxyfen** Tolylfluanid Toxaphene **Trifloxystrobin** Zoxamid	2,4-D Amitrole Bentazone Bromoxynil Chlormequat chloride Clopyralid Dicamba Ethephon Flonicamid Fosetyl-aluminium Glufosinate Glyphosate Mecoprop Prohexadione-calcium Quinmerac	6-benzyladenine Benalaxyl-M **Boscalid** Carfentrazone-ethyl Cyproconazole **Dimethomorph** Epoxiconazole Fenarimol **Fenbuconazole** Flufenacet Fluopicolide Fluopyram Mandipropamid Mefenpyr-diethyl Metconazole Myclobutanil Napropamide Penconazole Picoxystrobin Pinoxaden Prochloraz **Propiconazole** Spirotetramat **Tebuconazole** **Tetraconazole** Triadimenol	**Bromoxynil octanoate** Butralin Chlorpyrifos Ethion Meptyldinocap Oxadiazon Oxyfluorfen **Pendimethalin** Proquinazid Trifluralin	Abamectin
Number of atoms	42.5	28.5	42	28	50	38	20	39	39	134
Number of non-hydrogen atoms	27	16	27	16	29	23	13	23	20.5	62
Number of hydrogen	15	12.5	15	14	19	14	8	17	17.5	72

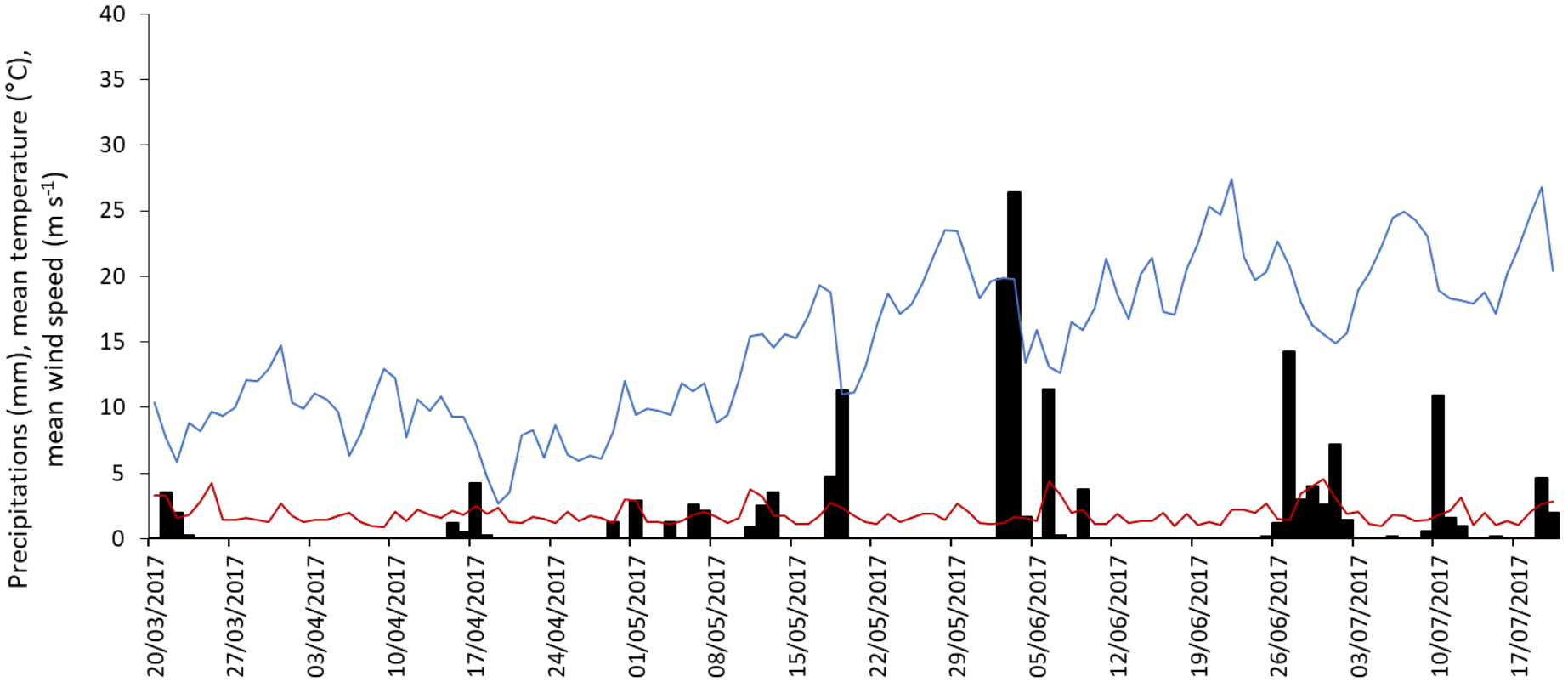
atoms										
Number of carbon atoms	19	10.5	14	10	23	16	7	16	14	48
Number of nitrogen atoms	2.5	1	5	1	1	2	1	3	2	0
Number of oxygen atoms	2.5	1.5	6	2	3	2	3	1.5	4	14
Number of chlorine atoms	1.5	1	0	0	1	0	0	1	0	0
Number of fluorine atoms	0	0	0	0	1	0	0	0	0	0
Number of halogen atoms	4.5	1	1	0	3	2	1	1.5	1.5	0
Number of phosphorus atoms	0	0	0	0	0	0	0	0	0	0
Number of sulfur atoms	0	0	1	0	0	0	0	0	0	0
Number of bonds	44.5	29.5	44	28	52	39	19	40.5	38	140
Number of non-hydrogen bonds	29.5	16	28	16	31	23	13	24.5	20	68
Number of double bonds	1	1	4	1	2	2	1	1	2	6
Number of triple bonds	0	0	0	0	1	0	0	0	0	0
Number of multiple bonds	17.5	7	16	7	15	13	7	12	8	6
Number of rotatable bonds	5	3	6	3	7	4	2	5	6	8
Number of aromatic bonds	17	6	12	6	12	11	6	11	6	0
Sum of conventional bond order	38.5	21	38	21	41	31.5	17	31.25	26.5	74

Number of rings	3	1	2	1	3	2	1	2	1	7
Number of circuits	4	1	2	1	3	2	1	2	1	15
Molecular weight ($g\ mol^{-1}$)	411.1	258.3	410.5	249.1	434.3	338.5	214.6	342.7	356.2	873.2
Connolly molecular surface area ($Å^2$)	321.4	222.8	315.3	218.2	381.3	287.7	167.9	294.5	287.0	698.8
MCI order 0	19.57	11.69	20.24	11.64	21.18	16.66	9.85	16.82	15.91	44.67
MCI order 1	13.08	7.32	12.69	7.77	13.73	10.63	6.07	11.09	9.58	29.50
MCI order 2	12.22	6.84	12.31	6.60	13.02	9.48	5.43	10.16	9.07	27.87
MCI order 3	9.97	5.05	9.16	5.09	9.94	7.90	3.78	8.25	6.55	24.49
MCI order 4	8.14	3.69	7.33	3.69	7.96	6.27	2.70	6.51	5.22	20.34
MCI order 5	6.59	2.53	5.59	2.95	6.24	4.96	1.90	4.84	4.38	16.52
Valence MCI order 0	15.46	10.95	15.77	10.00	17.25	13.57	7.97	13.57	13.47	38.22
Valence MCI order 1	8.63	6.09	9.07	5.43	9.70	7.74	4.32	7.59	7.32	22.86
Valence MCI order 2	6.90	4.51	6.93	4.49	8.34	5.95	3.39	5.99	6.09	18.96
Valence MCI order 3	4.44	2.94	4.73	2.81	5.32	4.11	2.02	4.08	3.47	14.50
Valence MCI order 4	2.86	1.86	3.34	1.69	3.31	2.63	1.21	2.74	2.33	10.56
Valence MCI order 5	1.91	1.08	2.11	1.07	2.32	1.85	0.69	1.70	1.57	7.45
Polarizability ($Å^3$)	40.717	25.975	36.352	25.269	45.764	34.096	19.970	35.362	32.802	94.851
Dipole moment (D)	3.194	3.432	5.688	3.174	2.504	3.832	3.370	3.255	3.977	5.154
HOMO energy (eV)	-9.415	-9.116	-10.020	-9.404	-9.216	-9.175	-9.789	-9.416	-9.755	-9.238
LUMO energy (eV)	-0.606	-0.529	-1.358	-0.411	-0.486	-0.534	-0.534	-0.428	-1.396	-0.150
Total energy (eV)	-5441.0	-3027.7	-5524.0	-2971.2	-5462.2	-4134.5	-2739.8	-4156.2	-3947.6	-11625.4
P_{vap} (mPa)	$2.94\ 10^{-5}$	0.17	$1.1\ 10^{-5}$	0.12	$2.00\ 10^{-4}$	$8.00\ 10^{-3}$	0.031	$2.67\ 10^{-3}$	0.37	$3.70\ 10^{-3}$
Sw ($mg\ L^{-1}$)	0.50	18.2	3200	1210	$1.20\ 10^{-3}$	0.80	100000	30.1	0.32	1.21

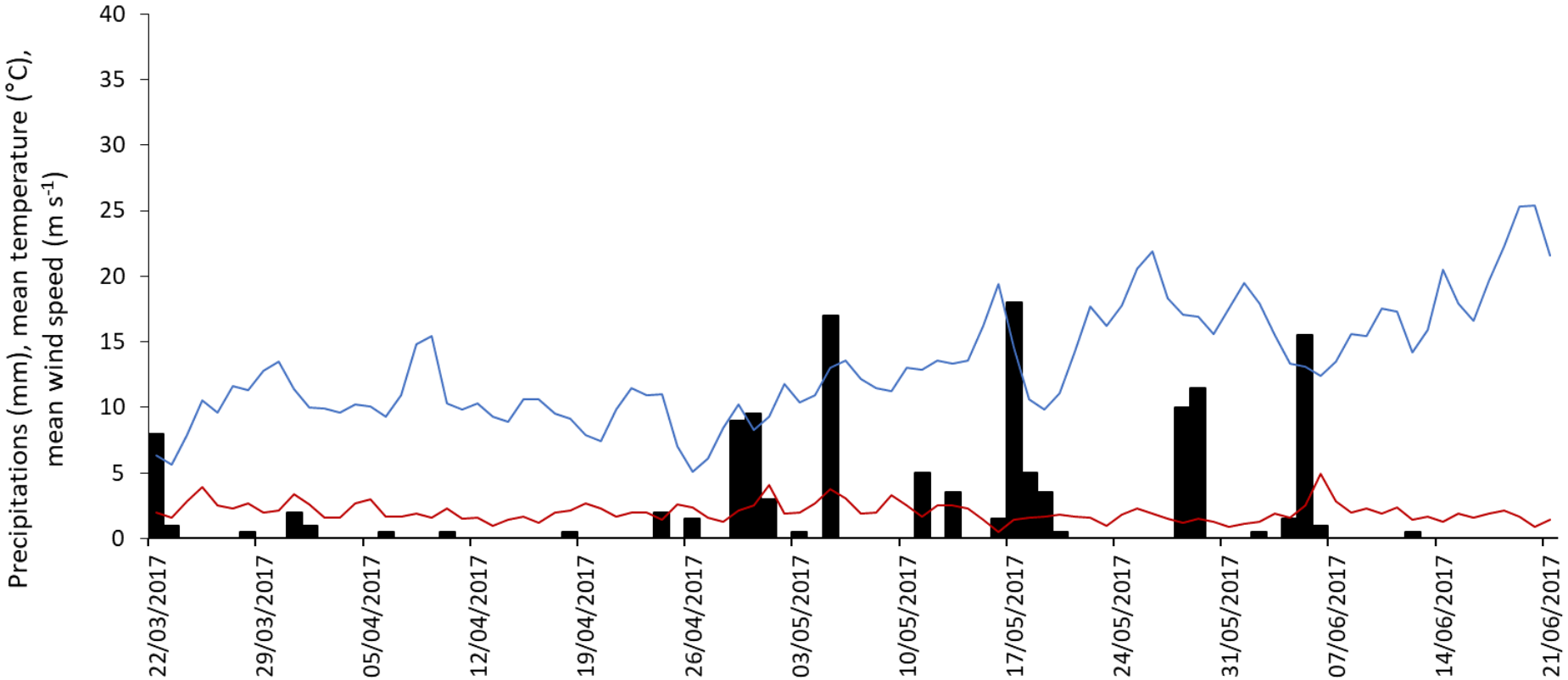
log Kow (-)	3.84	3.00	-0.70	1.26	6.0	3.94	-1.88	3.40	5.29	4.40



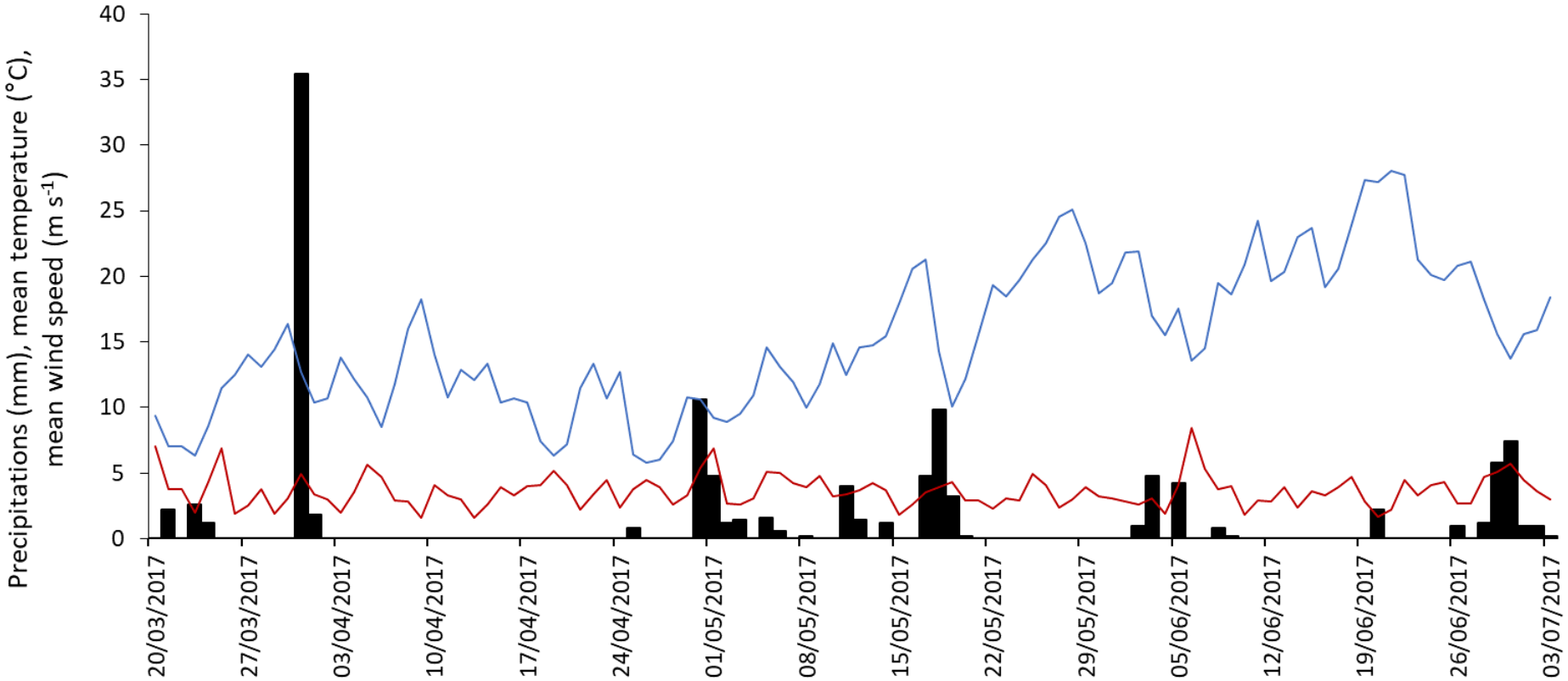
(a) Alsace (daily precipitations (mm) ■, daily mean temperature (°C) —, daily mean wind speed (m s^{-1}) —)



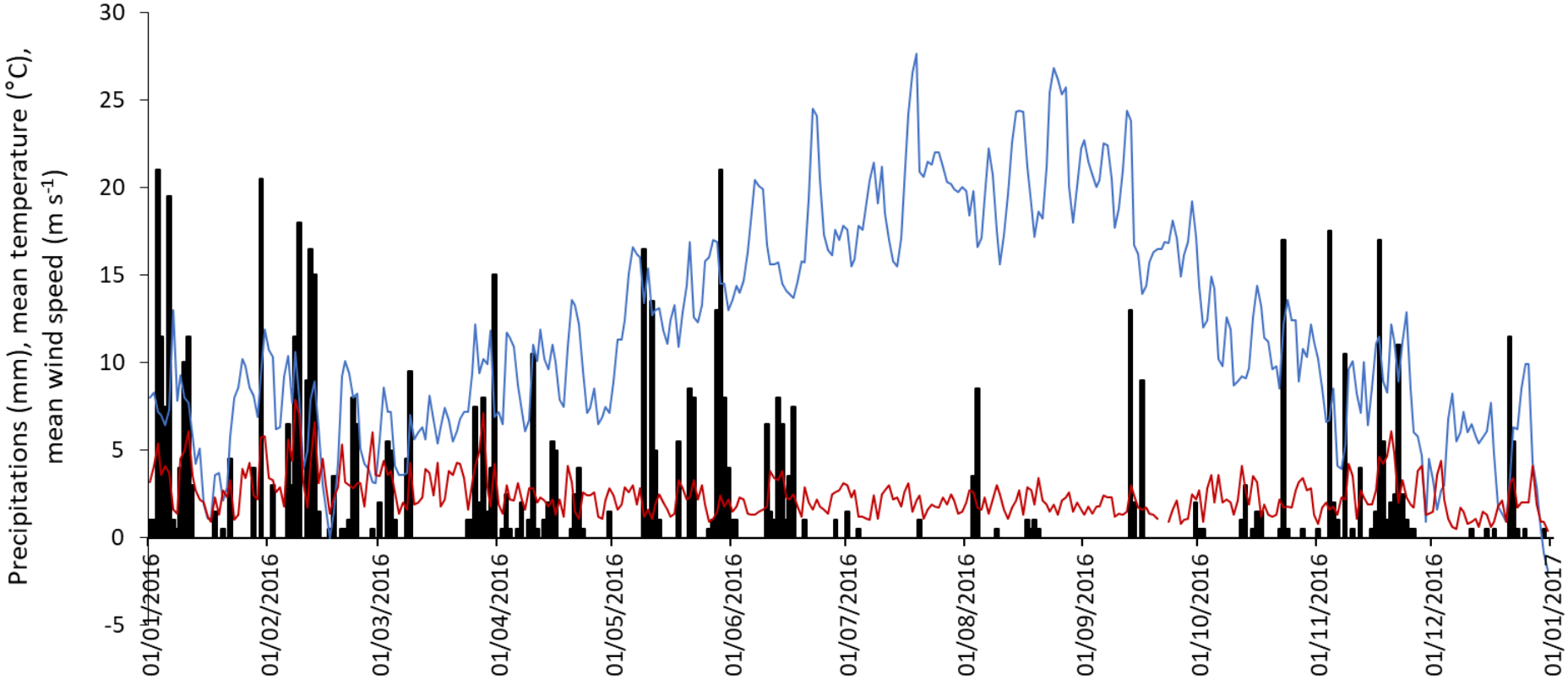
(b) Lorraine (daily precipitations (mm) ■, daily mean temperature (°C) —, daily mean wind speed (m s^{-1}) —)



(c) Bretagne (daily precipitations (mm) ■, daily mean temperature (°C) —, daily mean wind speed (m s^{-1}) —)

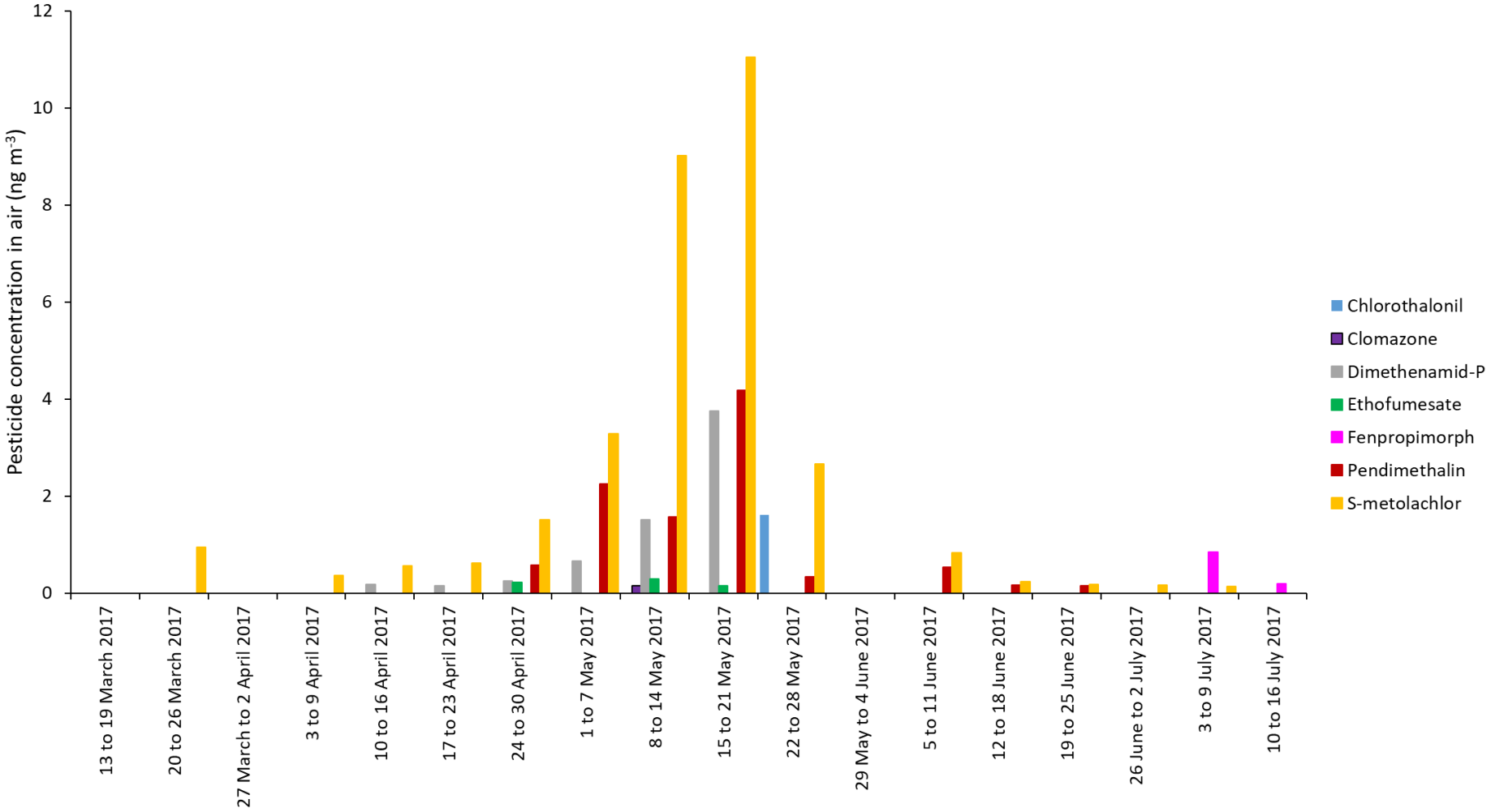


(d) Centre-Val de Loire (daily precipitations (mm) ■, daily mean temperature (°C) —, daily mean wind speed (m s^{-1}) —)

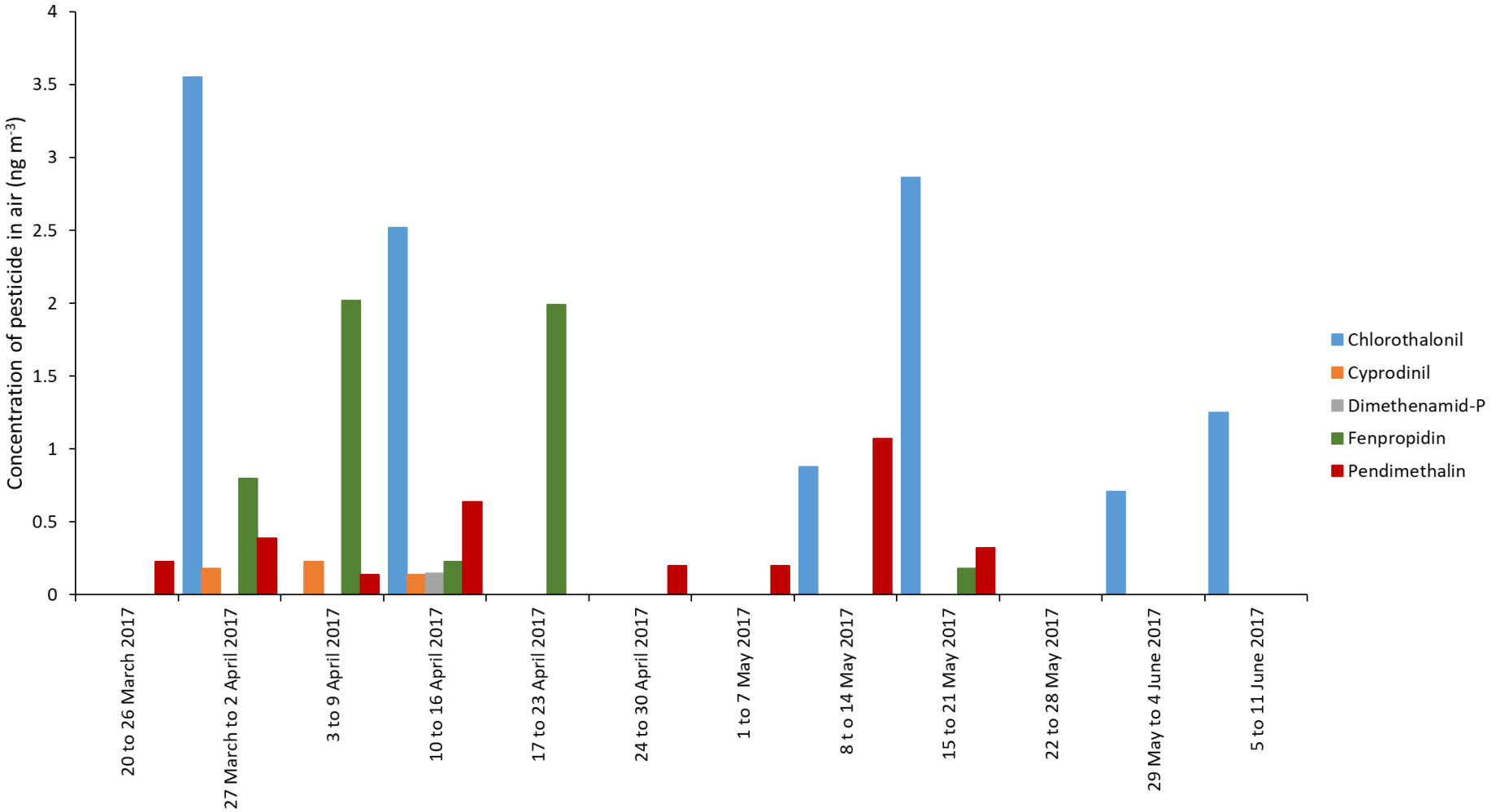


(e) Nouvelle Aquitaine

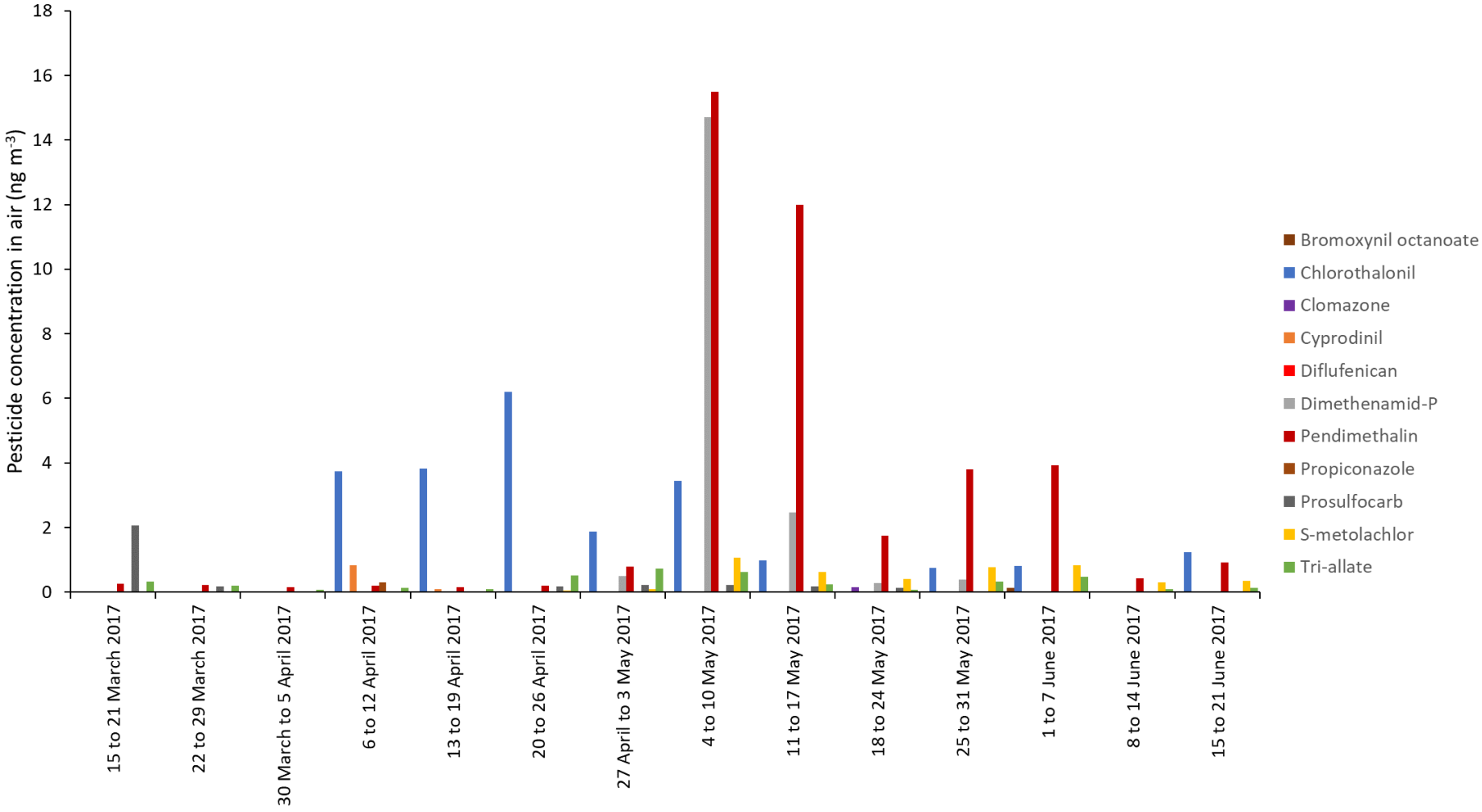
Fig. S1. Meteorological data (daily precipitations (mm) ■, daily mean temperature (°C) —, daily mean wind speed (m s^{-1}) —) measured in the five experimental sites: (a) Alsace, (b) Lorraine, (c) Bretagne, (d) Centre-Val de Loire, (e) Nouvelle Aquitaine.


Pesticide concentration in air (ng m-3)
12
10
8
6
4
2
0
13 to 19 March 2017
20 to 26 March 2017
27 March to 2 April 2017
3 to 9 April 2017
10 to 16 April 2017
17 to 23 April 2017
24 to 30 April 2017
1 to 7 May 2017
8 to 14 May 2017
15 to 21 May 2017
22 to 28 May 2017
29 May to 4 June 2017
5 to 11 June 2017
12 to 18 June 2017
19 to 25 June 2017
26 June to 2 July 2017
3 to 9 July 2017
10 to 16 July 2017
Chlorothalonil
Clomazone
Dimethenamid-P
Ethofumesate
Fenpropimorph
Pendimethalin
S-metolachlor

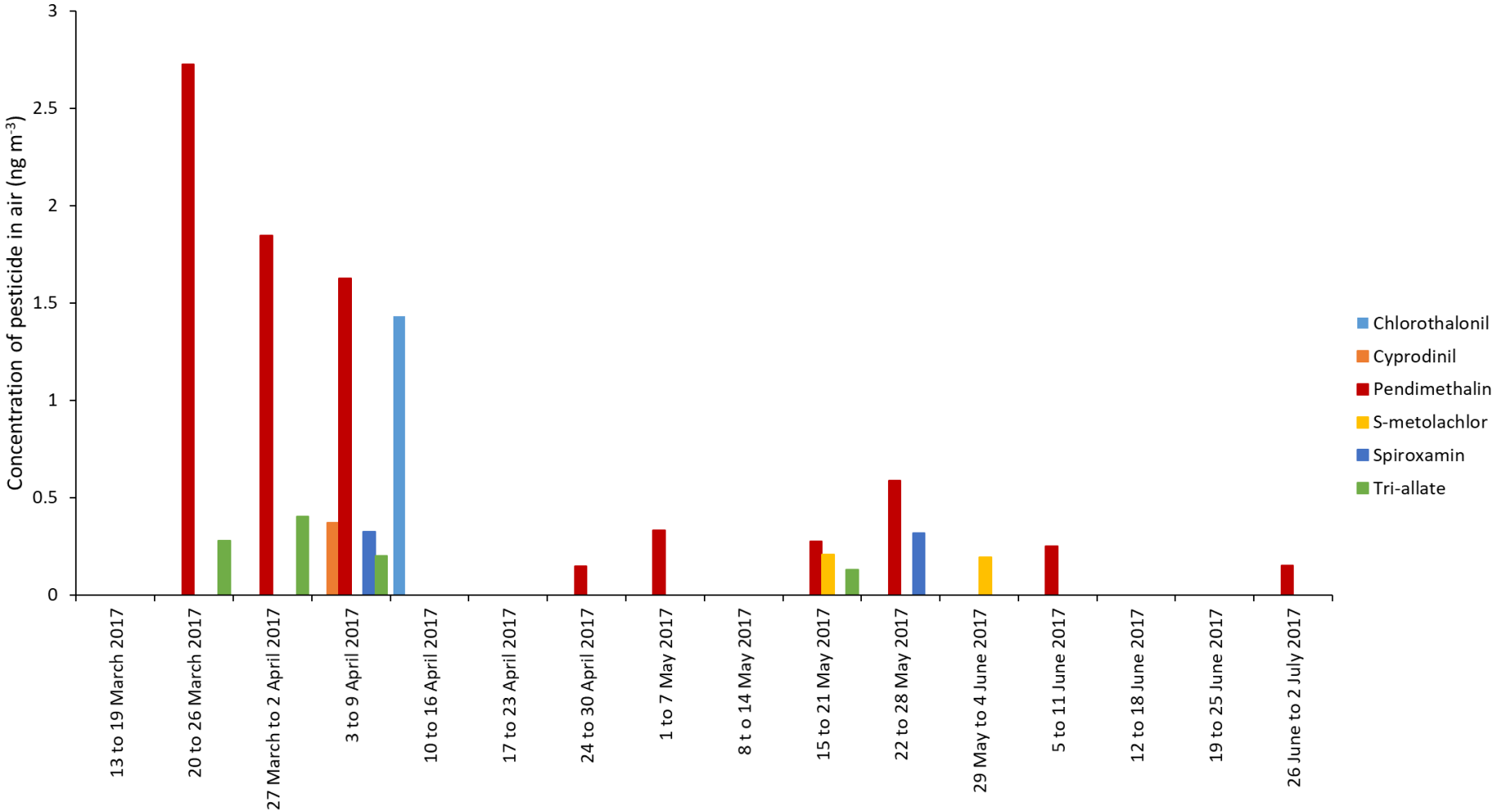
(a) Alsace


Concentration of pesticide in air (ng m-3)
4
3.5
3
2.5
2
1.5
1
0.5
0
20 to 26 March 2017
27 March to 2 April 2017
3 to 9 April 2017
10 to 16 April 2017
17 to 23 April 2017
24 to 30 April 2017
1 to 7 May 2017
8 t o 14 May 2017
15 to 21 May 2017
22 to 28 May 2017
29 May to 4 June 2017
5 to 11 June 2017
Chlorothalonil
Cyprodinil
Dimethenamid-P
Fenpropidin
Pendimethalin

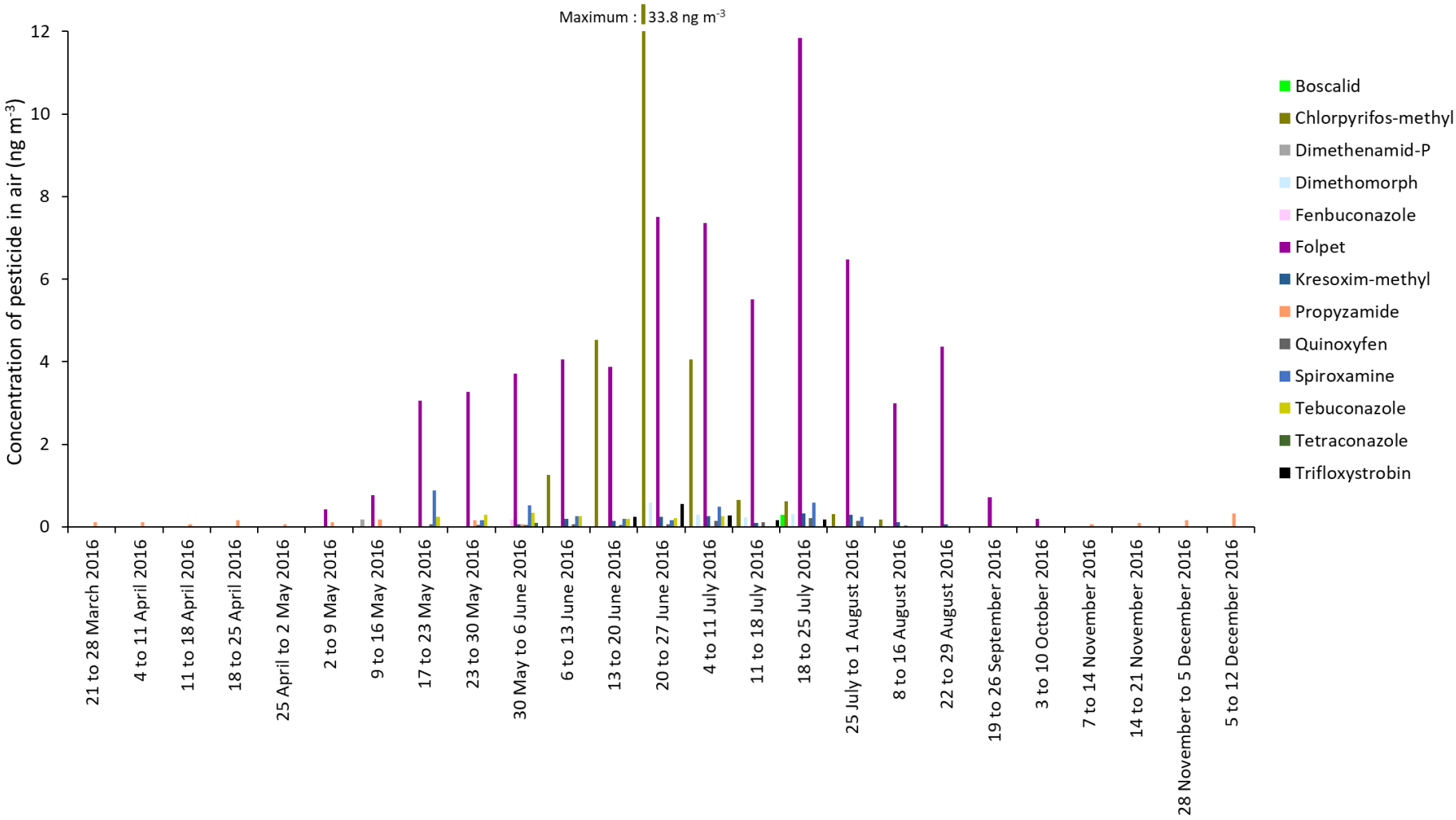
(b) Lorraine


Pesticide concentration in air (ng m-3)
18
16
14
12
10
8
6
4
2
0
15 to 21 March 2017
22 to 29 March 2017
30 March to 5 April 2017
6 to 12 April 2017
13 to 19 April 2017
20 to 26 April 2017
27 April to 3 May 2017
4 to 10 May 2017
11 to 17 May 2017
18 to 24 May 2017
25 to 31 May 2017
1 to 7 June 2017
8 to 14 June 2017
15 to 21 June 2017
Bromoxynil octanoate
Chlorothalonil
Clomazone
Cyprodinil
Diflufenican
Dimethenamid-P
Pendimethalin
Propiconazole
Prosulfocarb
S-metolachlor
Tri-allate

(c) Bretagne

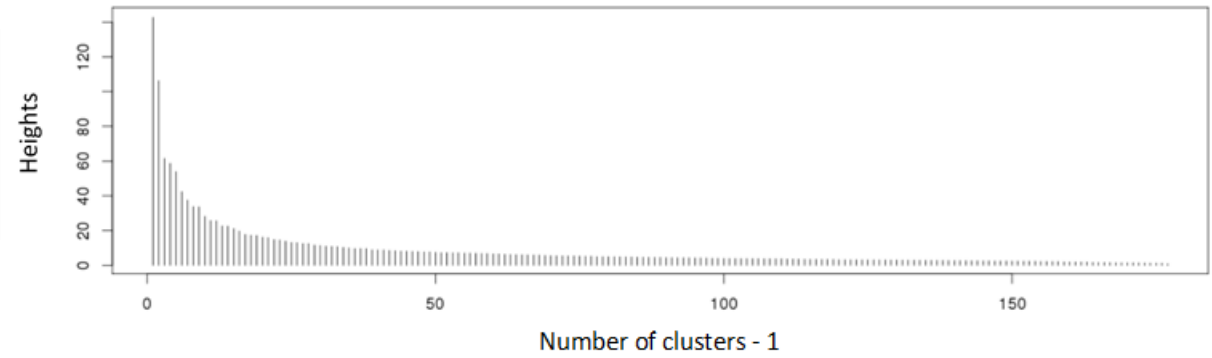


(d) Centre-Val de Loire

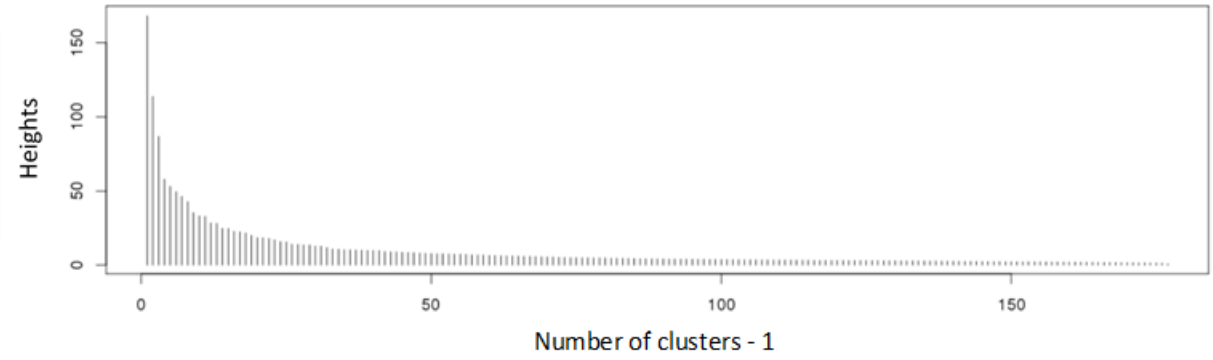


(e) Nouvelle Aquitaine

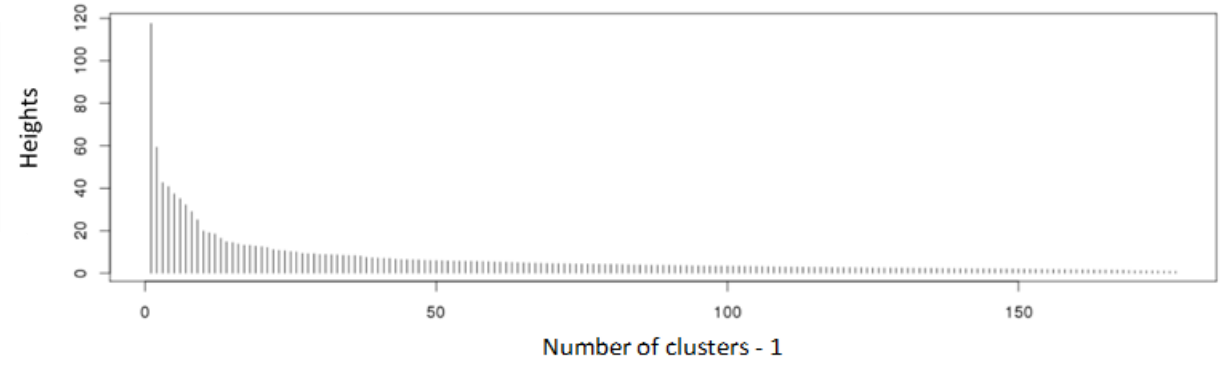
Fig. S2. Dynamics of pesticide concentrations measured in the air of the five experimental sites: Alsace (a), Lorraine (b), Bretagne (c), Centre-Val de Loire (d), and Nouvelle Aquitaine (e).



(a) Global potential emission to air (six clusters)

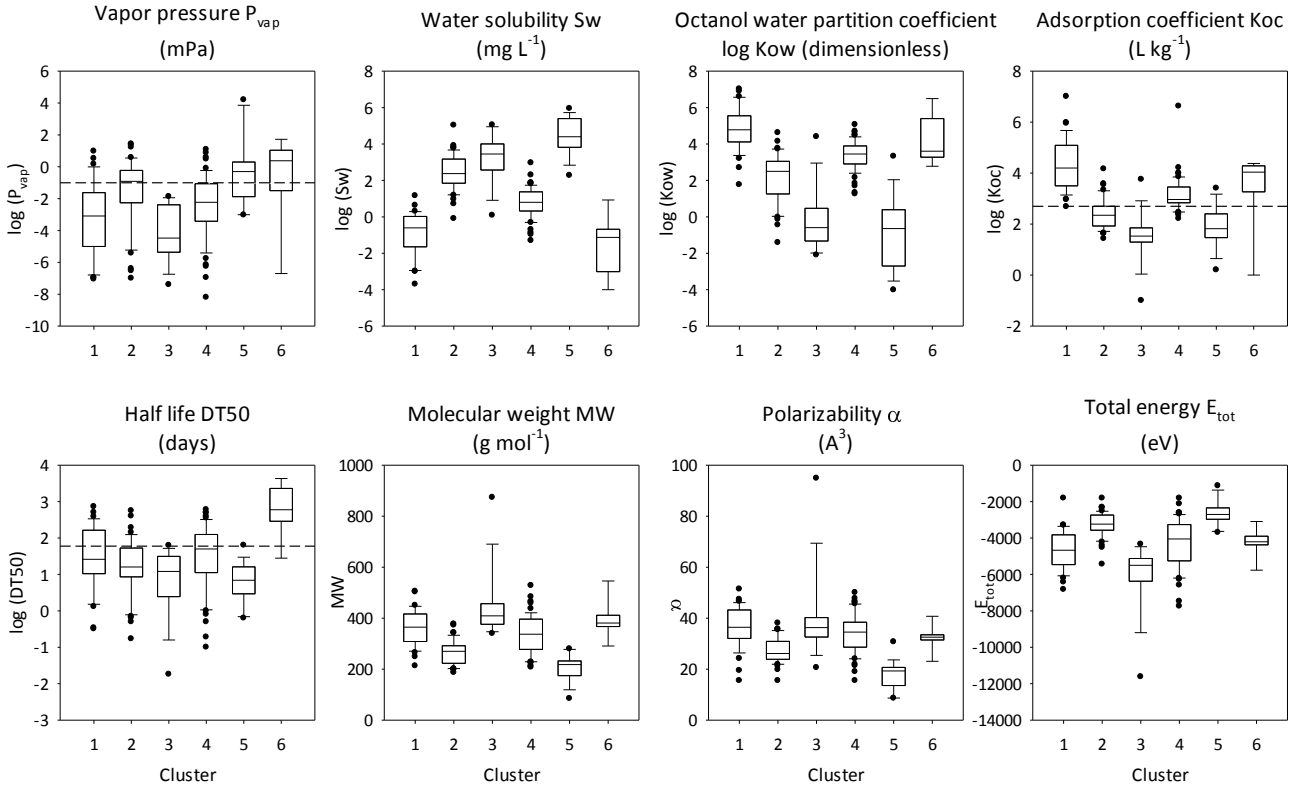


(b) Soil potential emission to air (nine clusters)



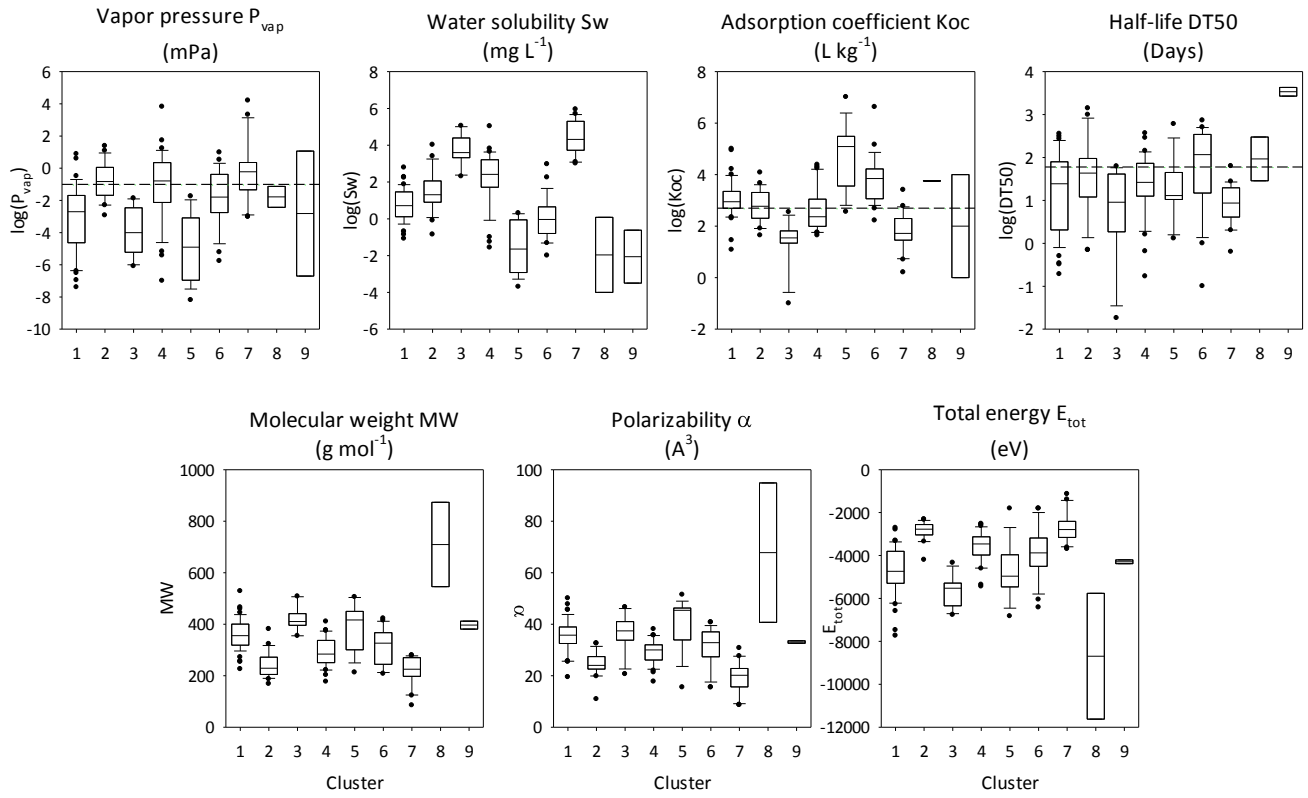
(c) Plant potential emission to air (ten clusters)

Fig. S3. TyPol barplots for the heights of the dendrograms obtained for global (a), soil (b) and plant (c) potential emission to air analyses.



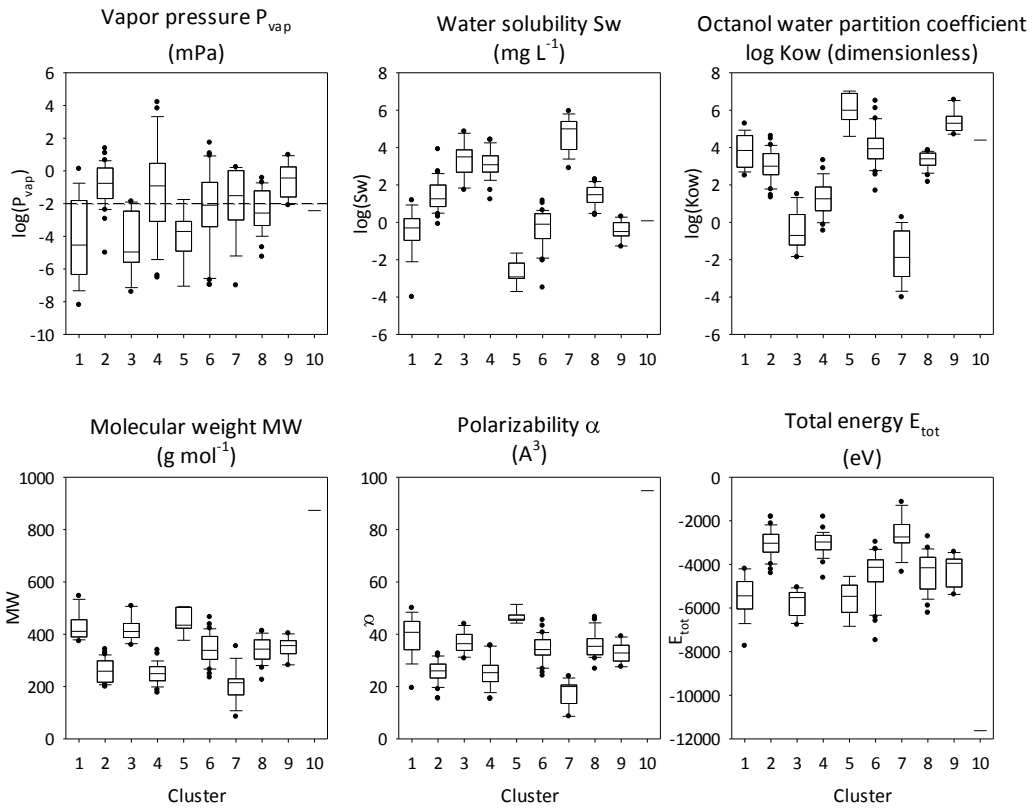
Cluster	1	2	3	4	5	6
Total number of pesticides	35	47	14	56	18	8
Number of applied and detected pesticides	4	9	0	13	0	0
Number of applied but not detected pesticides	8	9	5	8	2	0

Fig. S4. Range of variation (box-and-whisker plots) of the values of the five parameters considered into TyPol (water solubility Sw, octanol water partition coefficient log Kow, vapor pressure P_{vap}, adsorption coefficient normalized to soil carbon organic content Koc, and degradation half-life in soil DT50) and of some relevant molecular descriptors (molar mass, polarizability, total energy) for each cluster after analysis of the 178 pesticides for global emission potential to air. Dotted lines represent the limits between volatile (log P_{vap} > -1) and non-volatile compounds (log P_{vap} < -1) (FOCUS, 2008); mobile (log Koc < 2.7) and non-mobile compounds (log Koc > 2.7) (Mc Call et al., 1980); persistent (log DT50 > 1.78) and non-persistent compounds in soil (log DT50 < 1.78) (Regulation (EC) No 1107/2009, 2009). Table summarizes the number of pesticides in each cluster and the number of applied, detected and not detected pesticides.



Cluster	1	2	3	4	5	6	7	8	9
Total number of pesticides	49	22	11	32	15	25	20	2	2
Number of applied and detected pesticides	7	6	0	6	0	5	2	0	0
Number of applied but not detected pesticides	9	1	4	6	5	5	2	0	0

Fig. S5. Range of variation (box-and-whisker plots) of the values of the four parameters considered into TyPol (water solubility Sw, vapor pressure P_{vap}, adsorption coefficient normalized to soil carbon organic content Koc, and pesticide degradation half-life in soil DT50) and of some relevant molecular descriptors (molar mass, polarizability, total energy) for each cluster after analysis of the 178 pesticides for soil emission potential to air. Dotted lines represent the limits between volatile (log P_{vap} > -1) and non-volatile compounds (log P_{vap} < -1) after emission from soil (FOCUS, 2008); mobile (log Koc < 2.7) and non-mobile compounds (log Koc > 2.7) (Mc Call et al., 1980); persistent (log DT50 > 1.78) and non-persistent compounds in soil (log DT50 < 1.78) (Regulation (EC) No 1107/2009, 2009). Table summarizes the number of pesticides in each cluster and the number of applied, detected and not detected pesticides.



Cluster	1	2	3	4	5	6	7	8	9	10
Total number of pesticides	16	32	11	29	7	31	15	26	10	1
Number of applied and detected pesticides	1	8	0	4	0	5	0	6	2	0
Number of applied but not detected pesticides	3	4	4	6	2	6	2	4	1	0

Fig. S6. Range of variation (box-and-whisker plots) of the values of the three parameters considered into TyPol (water solubility Sw, octanol water partition coefficient log Kow, and vapor pressure P_{vap}) and of some relevant molecular descriptors (molar mass, polarizability, total energy) for each cluster after analysis of the 178 pesticides for plant emission potential to air. Dotted line represents the limit between volatile (log P_{vap} > -2) and non-volatile compounds (log P_{vap} < -2) following emission from plant (FOCUS, 2008). Table summarizes the number of pesticides in each cluster and the number of applied, detected and not detected pesticides.

References

FOCUS, 2008. Pesticides in air: considerations for exposure assessment. Report of the FOCUS Working Group on Pesticides in Air, EC Document Reference SANCO/10553/ 2006 Rev 2, June 2008.

McCall, P.J., Swann, R.L., Laskowski, D.A., Unger, S.M., Vrona, S.A., Dishburger, H.J., 1980. Estimation of chemical mobility in soil from liquid chromatographic retention times. Bull. Environ. Contam. Toxicol. 24, 190-195.

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Regulation (EC) No 1107/2009, 2009. Regulation (EC) No 1107/2009 of the European Parliament and of the Council of 21 October 2009 concerning the placing of plant protection products on the market and repealing Council Directives 79/117/EEC and 91/ 414/EEC.