Supporting Information

for

Organic chemicals jeopardize the health of freshwater ecosystems on the continental scale

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This file includes:

Data deposition: Datasets and R code are deposited at https://www.uni-koblenz-landau.de/campus-landau/faculty7/environmental-sciences/landscape-ecology/publications/Malaj/at_download/file

1. SI Methods

1.1 Chemical data

Monitoring data for chemical concentrations in the European River Basins were retrieved from the European Environmental Agency (EEA) in July 2012 as part of the Waterbase (version 12) dataset, table *HazSubs* (1). In total, this dataset comprises > 8,200 monitoring sites, covering 34 European countries. Quality control of the reported concentrations was performed following the decision flow chart in Fig. S1, which also provides the number of sites omitted for each step. The dataset was restricted to organic compounds that were identified by the Chemical Abstract Service (CAS) registry number. CAS numbers were checked for consistency and harmonised if necessary. Entries without CAS numbers, which was typically the case when organic compounds are reported as the sum of individual compounds (e.g., PCB congeners), were also removed from the dataset (Fig. S1).

The chemical concentrations were reported in µg/L as mean, minimum and maximum annual values for each monitoring site. The quality control document of the EEA provided guidance on the entries that were problematic, such as entries with missing concentrations or duplicate entries (2) that were consequently removed from the analysis (Fig. S1).

For entries with limit of quantification (LOQ) or limit of detection (LOD) not reported (or reported as zero) the original files submitted by the national authorities to the EEA were checked and, when available, the LOQ was added to the dataset. Otherwise, the entries were omitted. Mean and maximum concentrations above the LOQ (or LOD) were considered as reliable measurements and were included in the analysis. These values were referred to as quantified concentrations. Mean and maximum concentrations below the LOQ (or LOD) were considered as unreliable measurements and were set to zero. These cases were referred to as non-detects. We note that this procedure is likely to underestimate the real exposure.

Analytical measurements, and consequently LOQ/LOD values, are highly dependent on the monitoring programs of the countries and on the laboratories involved. Given that a non-quantified or non-detected chemical is generally reported as equal to or a fraction of the LOQ/LOD value (e.g., ½, ¼; ref. 3), the ratios between the minimum reported concentrations and the LOQ/LOD values usually result in integer values (e.g., 1, 2, 4), which was the case for all countries, except Spain. In the case of Spain, no integer ratios were obtained, thus indicating that the reported LOQ values were incorrect. The error in reported LOQ values was further underpinned by the fact that the LOQ values did not follow the general rule of rounded values (e.g., 0.05 µg/L) but had rather odd entries (e.g., 0.86 µg/L). Moreover, due to several sub-basins in the Spanish dataset, more than one LOQ value was reported for each compound. Therefore, the frequency distribution of all maximum concentrations was calculated for each compound to identify LOQ values empirically. In the case of >3 identical maximum values, these repeatedly occurring values were considered to be LOQ values and, in turn, flagged as non-detects. Due to these considerations, the majority (94 %) of entries for Spain were flagged as non-detects, which was higher than the average of the other countries (81 %). This approach allowed to consider the remaining entries as real maximum concentrations. From this remaining Spanish dataset, 10 entries were removed for the chemical cyanide due to concentration values that were three order of magnitude higher than the mean value found in the other sub-basins.

Geographic coordinates for each site were retrieved from the EEA, Waterbase database, table *Station* (1), which was connected with the *HazSubs* dataset via the unique site identifier *WatebaseID*. For 148 sites (all in Hungary), the *WatebaseID* was decapitalised to allow matching. Sites were linked to the river basins of the European Catchments and Rivers Network System database (ECRINS) version 1.0 (4), which defined the river basins as *"the area of land from which all surface run-off flows through a sequence of streams, rivers and, possibly, lakes into the sea at a single river mouth, estuary or delta"* (see ref. 3, Article 2). A few sites (41) were removed due to missing coordinates or coordinates outside Europe.

Sampling sites were considered as spatially autocorrelated when they were (i) less than 5 km apart from each other and (ii) analyzed in the same year. Sites that exhibited autocorrelation with several other sites were removed, whereas for pairs of autocorrelated sites, we removed one of the sites randomly. This process led to the omission of 532 sites (Fig. S1). Finally, 4,004 sites were available, covering 91 river basins in 27 European countries.

1.2 Concentrations for acute and chronic exposure

The number of samples taken in any monitoring program strongly biases the estimation of chronic exposure. To ensure that the mean annual concentration (C_{mean}) was related to multiple detections of a chemical and was not based on a single quantified concentration (i.e., the maximum concentration), we computed a test mean concentration (C_t) assuming that all other values were non-detects. As outlined above, in the regulatory context, non-detects were usually set as a fraction of the LOQ/LOD and reported as the minimum, which would consequently influence the reported C_{mean} (see ref. 3, Article 5). To check whether the reported C_{mean} was determined solely by a single maximum and otherwise minimum annual concentrations (C_{min} and C_{max}), we estimated C_t by:

$$C_t = ((n-1)\, C_{min} + C_{max})/n \quad (1)$$

where n is the number of measurements for each entry.

A ratio $C_{mean}/C_t > 1$ would indicate that C_{max} was not the only quantified concentration. However, given that the probability of measuring a compound likely depends on the *n*, we checked this relationship for sites with > 12 measurements. For the cases where the *n* was > 12 (342 sites) and > 24 (25 sites), we found that 54 % and 60 % of the sites with quantified concentrations had a ratio $C_{mean}/C_t > 1$, respectively. Due to the high uncertainty when drawing conclusions from a small number of sites (e.g., only 5 sites had n > 48), we considered n > 12 as the best compromise between the number of measurements and the representativeness in terms of number of sites. The ratio C_{mean}/C_t for these sites indicated that at least two quantified values (the maximum annual concentration and another concentration between the maximum and minimum) were used for estimating the reported mean in approximately half of the samples. Thus, the mean can be considered representative for the exposure concentration of at least a few weeks.

However, only 20 % of sites had n >12. To remove the dependency of the mean on the LOQ for sites with less frequent sampling (i.e., $n \leq 12$), we estimated a corrected mean concentration $C_{c\text{-}mean}$ using the C_{max}/C_{mean} relationship for the sites with n > 12. The median for this relationship was estimated as approximately three. Thus, $C_{c\text{-}mean}$ for sites with $n \leq 12$ was estimated as:

$$C_{c\text{-}mean} = C_{max}/3 \quad (2)$$

To assess the short-term (acute) exposure, the reported C_{max} was used. For 103 cases where this concentration was not reported, the C_{mean} was used instead. Although episodic peak exposures were likely to be missed (see above), we considered C_{max} as the best approximation of acute exposure in the investigated monitoring programs, especially when considering that several studies have reported a strong relationship between C_{max} and ecological effects (5-7). C_{max} exhibits a higher analytical precision, as it often strongly exceeds the LOQ. The analytical methods are given in Table S1, and although they were not reported for all compounds, analytical methods for chemical monitoring in Europe are considered to be well established and highly standardised (8). Unless data for only one year were reported, the maximum concentration of each chemical over all years was used to represent the maximum exposure of a site.

1.3 Toxicity data

The standard test species used in this analysis (*Pimephales promelas, Daphnia magna,* and

Pseudokirchneriella subcapitata) were selected because they are (i) standard test species for which a vast amount of experimental toxicity data are available; (ii) representatives of the three major organism groups of vertebrates, invertebrates, and plants; (iii) representatives of three major trophic levels of secondary consumers, primary consumers, and primary producers in freshwater ecosystems; and (iv) considered as relatively sensitive to chemical stressors (9).

The endpoints used were either the LC50 (median lethal concentration) or the EC50 (median effect concentration). The LC50 is the concentration at which 50 % of the test population suffers a lethal response (in the case of fish and invertebrate). The EC50 is the concentration at which 50 % of the population suffers an equivalent effect, i.e., immobility for fish and invertebrate, or inhibition of cellular reproduction by 50 % for primary producers. To improve readability, we refer to all endpoints as the LC50.

Experimental toxicity data were available for 80 % of the compounds for *D. magna* and for 54 % of the compounds for both *P. promelas* and *P. subcapitata* (see Table S1 for sources). Predicted values based on a read-across methodology (10, 11) were used for 15 %, 46 % and 31 % of the compounds for *D. magna*, *P. promelas* and *P. subcapitata*, respectively. Read-across models extrapolate the acute toxicity of non-tested compounds based on the structural similarity of compounds for which the acute toxicity is available. The similarity of two compounds is obtained by comparing the occurrence of identical atom-centred fragments (ACFs; see ref. 10 for details). An algorithm employing ACFs has been developed for the standard test species (10, 11) and the method is fully automated in ChemProp (12). The latter was also used to extract physicochemical parameters of compounds (e.g, water solubility and the octanol-water partitioning coefficient: K_{ow}; Table S1). The level of similarity between compounds would establish the reliability of the predicted values, which were classified from very high to low reliability (see ref. 11 for details) and are presented in Table S1. The prediction performance of the read-across models were assessed using a leave-one-out cross validation technique and explained 75-90 % of the variance (10, 11).

For the compounds where the read-across models were not applicable, baseline toxicity was estimated from the compounds' logK_{ow} using the species specific quantitative structure-activity relationship (QSAR; 5 % for *D. magna*, and 15 % for *P. subcapitata*; see Table S1 for sources). Baseline toxicity assumes a narcotic mode of action (partioning into membranes), which is typically regarded as the minimal toxicity of an organic compound (13). Hence, this approach tends to underestimate the true toxicity. If the log K_{ow} was outside of the application domain of the baseline predictions ($1 < \log K_{ow} < 6$), then this compound was excluded from the anaylsis (Table S1; 3 compounds for *P. promelas*, 4 compounds for *D. magna*, and 28 compounds for *P. subcapitata*).

Furthermore, compounds were removed when the respective experimental, predicted or baseline toxicity values were ≥ 10-fold higher (Table S1; 18 compounds for *P. promelas*, 13 compounds for *D. magna*, 15 compounds for *P. subcapitata*). For three active enantiomers (metalaxyl-m, dichlorprop-p, and mecoprop-p) the measured or predicted values for the enantiomer mixtures were used.

Finally, 223 compounds with acute toxicity values for at least one species were used in the analysis, covering 4,001 European sites.

1.4 Threshold selection for the assessment of chemical risk

Chemical concentrations above the acute risk threshold (ART -1/10 of the LC50) are generally recognised to result in acute ecological effects (5, 14, 15). Difficulties arise to estimate the threshold levels for ecological communities exposed to mixtures of chemicals for longer periods at lower concentrations. To our knowledge, there is only one meta-analysis that provides a potential threshold for such effects (5). These studies reported shifts in invertebrate communities towards more tolerant species when exposed to pesticides at 1/1,000 of the *D.magna* LC50

values. Furthermore, a recent study confirmed losses in biodiversity at 1/1,000 of the LC50 values (16). Hence, this value was used as the chronic risk threshold (CRT) for invertebrates. In the absence of similar studies for fish and algae, we used the acute-to-chronic-ratio (ACR) from laboratory data to derive chronic effect thresholds for these organism groups. This method is based on the empirical calculation of the ratio between the acute toxicity data used here (e.g., LC50/EC50 values) and Chronic No Observed Effect Concentration (NOEC) values or Lowest Observed Effect Concentration (LOEC) for the same species and the same compound. Typically, the ACR is a factor of 10 for fish (17-20), while for algae, the ACR is a factor of 4 to 5 (17, 20). Algae ACRs are limited due to insufficient acute data (21). In the absence of field studies, which help in validating laboratory-driven thresholds, it is difficult to assess the magnitude of chronic effects for algae and fish, because (i) the test species used here are most likely not the most sensitive species for all substances consisting of various modes of action, (ii) laboratory chronic studies cover still only a short period compared to potential field exposures and the life cycle of many invertebrates and fish, and (iii) toxicity tests for single species cannot integrate ecological concepts, such as recovery or species interaction and the resulting indirect effects (9, 22-25).

The chronic risk for fish and algae estimated from the ACR-based threshold could be underestimated in our study, if field studies established lower effect thresholds for these organism groups. For instance, the use of the ACR-based threshold for invertebrates (1/100 of the LC50 values; ACR is approximately a factor of 10 (17)) would underestimate the chronic risk by approximately 68 % compared to the field-based threshold (1/1,000 of the LC50 values).

1.5 Likelihood definition

We defined the likelihood for acute and chronic effects in field conditions based on the available literature on the ecological risk thresholds (Table S3). Observation of acute effects was likely at sites exceeding 1/10 of the LC50 values, because on average in 55 % of the cases, such concentrations led to adverse effects on organisms from insecticides and herbicides (Table S3; Overall chemical). Similarly, it was likely to observe chronic effects on invertebrates at sites that exceed 1/1,000 of the LC50 values, as 71 % of the cases reported shifts in invertebrate communities when exposed to pesticides (Table S3). We note that only pesticide-related threshold studies were available, and this limited availability should be considered when interpreting our results, which relate to organic chemicals in general. However, pesticides were the major contributors to the chemical risk in our study, and in the absence of other studies, we deem our analysis to be based on the best available knowledge.

1.6 Suitability of reported limits of quantification for chemical risk assessment

No risk is generally assumed from a compound that is reported below the limit of quantification. However, if the LOQ (and, when not available, the LOD) is greater than any of the two risk thresholds (ART or CRT) for any of the three organism groups, the real concentration might still exceed the respective risk threshold(s). Therefore, for each chemical, we calculated the frequency of sites with non-detects, where the LOQ values exceeded one of the risk thresholds. This procedure was not followed for Spain because the LOQ values for Spain were considered unreliable.

1.7 Influence of acute-risk chemicals (ARCs) on chemical risk

The chemical risk was calculated for groups of sites for each river basin at which a given number of ARCs were analyzed as:

$$CR_{r,j,b} = N_{r,j,b}/N_{total,r,b} \quad (3)$$

where N represents the number of sites for which one of the chemical concentrations exceeded the respective risk threshold j within a river basin b, N_{total} represents the total number of sites

within that river basin, and r = 0 to 36 and comprises all sites within a river basin with the respective number of analyzed ARCs. A value of r = 0 represents sites where no ARCs were analyzed, while r = 36 represents sites where all ARCs were analyzed. The risk threshold *j* is either the CRT or the ART. All basins that had less than three sites for each *r* group were excluded from this analysis.

The overall chemical risk in each ARC group *r* for each threshold *j* was subsequently calculated as the mean of all basins:

$$CR_{r,j} = \frac{1}{m} \sum_{i=1}^{m} CR_{r,j,i} \quad (4)$$

where i = 1,...,m indicates the number of river basins. For each *r* group, at least three basins were required for the calculation of the mean ($CR_{r,j}$).

2. SI Discussion

Influence of hydrophobic compounds on chemical risk: Compounds with experimental or predicted effect concentrations that strongly exceeded the water solubility were omitted from the analysis (17, 13 and 15 compounds for fish, the invertebrate and algae, respectively, Table S1). Exceedance of the water solubility usually results in suspensions in the form of undissolved test material, which compromises the quantification of exposure concentrations (26). However, removal of these hydrophobic compounds from the dataset had only a negligible influence on the chemical risk, except for di-(2-ethylhexyl) phthalate (DEHP). This plasticizer is widely found at measurable concentrations in aquatic ecosystems because of its high production volume (included in more than 50 % of the European plasticizers; ref. 27). In addition, it has a high potential to persist in the environment and to bioaccumulate in biota (especially for invertebrates; ref. 28) due to its high lipophilicity. Large discrepancies are reported for the experimental and predicted lethal concentrations of DEHP, which will be discussed below.

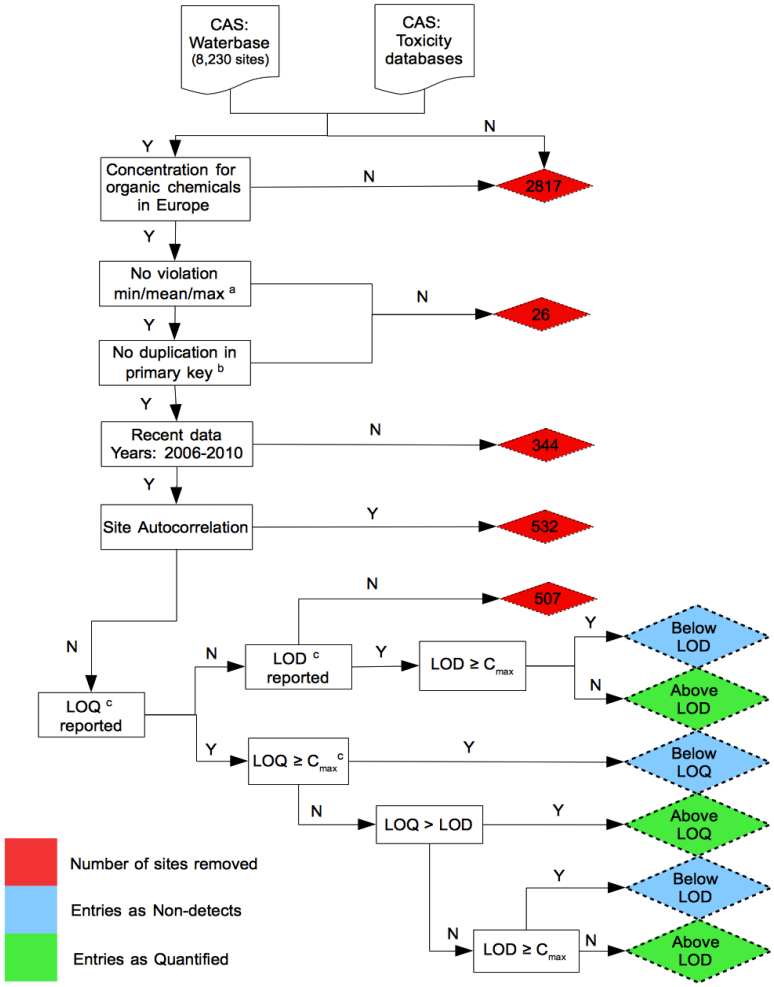
Short-term experimental toxicity values for DEHP exceeded the water solubility of 3 µg/L (at 20°C; ref. 28) by up to five-orders of magnitude for fish, and by up to three-orders of magnitude for the invertebrate and algae (e.g., ref. 29). In several studies, a clear dose-response relationship could not be established for DEHP, suggesting that the reported lethal effects were caused through physical mechanisms, such as coating on fish (26, 28). The unrealistically high effect concentrations reported are typically nominal instead of measured concentrations, which leads to an underestimation of DEHP toxicity (28). Given the high uncertainty associated with the experimental effect concentrations for DEHP, we suggest that the risk assessment should be based on QSAR predictions instead.

Using baseline toxicity based on the log K_{ow} of DEHP (recommended value: 7.5; ref. 28), LC50 values resulted in 8.5 µg/L, 2.2 µg/L and 2.1 µg/L, for fish, invertebrate and algae, respectively. Note that the quantitative structure-activity relationship (QSAR) models used for prediction are typically linear extrapolations, while it is argued that for hydrophobic compounds with a log K_{ow} > 5.5, this relationship is parabolic (see ref. (26) and the references therein). Accounting for the deviation from linearity would increase the predicted LC50, and consequently reduce the chemical risk from DEHP. Hence, there is great uncertainty regarding the prediction of effect concentrations and the risk predictions derived from that.

By including the highly uncertain QSAR based LC50 for DEHP in our assessment, the acute and chronic chemical risk would increase by 6 % and 2 %, respectively, and render this compound responsible for the majority of exceedances (53 %) for the acute chemical risk. Thus, DEHP has the clear potential to increase the overall risk, although the quantification of risk with the current knowledge is highly uncertain. To avoid overestimation caused by highly uncertain predicted

values, we omitted DEHP from the main analysis, which is also in line with the above mentioned criteria for baseline toxicity predictions' domain ($1<\log K_{ow}<6$). However, this does not rule out the potential of the DEHP or other hydrophobic compounds to cause ecological effects as a result of lethal or sublethal (e.g., endocrine disruption) effects (e.g., refs. 30, 31) .

3. SI Figures



[a] The reported concentrations which had the following violations: (i) the mean is missing, (ii) the mean is negative which is not allowed or possible, (iii) the mean is zero which is not allowed or possible, (iv) the minimum is higher than the mean, (v) the mean is higher than the maximum and (vi) the minimum is higher than the maximum (2)
[b] Primary key is a field or combination of fields with values which have to be unique in the dataset.
[c] LOQ: limit of quantification, LOD: Limit of detection, C_{max} maximum concentration analyzed

Figure S1: Flow chart visualising the quality control of the chemical dataset.

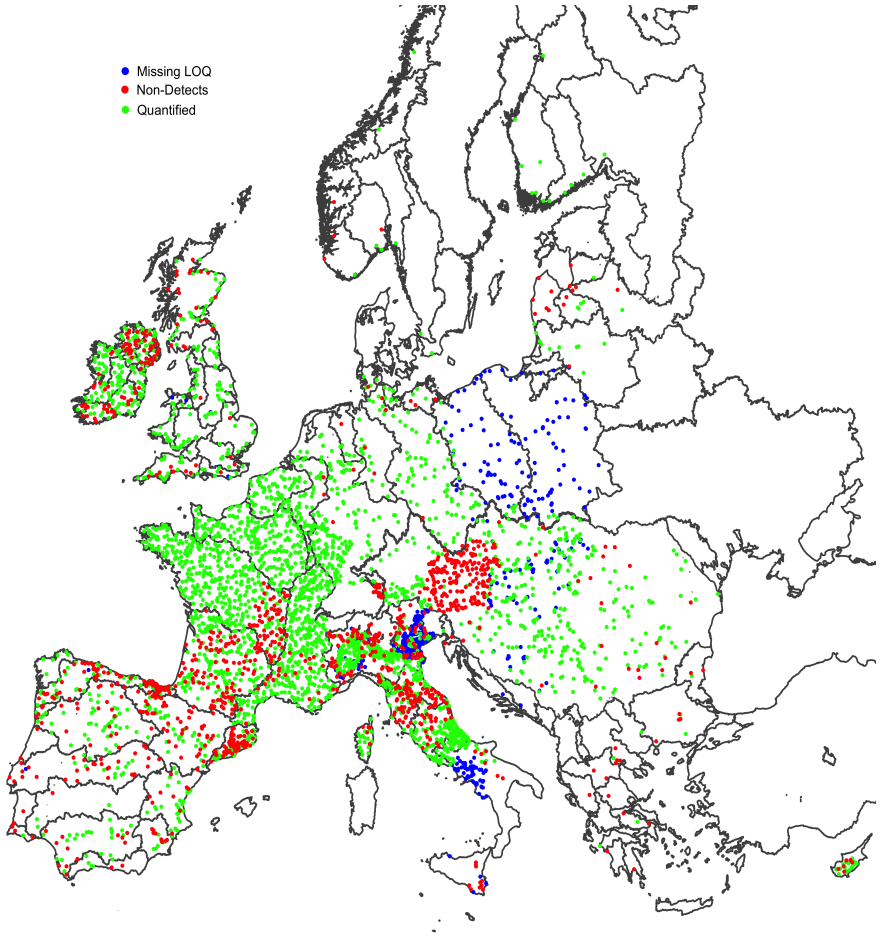


Figure S2: Overview of monitoring sites in Europe. Sites that have at least one chemical with a maximum concentration above the limit of quantification/limit of detection are classified as "quantified"(n = 2890). Sites with all measurements below the limit of quantification/limit of detection are classified as "non-detects" (n = 1114), and "missing LOQ" represents the sites which have no information on the limit of quantification/limit of detection (n = 506).

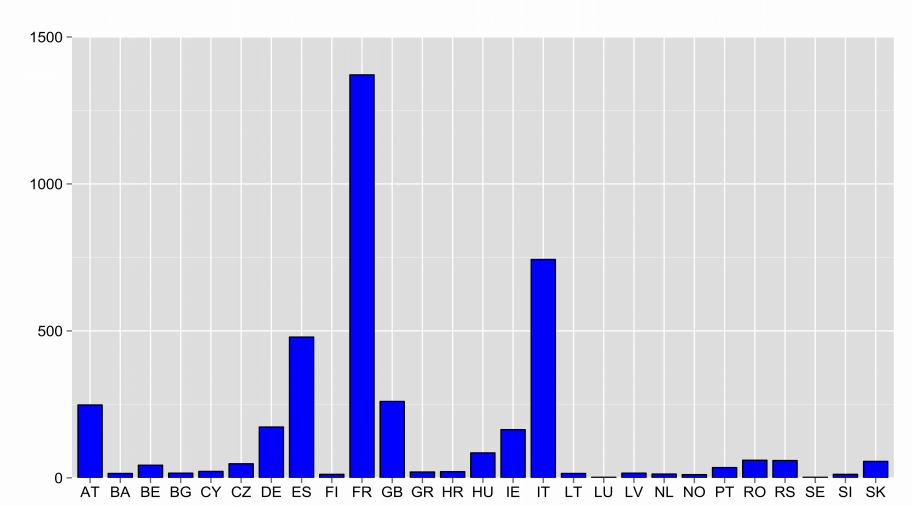


Figure S3: Number of sites monitored in each country during the 2006-2010 period. The codes correspond to AT: Austria, BA: Bosnia and Herzegovina, BE: Belgium, BG: Bulgaria, CY: Cyprus, CZ: Czech Republic, DE: Germany, ES: Spain, FI: Finland, FR: France, GB: Great Britain, GR: Greece, HR: Croatia, HU: Hungary, IE: Ireland, IT: Italy, LT: Lithuania, LU: Luxembourg, LV: Latvia, NL: Netherlands, NO: Norway, PT: Portugal, RO: Romania, RS: Serbia, SE: Sweden, SI: Slovenia, SK: Slovakia.

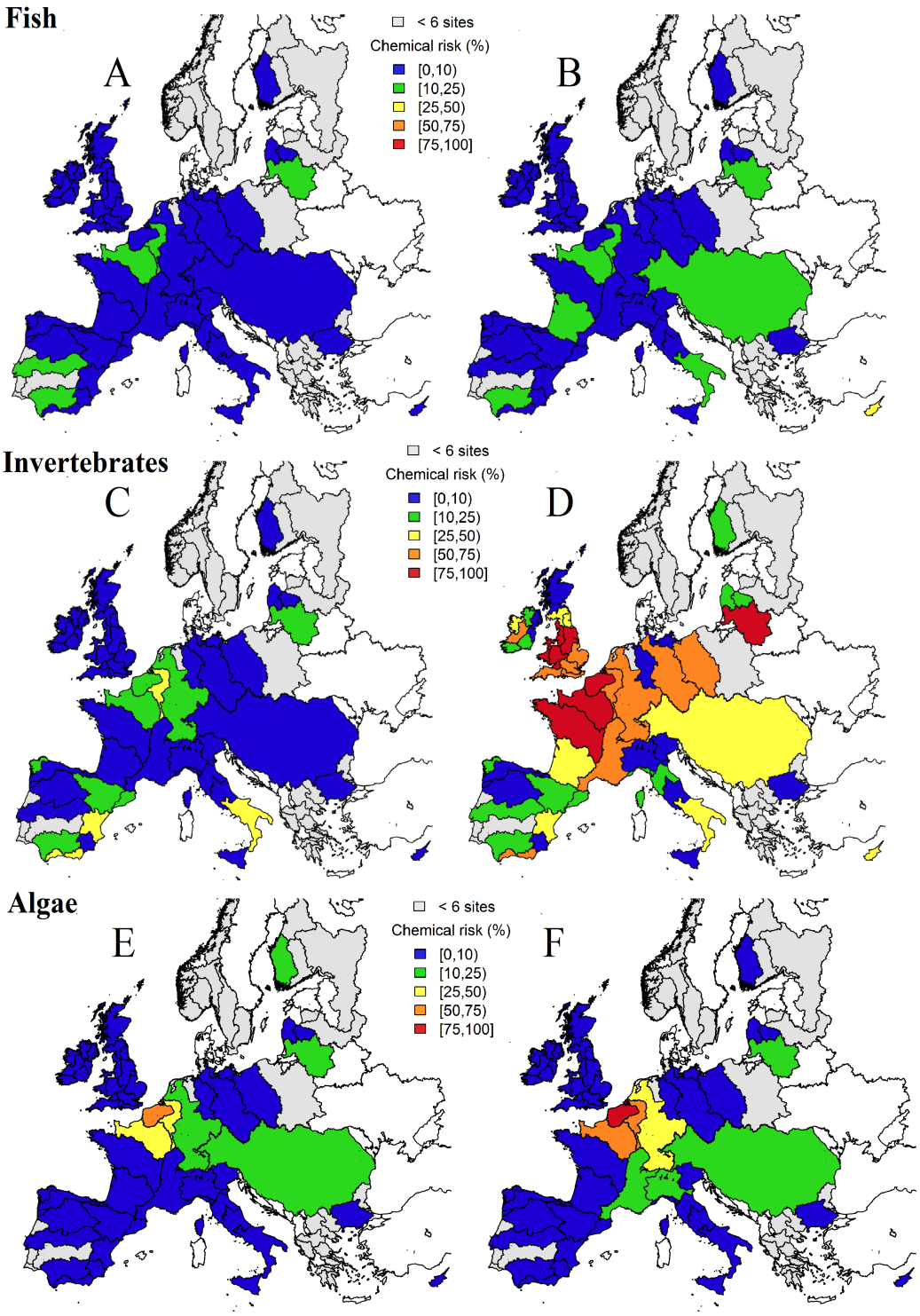


Figure S4: Chemical risk (by percentage range) in the European river basins separately for the three organism groups. The map displays the fraction of sites which exceed the acute risk threshold (A, C, and E) and the chronic risk threshold (B, D and F) for fish (represented by *P. promelas*; A and B), invertebrates (represented by *D. magna*; C and D), and algae (represented by *P. subcapitata*; E and F). The colour range shows the level of chemical risk, from low chemical risk (blue) to high chemical risk (red). River basins with up to six sites are displayed in grey, whereas river basins without data are displayed in white. Direct comparisons between river systems is potentially biased by the ecotoxicologically relevant compounds analysed and the limit of quantification of the compounds.

4. SI Tables

Table S1: Overview of chemicals analyzed and their toxicity. Information on the chemical group, the main applications, the octanol-water partitioning coefficient (K_{ow}), the water solubility and the analytical methods are given for each chemical, identified by the Chemical Abstract Service (CAS) number. Information on the toxicity comprises the median lethal concentration (LC50) in µg/L, sources of the toxicity values and the type of data for each chemical and each organism group represented by the fish *P. promelas* (PP), the invertebrate *D. magna* (DM), and the algae *P. subcapitata* (PS).

Chemical Group [a]	Main Application [b]	CAS	Chemical Name	log K_{ow}	Water Solubility [µg/L]	LC50 [µg/L] PP	Source PP	Type of data PP [c]	LC50 [µg/L] DM	Source DM	Type of data DM [c]	LC50 [µg/L] PS	Source PS	Type of data PS [c]	Analytical Methods [d]
A	Ins	50293	4,4'- DDT	6.79	8.62	22.0	(32)	E	5.00	(14)	E	-	-	D	-
A	Ins	53190	2,4'-DDD	5.87	83.38	463	(12)	P/1	9.10	(12)	P/4	145	(33)	B	EN ISO 6468:1996
A	Ins	56382	Parathion-ethyl	3.73	3669	1519	(32)	E	2.50	(14)	E	1436	(12)	P/2	EN ISO 6468:1996
A	Ins	57125	Cyanide	-0.69	352690000	155	(32)	E	517	(32)	E	-	-	D	EN ISO 6468:1996
A	Ins	57749	Chlordane	6.26	33.14	96.0	(32)	E	98.4	(32)	E	-	-	WS	-
A	Ins	58899	g-Hexachlorocyclohexane	4.26	3194	82.0	(32)	E	1600	(14)	E	3385	(33)	B	-
A	Ins	60515	Dimethoate	0.72	7454800	34548	(12)	P/1	2000	(14)	E	37000	(32)	E	-
A	Ins	60571	Dieldrin	5.45	120	24.0	(32)	E	250	(14)	E	39.0	(12)	P/2	-
A	Ins	62737	Dichlorvos	0.60	10452000	6230	(32)	E	0.19	(14)	E	737	(32)	E	-
A	Ins	72208	Endrin	5.45	120	1.00	(32)	E	117	(32)	E	39.0	(12)	P/2	-
A	Ins	72435	Methoxychlor	5.67	264	24.0	(32)	E	50.0	(14)	E	1763	(12)	P/1	EN ISO 6468:1996
A	Ins	72548	4,4'- DDD	5.87	83.38	375	(12)	P/1	9.00	(32)	E	614	(12)	P/2	EN ISO 6468:1996
A	Ins	72559	4,4'- DDE	6.00	72.31	91.0	(12)	P/1	13.3	(12)	P/4	240	(12)	P/1	EN ISO 6468:1996
A	Ins	76448	Heptachlor	5.86	103	68.0	(32)	E	42.0	(14)	E	27.0	(14)	E	-
A	Ins	77474	Hexachlorocyclopentadiene	4.63	1241	74.0	(32)	E	46.0	(32)	E	190	(12)	P/4	EN ISO 17993:2003/6468:1996
A	Ins	87865	Pentachlorophenol	4.74	27202	245	(12)	P/4	450	(14)	E	347	(32)	E	-
A	Ins	115297	Endosulfan	3.50	75.69	1.00	(32)	E	440	(14)	E	427.8	(32)	E	-
A	Ins	115322	Dicofol	5.81	9.28	-	-	WS	-	-	WS	-	-	WS	-
A	Ins	121755	Malathion	2.29	6174200	14100	(14)	E	0.70	(14)	E	13000	(14)	E	EN ISO 6468:1996
A	Ins	122145	Phenitrothion	3.30	38355	4000	(14)	E	8.60	(14)	E	1300	(14)	E	-
A	Ins	143500	Kepon	4.91	4258	380	(32)	E	531	(32)	E	1539	(33)	B	-
A	Ins	297789	Isobenzan	4.51	84.38	-	-	WS	8.07	(12)	P/4	-	-	WS	EN ISO 10695:2000/6468:1996
A	Ins	298000	Methyl parathion	2.75	36445	7741	(14)	E	7.30	(14)	E	5400	(32)	E	-
A	Ins	309002	Aldrin	6.06	120	24.0	(32)	E	28.0	(14)	E	74.0	(12)	P/3	-
A	Ins	319846	a-Hexachlorocyclohexane	4.26	3194	82.0	(12)	P/4	370	(14)	E	3385	(33)	B	EN ISO 10695:2000
A	Ins	319857	b-Hexachlorocyclohexane	4.26	3194	82.0	(12)	P/4	1084	(12)	P/4	3385	(33)	B	-
A	Ins	319868	d-Hexachlorocyclohexane	4.26	3194	82.0	(12)	P/4	1084	(12)	P/4	3385	(33)	B	-
A	Ins	465736	Isodrin	6.06	120	167	(12)	P/1	69.3	(12)	P/4	74.0	(12)	P/3	-
A	Ins	470906	Chlorfenvinfos	4.15	1549	360	(12)	P/1	0.25	(14)	E	5226	(33)	B	EN ISO 6468:1996

Chemical Group [a]	Main Application [b]	CAS	Chemical Name	log K_{ow}	Water Solubility [µg/L]	LC50 [µg/L] PP	Source PP	Type of data PP [c]	LC50 [µg/L] DM	Source DM	Type of data DM [c]	LC50 [µg/L] PS	Source PS	Type of data PS [c]	Analytical Methods [d]
A	Ins	608731	Hexachlorocyclohexane	4.26	3194	125	(32)	E	1084	(12)	P/4	3385	(33)	B	-
A	Ins	789026	2,4'-DDT	6.79	8.62	85.0	(12)	P/3	5.07	(12)	P/4	-	-	D	-
A	Ins	919868	Demeton-S-Methyl	1.01	4161300	295850	(12)	P/1	23.0	(14)	E	1888914	(33)	B	EN ISO 6468:1996
A	Ins	959988	Endosulfan I	3.50	75.69	1.00	(32)	E	440	(12)	P/4	43.0	(12)	P/2	-
A	Ins	1024573	Heptachloro Epoxide B	4.56	219	471	(12)	P/1	240	(14)	E	40.0	(12)	P/3	-
A	Ins	1113026	Omethoate	-0.79	176770000	-	-	D	21.0	(32)	E	-	-	D	-
A	Ins	1563662	Carbofuran	2.30	368070	844	(34)	E	9.40	(14)	E	6500	(14)	E	-
A	Ins	2310170	Phosalone	4.29	1048	231	(32)	E	0.74	(35)	E	880	(32)	E	-
A	Ins	2385855	Mirex	7.35	246	2.16	(12)	P/1	65.3	(12)	P/4	-	-	D	-
A	Ins	2921882	Chlorpyrifos	5.11	266	500	(14)	E	0.10	(14)	E	1586	(12)	P/3	-
A	Ins	3424826	2,4'-DDE	6.00	72.31	91.8	(12)	P/1	19.3	(12)	P/4	487	(12)	P/1	-
A	Ins	8001352	Toxaphene	6.79	10.37	12.0	(32)	E	14.1	(35)	E	-	-	WS	-
A	Ins	10265926	Methamidophos	-0.93	515720000	465820	(12)	P/1	270	(35)	E	-	-	D	EN ISO 10301:1997
A	Ins	13071799	Terbufos	4.49	2098	142	(32)	E	0.31	(35)	E	2111	(33)	B	-
A	Ins	13356086	Fenbutatin oxide	13.63	0.00	-	-	WS	-	-	WS	-	-	WS	EN ISO 10301:1997
A	Ins	16752775	Methomyl	0.61	20149000	2110	(34)	E	7.60	(35)	E	60000	(32)	E	-
A	Ins	17040196	Demeton-S-methylsulfon	-0.91	120920000	295850	(12)	P/1	259	(12)	P/4	-	-	D	-
A	Ins	18181709	Iodofenphos	5.39	63.43	139	(12)	P/1	1.60	(35)	E	-	-	WS	-
A	Ins	23103982	Pirimicarb	1.40	1748900	100000	(14)	E	17.0	(14)	E	140000	(14)	E	-
A	Ins	39765805	Trans-nonachlor	6.44	9.54	20.0	(12)	P/1	-	-	D	-	-	D	-
A	Ins	52645531	Permethrin	7.43	1.57	16.0	(34)	E	0.60	(35)	E	-	-	D	EN ISO 17353:2005
A	Ins	112410238	Tebufenozide	4.62	679	2116	(12)	P/1	3800	(35)	E	640	(32)	E	-
A	Ins	120928098	Fezaquin	5.76	136	179	(12)	P/1	4.10	(35)	E	208	(35)	E	-
A	Her	75990	Dalapon	1.68	74590000	290000	(32)	E	176220	(12)	B	303432	(33)	B	-
A	Her	88857	Dinoseb	3.67	19662	700	(34)	E	240	(36)	E	20496	(12)	P/3	-
A	Her	93721	Fenoprop	3.68	59374	23000	(14)	E	4379	(12)	B	218197	(12)	P/3	-
A	Her	93765	2,4,5-Trichlorophenoxyacetic Acid	3.26	193480	57711	(12)	P/3	5000	(14)	E	28042	(12)	P/3	-
A	Her	94746	MCPA	2.52	836260	134550	(12)	P/2	190000	(14)	E	15756	(32)	E	-
A	Her	94757	2,4-D	2.62	495230	63400	(35)	E	148281	(36)	E	30624	(32)	E	-
A	Her	94815	MCPB	3.50	117730	12500	(32)	E	55000	(14)	E	41000	(14)	E	EN ISO 6468:1996
A	Her	94826	2,4'-DB	3.60	127100	18000	(14)	E	25000	(14)	E	33636	(12)	P/3	-
A	Her	120365	Dichlorprop	3.03	690320	71895	(12)	P/3	100000	(35)	E	194000	(32)	E	-
A	Her	122349	Simazine	2.40	34471	34921	(12)	P/1	94000	(14)	E	275	(14)	E	-
A	Her	139402	Propazine	3.24	6371	5017	(12)	P/1	11000	(14)	E	29.0	(14)	E	-
A	Her	314409	Bromacil	1.68	680850	186000	(14)	E	121000	(32)	E	7.00	(14)	E	-
A	Her	330541	Diuron	2.67	63509	14200	(14)	E	5700	(14)	E	2.00	(14)	E	-
A	Her	330552	Linuron	2.91	117270	9481	(12)	P/1	477	(14)	E	16.0	(14)	E	-
A	Her	534521	Dinitro-o-Cresol	2.27	515150	1745	(34)	E	3200	(36)	E	50000	(12)	P/4	-
A	Her	834128	Ametryne	3.32	183640	10850	(32)	E	28000	(14)	E	4.00	(14)	E	EN ISO 6468:1996
A	Her	886500	Terbutryn	3.77	15673	3441	(12)	P/1	7100	(32)	E	3.00	(32)	E	-

Chemical Group [a]	Main Application [b]	CAS	Chemical Name	log K_{ow}	Water Solubility [µg/L]	LC50 [µg/L] PP	Source PP	Type of data PP [c]	LC50 [µg/L] DM	Source DM	Type of data DM [c]	LC50 [µg/L] PS	Source PS	Type of data PS [c]	Analytical Methods [d]
A	Her	1007289	Desisopropylatrazine	1.36	1213500	89255	(12)	P/1	132340	(12)	P/3	77.0	(12)	P/3	EN ISO 6468:1996
A	Her	1014693	Desmetryn	2.82	114350	2859	(12)	P/1	26000	(32)	E	25.0	(35)	E	EN ISO 6468:1996
A	Her	1066519	Aminomethylphosphonic Acid	-2.47	141410000000	-	-	D	-	-	D	-	-	D	-
A	Her	1071836	Glyphosate	-4.77	6263500000	29867	(32)	E	40000	(35)	E	38964	(32)	E	EN ISO 6468:1996
A	Her	1194656	Dichlobenil	2.83	62544	6532	(14)	E	6200	(14)	E	11024	(12)	P/3	EN ISO 6468:1996
A	Her	1582098	Trifluralin	5.31	284	119	(14)	E	245	(14)	E	12.2	(14)	E	-
A	Her	1610180	Prometon	3.57	119970	6611	(12)	P/1	41167	(32)	E	98.0	(32)	E	-
A	Her	1689834	Ioxynil	3.94	128340	6800	(34)	E	3900	(35)	E	7276	(12)	P/1	-
A	Her	1689845	Bromoxynil	3.39	43879	12500	(14)	E	12500	(14)	E	4229	(32)	E	EN ISO 17993:2003
A	Her	1689992	Bromoxynil Octanoate	5.86	15.75	-	-	WS	46.0	(35)	E	-	-	WS	-
A	Her	1698608	Chloridazon	0.76	370690	545230	(12)	P/1	132000	(14)	E	3000	(14)	E	EN ISO 17993:2003
A	Her	1702176	Clopyralid	1.63	391450	63700	(12)	P/1	225000	(37)	E	30500	(35)	E	-
A	Her	1836755	Nitrofen	4.32	144	666	(12)	P/3	217	(14)	E	123	(12)	P/3	-
A	Her	1861401	Benfluralin	5.31	215	100.0	(32)	E	1143	(32)	E	-	-	WS	EN ISO 17993:2003
A	Her	1912249	Atrazine	2.82	14850	13525	(32)	E	54000	(14)	E	143	(14)	E	EN ISO 17993:2003
A	Her	1918009	Dicamba	2.14	497360	45796	(12)	P/1	110300	(12)	P/4	3700	(32)	E	-
A	Her	1918134	Chlorthiamid	2.96	8414	6444	(12)	P/1	6343	(12)	P/3	6538	(12)	P/1	-
A	Her	2008584	2,6-dichlorobenzamide	0.90	73738	469000	(14)	E	180000	(14)	E	5222	(12)	P/2	-
A	Her	2164081	Lenacil	3.09	158330	19357	(12)	P/1	8400	(14)	E	7.70	(14)	E	-
A	Her	3397624	Deisopropyldeethylatrazine	0.32	42275000	498310	(12)	P/1	-	-	D	115	(12)	P/2	EN ISO 6468:1996
A	Her	5915413	Terbutylazine	3.27	924	8782	(12)	P/1	13100	(32)	E	12.0	(14)	E	EN ISO 10301:1997
A	Her	6190654	Desethylatrazine	1.78	31628	86693	(12)	P/1	76529	(12)	P/4	2000	(32)	E	-
A	Her	7085190	Mecoprop	2.94	281400	35134	(12)	P/2	200000	(35)	E	10000	(32)	E	-
A	Her	7287196	Prometryn	3.73	23565	2513	(12)	P/1	12660	(14)	E	16.0	(14)	E	EN ISO 10301:1997
A	Her	13684565	Desmedipham	3.22	12861	9041	(35)	E	450	(35)	E	10	(35)	E	EN ISO 6468:1996
A	Her	15972608	Alachlor	3.37	170160	5000	(14)	E	10000	(14)	E	5.00	(14)	E	-
A	Her	16672870	2-Chloroethylphosphonic Acid	-0.25	131050000	130000	(32)	E	31700	(35)	E	1400	(32)	E	-
A	Her	21087649	Metribuzin	1.49	1970200	247100	(12)	P/1	49000	(14)	E	48.0	(14)	E	-
A	Her	21725462	Cyanazine	2.51	6754	18625	(32)	E	49000	(14)	E	22.0	(14)	E	-
A	Her	23950585	Propyzamide	3.57	19546	1658	(12)	P/1	5600	(32)	E	760	(32)	E	-
A	Her	25057890	Bentazone	1.67	1003000	185940	(12)	P/1	125000	(14)	E	4500	(14)	E	-
A	Her	26225796	Ethofumesate	2.89	119440	38663	(12)	P/1	14000	(14)	E	3900	(14)	E	-
A	Her	26259450	Secbumeton	3.64	96381	8527	(12)	P/1	3992	(12)	B	73.0	(12)	P/3	-
A	Her	30125634	Desethylterbutylazine	2.23	20915	41547	(12)	P/1	42000	(14)	E	11.0	(12)	P/3	-
A	Her	33693048	Terbumeton	3.60	83338	51500	(32)	E	40000	(35)	E	42.5	(32)	E	-
A	Her	34123596	Isoproturon	2.84	77471	17586	(12)	P/1	580	(14)	E	13.6	(32)	E	-
A	Her	34256821	Acetochlor	3.37	866070	6105	(12)	P/3	8600	(35)	E	1430	(32)	E	EN ISO 18857-1:2006
A	Her	40487421	Pendimethalin	4.82	1205	164	(12)	P/1	280	(14)	E	6.00	(14)	E	-
A	Her	41394052	Metamitron	1.44	2511300	133740	(12)	P/1	97000	(32)	E	34909	(12)	P/2	-
A	Her	51218452	Metolachlor	3.24	221820	8200	(32)	E	15595	(14)	E	38.0	(14)	E	-

Chemical Group [a]	Main Application [b]	CAS	Chemical Name	log K_{ow}	Water Solubility [µg/L]	LC50 [µg/L] PP	Source PP	Type of data PP [c]	LC50 [µg/L] DM	Source DM	Type of data DM [c]	LC50 [µg/L] PS	Source PS	Type of data PS [c]	Analytical Methods [d]
A	Her	51235042	Hexazinone	2.15	334940	274000	(32)	E	85000	(14)	E	14.0	(14)	E	-
A	Her	55512339	Pyridate	5.73	52.80	97.0	(12)	P/1	-	-	WS	227	(33)	B	-
A	Her	64902723	Chlorsulfuron	2.26	3198	-	-	WS	-	-	WS	68.0	(35)	E	-
A	Her	67129082	Metazachlor	2.38	153130	81650	(12)	P/1	33000	(14)	E	16.0	(14)	E	EN ISO 18856:2005
A	Her	74223646	Metsulfuronmethyl	2.00	3828	-	-	WS	-	-	WS	395	(32)	E	-
A	Fun	50000	Formaldehyde	0.35	57018000	24100	(32)	E	19200	(32)	E	4249	(32)	E	-
A	Fun	82688	Pentachloronitrobenzene	5.03	270	55.0	(12)	P/1	770	(14)	E	493	(12)	P/2	-
A	Fun	96457	Ethylenethiourea	-0.49	3076200000	1957000	(12)	P/1	21600	(35)	E	93800	(35)	E	-
A	Fun	118741	Hexachlorobenzene	5.86	18.20	56.9	(12)	P/2	5.70	(14)	E	30.0	(32)	E	-
A	Fun	133062	Captan	2.74	55683	120	(32)	E	7100	(35)	E	1180	(35)	E	-
A	Fun	137268	Thiram	1.70	9613000	24.0	(32)	E	11.0	(35)	E	65.0	(35)	E	-
A	Fun	137304	Ziram	1.14	12291000	8.00	(32)	E	48.0	(35)	E	66.0	(35)	E	-
A	Fun	57837191	Metalaxyl	1.70	10208000	171160	(12)	P/1	28000	(14)	E	688	(12)	P/2	-
A	Fun	60207901	Propiconazole	4.13	2051	3246	(12)	P/1	10200	(14)	E	5333	(32)	E	-
A	Fun	67306030	Fenpropimorph	5.50	2397	530	(12)	P/1	2240	(35)	E	327	(35)	E	-
A	Fun	136426545	Fluquincozole	3.73	137	-	-	WS	-	-	WS	46.0	(35)	E	-
B	Lub,Pla	2051243	PCB 209	10.20	0.0014	-	-	WS	-	-	WS	-	-	WS	-
B	Lub,Pla	7012375	PCB 28	5.69	241	74.0	(12)	P/4	160	(14)	E	120	(12)	P/3	-
B	Lub,Pla	31508006	PCB 118	6.98	9.38	9.00	(12)	P/4	10.1	(12)	P/4	-	-	D	-
B	Lub,Pla	32598133	PCB 77	6.34	1.14	2.00	(32)	E	2.00	(36)	E	-	-	D	-
B	Lub,Pla	32598144	PCB 105	6.98	9.38	8.94	(12)	P/4	10.1	(12)	P/4	-	-	D	EN ISO 18857-1:2006
B	Lub,Pla	32774166	PCB 169	7.62	1.80	0.60	(12)	P/4	5.06	(12)	P/4	-	-	D	-
B	Lub,Pla	35065271	PCB 153	7.62	3.07	1.00	(32)	E	1.30	(14)	E	-	-	D	-
B	Lub,Pla	35065282	PCB 138	7.62	3.07	0.60	(12)	P/4	6.08	(12)	P/4	-	-	D	-
B	Lub,Pla	35065293	PCB 180	8.27	0.46	0.53	(12)	P/3	2.10	(12)	P/4	-	-	D	-
B	Lub,Pla	35693993	PCB 52	6.34	19.66	30.0	(32)	E	30.0	(32)	E	-	-	D	-
B	Lub,Pla	35694087	PCB 194	8.91	0.05	0.20	(32)	E	0.20	(32)	E	-	-	D	-
B	Lub,Pla	37680732	PCB 101	6.98	9.38	10.0	(32)	E	10.00	(32)	E	-	-	D	-
B	Lub,Pla	38380084	PCB 156	7.62	2.27	0.60	(12)	P/4	6.66	(12)	P/4	-	-	D	-
B	Lub,Pla	57465288	PCB 126	6.98	9.38	8.94	(12)	P/4	10.1	(12)	P/4	-	-	D	-
B	Lub,Pla	69782907	PCB 157	7.62	2.27	0.60	(12)	P/4	6.66	(12)	P/4	-	-	D	-
C	Byprod	50328	Benzo[a]pyrene	6.11	1.90	6.00	(38)	E	1.80	(32)	E	15.0	(14)	E	EN ISO 6468:1996
C	Byprod	53703	Dibenz[ah]anthracene	6.70	0.33	-	-	WS	-	-	WS	-	-	WS	EN ISO 6468:1996
C	Byprod	56553	Benz[a]anthracene	5.52	7.56	-	-	WS	71.6	(32)	E	-	-	WS	EN ISO 6468:1996
C	Byprod	83329	Acenaphthene	4.15	5239	1730	(14)	E	2350	(14)	E	520	(14)	E	-
C	Byprod	85018	Phenanthrene	4.35	665	1016	(12)	P/3	598	(14)	E	411	(14)	E	-
C	Byprod	86737	Fluorene	4.02	4081	2457	(12)	P/1	430	(14)	E	3400	(32)	E	-
C	Byprod	90120	1-Methylnaphthalene	3.72	39933	9000	(32)	E	1422	(32)	E	12000	(32)	E	-
C	Byprod	91203	Naphthalene	3.17	90836	6140	(14)	E	15000	(14)	E	25000	(14)	E	-
C	Byprod	91576	2-Methylnaphthalene	3.72	10479	8993	(12)	P/4	1670	(32)	E	3281	(12)	P/2	-

Chemical Group [a]	Main Application [b]	CAS	Chemical Name	log K_{ow}	Water Solubility [µg/L]	LC50 [µg/L] PP	Source PP	Type of data PP [c]	LC50 [µg/L] DM	Source DM	Type of data DM [c]	LC50 [µg/L] PS	Source PS	Type of data PS [c]	Analytical Methods [d]
C	Byprod	120127	Anthracene	4.35	665	1015	(12)	P/3	428	(14)	E	225	(12)	P/3	-
C	Byprod	129000	Pyrene	4.93	27.52	200	(32)	E	195	(32)	E	-	-	WS	-
C	Byprod	135193	2-naphthalenol	2.69	204340	3500	(14)	E	3540	(14)	E	18800	(32)	E	-
C	Byprod	206440	Fluoranthene	4.93	16.83	-	-	WS	106	(14)	E	-	-	WS	-
C	Byprod	208968	Acephthylene	3.76	8394	3659	(12)	P/1	4204	(12)	P/3	509	(12)	P/3	-
C	Byprod	1634044	MTBE	1.43	59229000	672000	(34)	E	136000	(39)	E	73339	(12)	P/1	-
D	Sol	87616	1,2,3-Trichlorbenzene	3.93	27463	2987	(12)	P/4	1850	(14)	E	900	(14)	E	-
D	Sol	95501	1,2-Dichlorobenzene	3.28	118710	9470	(14)	E	2300	(14)	E	49800	(32)	E	-
D	Sol	108703	1,3,5-Trichlorobenzene	3.93	15096	2987	(12)	P/4	7295	(12)	P/4	1685	(12)	P/3	-
D	Sol	108907	Monochlorobenzene	2.64	199530	25185	(32)	E	19241	(14)	E	12500	(32)	E	-
D	Sol	120821	1,2,4-Trichlorobenzene	3.93	30356	2990	(14)	E	1700	(32)	E	16867	(32)	E	-
D	Sol	541731	1,3-Dichlorobenzene	3.28	118710	8030	(14)	E	9733	(14)	E	4509	(12)	P/3	-
D	Sol	608935	Pentachlorobenzene	5.22	821	306	(14)	E	1327	(32)	E	6600	(14)	E	-
E	Sol	56235	Carbon tetrachloride	2.44	388470	43000	(35)	E	29400	(14)	E	70443	(33)	B	EN ISO 6468:1996
E	Sol	67663	Trichloromethane	1.52	6622200	70700	(14)	E	228967	(14)	E	349909	(33)	B	-
E	Sol	71556	1,1,1-Trichloroethane	2.68	2276400	52900	(14)	E	11200	(32)	E	37645	(33)	B	EN ISO 6468:1996
E	Sol	75092	Dichloromethane	1.34	17630000	330000	(34)	E	220000	(14)	E	357960	(33)	B	-
E	Sol	75274	Bromodichloromethane	1.61	3215700	220912	(12)	P/1	234970	(12)	B	400476	(33)	B	EN ISO 6468:1996
E	Sol	75343	1,1-Dichloroethane	1.76	6154500	114673	(12)	P/1	92185	(12)	P/4	6460	(12)	P/1	EN ISO 6468:1996
E	Sol	75354	1,1-Dichloroethene	2.12	1846200	135060	(14)	E	51000	(14)	E	23923	(12)	P/1	-
E	Sol	75694	Trichlorofluoromethane	2.13	1120600	59442	(12)	P/1	63928	(12)	B	117591	(33)	B	EN ISO 6468:1996
E	Sol	75718	Dichlorodifluoromethane	1.82	503450	107990	(12)	P/1	110070	(12)	B	193462	(33)	B	-
E	Sol	79005	1,1,2-Trichloroethane	2.01	4998600	81600	(14)	E	107333	(14)	E	144600	(14)	E	-
E	Sol	79016	1,1,2-Trichloroethene	2.47	696870	44100	(14)	E	59000	(36)	E	56637	(33)	B	-
E	Sol	87683	Hexachlorobutadiene	4.72	1612	90.0	(34)	E	500	(14)	E	143	(12)	P/2	-
E	Sol	106934	1,2-Dibromoethane	2.01	3663400	5074	(12)	P/1	119000	(14)	E	204878	(33)	B	-
E	Sol	107062	1,2-Dichloroethane	1.83	9887600	136000	(14)	E	507000	(14)	E	16254	(12)	P/1	-
E	Sol	127184	Tetrachloroethylene	2.97	187090	13400	(14)	E	14000	(14)	E	5028	(12)	P/2	-
E	Sol	156592	Cis-1,2-Dichloroethylene	1.98	4980700	30498	(12)	P/1	62420	(12)	B	112317	(33)	B	-
E	Sol	156605	Trans-1,2-Dichloroethylene	1.98	4980700	30498	(12)	P/1	220000	(14)	E	112317	(33)	B	-
E	Sol	540590	1,2-Dichloroethene	1.98	4980700	30498	(12)	P/1	62420	(12)	B	112317	(33)	B	-
E	Sol	1070786	1,1,1,3-Tetrachloropropane	3.42	398470	6611	(12)	P/1	11184	(12)	P/4	11530	(33)	B	-
F	Sur	58902	2,3,4,6-Tetrachlorophenol	4.09	125820	1030	(34)	E	175	(14)	E	1300	(14)	E	EN ISO 10695:2000/6468:1996
F	Sur	59507	4-Chloro-3-Methylphenol	2.70	1055700	7380	(14)	E	2000	(14)	E	25157	(12)	P/3	EN ISO 10695:2000/6468:1996
F	Sur	80057	Bisphenol-a	3.64	367810	4650	(32)	E	10313	(32)	E	2900	(32)	E	-
F	Sur	87650	2,6-Dichlorophenol	2.80	8273000	7748	(12)	P/4	3400	(14)	E	29000	(14)	E	-
F	Sur	88062	2,4,6-Trichlorophenol	3.45	564320	2285	(12)	P/4	1710	(14)	E	3500	(14)	E	-
F	Sur	95487	2-Methylphenol	2.06	17303000	14000	(14)	E	14689	(14)	E	65000	(14)	E	EN 12918:1999/10695:2000
F	Sur	95874	2,5-Dimethylphenol	2.61	1749300	18457	(12)	P/4	6750	(32)	E	7053	(12)	P/3	-
F	Sur	95954	2,4,5-Trichlorophenol	3.45	550940	902	(14)	E	900	(14)	E	1200	(14)	E	-

Chemical Group [a]	Main Application [b]	CAS	Chemical Name	log K_{ow}	Water Solubility [µg/L]	LC50 [µg/L] PP	Source PP	Type of data PP [c]	LC50 [µg/L] DM	Source DM	Type of data DM [c]	LC50 [µg/L] PS	Source PS	Type of data PS [c]	Analytical Methods [d]
F	Sur	100027	4-Nitrophenol	1.91	7507500	45633	(32)	E	15200	(36)	E	4540	(32)	E	-
F	Sur	104405	4-Nonylphenol	5.99	215	140	(34)	E	135	(32)	E	515	(32)	E	-
F	Sur	106445	4-Methylphenol	2.06	15703000	16500	(14)	E	4550	(32)	E	10148	(12)	P/3	-
F	Sur	120832	2,4-Dichlorophenol	2.80	3602500	7750	(14)	E	2600	(14)	E	31520	(14)	E	-
F	Sur	140669	Para-tert-octylphenol	5.28	16110	48.0	(32)	E	90.0	(36)	E	1900	(12)	P/4	-
F	Sur	526750	2,3-Dimethylphenol	2.61	12016000	18457	(12)	P/4	22500	(32)	E	10215	(12)	P/3	-
F	Sur	732263	2,4,6-tri-tert-Butylphenol	6.39	268	61.0	(32)	E	110	(12)	P/4	-	-	D	-
F	Sur	1570645	4-Chloro-2-Methylphenol	2.70	1055700	5471	(12)	P/4	290	(14)	E	29706	(12)	P/3	-
F	Sur	1806264	4-Octylphenol	5.50	738	287	(12)	P/3	270	(12)	P/4	189	(12)	P/3	EN ISO 17993:2003
F	Sur	4901513	2,3,4,5-Tetrachlorophenol	4.09	122490	410	(14)	E	1760	(14)	E	877	(12)	P/3	EN ISO 10301:1997
F	Sur	84852153	4-Nonylphenol, branched	5.92	246	138	(32)	E	137	(12)	P/4	410	(32)	E	-
G	AOxi	71432	Benzene	1.99	1093300	24600	(14)	E	31277	(12)	E	35000	(14)	E	-
G	AOxi	95476	o-Xylene	3.09	189810	16400	(32)	E	17500	(14)	E	4450	(14)	E	-
G	AOxi	100414	Ethylbenzene	3.03	166690	12100	(14)	E	18870	(32)	E	5300	(14)	E	-
G	AOxi	100425	Styrene	2.89	292600	15928	(14)	E	4721	(12)	E	1218	(14)	E	-
G	AOxi	106423	p-Xylene	3.09	189880	8400	(32)	E	32400	(14)	E	3752	(14)	E	-
G	AOxi	108383	m-Xylene	3.09	189790	16000	(32)	E	17584	(32)	E	4368	(14)	E	-
G	AOxi	1330207	Xylene	3.09	189790	27710	(32)	E	17500	(14)	E	13099	(33)	B	EN ISO 6468:1996
G	AOxi	1825214	Pentachloroanisole	5.30	139	650	(32)	E	27.0	(36)	E	326	(12)	P/3	-
H	Sol	106434	4-Chlorotoluene	3.18	60804	3596	(12)	P/2	3570	(14)	E	7243	(12)	P/3	-
H	Sol	108883	Toluene	2.54	461360	36200	(14)	E	6000	(32)	E	10950	(14)	E	-
H	Sol	118967	2,4,6-Trinitrotoluene	1.99	215060	2190	(14)	E	9250	(14)	E	729	(14)	E	EN ISO 6468:1996
H	Sol	121142	2,4-Dinitrotoluol	2.18	301100	24300	(14)	E	35000	(14)	E	807	(32)	E	-
I	AFun	14488530	Dibutyltin	0.57	9566900	1776100	(12)	P/1	900	(14)	E	6544	(12)	P/3	EN ISO 10301:1997
I	AFun	56573854	Tributyltin	7.35	7.41	4.00	(32)	E	4.30	(14)	E	3.00	(32)	E	-
J	FlRet	85223	Pentabromoethylbenzene	7.48	0.29	-	-	WS	2.18	(12)	P/4	-	-	WS	-
J	FlRet	101553	4-Bromophenyl phenyl ether	4.94	2284	575	(32)	E	360	(36)	E	2339	(12)	P/2	-
J	FlRet	41318756	PBDE 28	5.88	38.91	88.7	(12)	P/1	248	(12)	P/4	180	(33)	B	-
J	FlRet	5436431	PBDE 47	6.77	0.31	-	-	WS	-	-	WS	-	-	D	-
J	FlRet	60348609	PBDE 99	7.66	0.01	-	-	WS	-	-	WS	-	-	D	-
J	FlRet	68631492	PBDE 153	8.55	3.07	-	-	WS	-	-	WS	-	-	D	-
J	FlRet	182346210	PBDE 85	7.66	0.01	-	-	WS	-	-	WS	-	-	D	-
K	Pla	84662	Di-ethyl phthalate	2.65	531890	21867	(32)	E	54235	(36)	E	48603	(32)	E	-
K	Pla	84742	Di-(n-butyl) phthalate	4.61	14851	1610	(32)	E	3700	(36)	E	400	(32)	E	-
K	Pla	85687	Butyl benzyl phthalate	4.84	2272	1533	(32)	E	2000	(36)	E	120	(32)	E	EN ISO 6468:1996
K	Pla	117817	Di-(2-ethylhexyl) phthalate	7.5	3	-	-	WS	-	-	WS	-	-	WS	-
K	Pla	131113	Dimethyl phthalate	1.66	1790100	121000	(34)	E	33000	(36)	E	70367	(32)	E	-
K	Pla	131168	Dipropyl phthalate	3.63	419510	5523	(12)	P/3	9274	(12)	P/4	15200	(12)	P/3	-
K	Pla	131180	Dipentyl phthalate	5.59	1162	153	(12)	P/3	391	(12)	P/4	5872	(12)	P/3	-
L	Mis	60004	EDTA	-3.86	4848600	59800	(32)	E	-	-	D	40842	(12)	P/1	-

Chemical Group [a]	Main Application [b]	CAS	Chemical Name	log K_{ow}	Water Solubility [µg/L]	LC50 [µg/L] PP	Source PP	Type of data PP [c]	LC50 [µg/L] DM	Source DM	Type of data DM [c]	LC50 [µg/L] PS	Source PS	Type of data PS [c]	Analytical Methods [d]
L	Mis	75014	Vinylchloride	1.62	4837500	26624	(12)	P/1	87715	(12)	B	149716	(33)	B	-
L	Mis	107131	Acrylonitrile	0.21	69155000	16980	(32)	E	8800	(36)	E	2186680	(33)	B	-
L	Mis	139139	Nitrilotriacetic acid	-3.81	1839000000	-	-	D	-	-	D	30695	(12)	P/1	-
L	Mis	2599113	Hydroxysimazine	1.67	833040	132410	(12)	P/1	165760	(12)	P/3	36.0	(12)	P/3	-

[a] **A**: Pesticides and transformation products, **B**: Polychlorinated biphenyls, **C**: Polycyclic aromatic hydrocarbons and derivates, **D**: Halogenated benzenes and nitrobenzenes, **E**: Halogenated alkanes, **F**: Phenols and chlorophenols, **G**: Anilines, anisoles and alkylated benzenes, **H**: Toluenes and halogenated derivatives, **I**: Organotin compounds, **J**: Brominated flame retardants, **K**: Phthalates, **L**: Miscellaneous.

[b] **Her**: Herbicides, **Fun**: Fungicides, **Ins**: Insecticides, **Lub,Pla**: Lubricants, plasticizers, **Byprod**: Byproducts of petroleum processing or combustion, **Sol**: Solvent, **Sur**: Surfactant, **AOxi**: Anti-oxidants, **AFun**: Anti-fungal, **FlRet**: Flame retardants, **Pla**: Plasticizer, **Mis**: Miscellaneous

[c] **E**: Experimental toxicity data from literature, **B**: Baseline toxicity data estimated from the octanol/water partitioning coefficient, **P**: Predicted toxicity data from read across together with the level of reliability (1: low ; 2: moderate ; 3: high and 4: very high). Toxicity values were removed when they lay outside of the model domain ($1 < \log K_{ow} < 6$) for the baseline prediction (**D**), or when they exceed water solubility by a factor of 10 (**WS**).

[d] **DIN EN ISO 6468:1996** - Water quality. Determination of certain organochlorine insecticides, polychlorinated biphenyls and chlorobenzenes - Gas-chromatographic method after liquid-liquid extraction; **DIN EN ISO 17993:2003** - Water quality. Determination of 15 polycyclic aromatic hydrocarbons (PAH) in water by HPLC with fluorescence detection after liquid-liquid extraction; **DIN EN ISO 10301:1997** - Water quality. Determination of highly volatile halogenated hydrocarbons – Gas chromatographic methods; **EN ISO 10695:2000** - Water quality. Determination of selected organic nitrogen and phosphorus compounds -- Gas chromatographic methods; **EN ISO 18856:2005** - Water quality. Determination of selected phthalates using gas chromatography/mass spectrometry; **EN ISO 17353:2005** - Water quality. Determination of selected organotin compounds. Gas chromatographic method; **EN ISO 18857-1:2006** - Water quality. Determination of selected alkylphenols - Part 1: Method for non-filtered samples using liquid-liquid extraction and gas chromatography with mass selective detection; **DIN EN 12918:1999** - Water quality. Determination of parathion, parathion-methyl and some other organophosphorus compounds in water by dichloromethane extraction and gas chromatographic analysis

Table S2: Number of sites with quantified and non-detected concentrations for each chemical. The frequency of exceedance (%; in parentheses) and the number of sites are given for each chemical after comparing the limit of quantification (LOQ) for the non-detects with the chronic risk threshold (CRT) and the acute risk threshold (ART).

Chemical Name	No. Cases[a]			
	Quantified	Non-Detects	LOQ>CRT[b]	LOQ>ART[b]
Fluoranthene	976	67	67(100)	12(18)
Benzo[a]pyrene	924	967	838(87)	65(7)
Diuron	859	1201	264(22)	32(3)
Naphthalene	826	919	17(2)	1(0)
Atrazine	820	2016	23(1)	14(1)
Isoproturon	727	1233	19(2)	0(0)
Metolachlor	480	736	23(3)	10(1)
Tributyltin	479	1005	581(58)	0(0)
Simazine	473	2284	14(1)	4(0)
g-Hexachlorocyclohexane	457	1904	33(2)	14(1)
MCPA	432	1024	0(0)	0(0)
Mecoprop	407	1082	0(0)	0(0)
Glyphosate	397	326	0(0)	0(0)
Phenanthrene	391	313	15(5)	0(0)
Pyrene	361	15	15(100)	0(0)
Alachlor	341	2261	18(1)	18(1)
Anthracene	327	1585	70(4)	4(0)
Terbutylazine	316	1008	12(1)	6(1)
Trichloromethane	299	1700	16(1)	0(0)
Bentazone	295	857	0(0)	0(0)
Benz[a]anthracene	289	7	7(100)	0(0)
Desethylatrazine	286	772	0(0)	0(0)
Metazachlor	285	693	0(0)	0(0)
Tetrachloroethylene	276	1753	21(1)	17(1)
2,4-D	265	892	0(0)	0(0)
Endrin	257	2158	436(20)	73(3)
Dichloromethane	254	1650	14(1)	0(0)
Linuron	233	1555	35(2)	0(0)
Pentachlorophenol	221	1704	186(11)	4(0)
4,4'- DDT	206	1005	1005(100)	61(6)
Carbofuran	204	780	753(97)	0(0)
Isodrin	201	1984	80(4)	4(0)
Chlorpyrifos	191	1935	1934(100)	1149(59)
Hexachlorobenzene	188	2139	1248(58)	81(4)
a-Hexachlorocyclohexane	183	1156	10(1)	10(1)
Toluene	183	1351	31(2)	17(1)
Para-tert-octylphenol	180	1066	370(35)	7(1)
1,3,5-Trichlorobenzene	177	874	0(0)	0(0)
Benzene	174	1975	21(1)	0(0)
b-Hexachlorocyclohexane	169	1146	10(1)	10(1)
Dieldrin	167	2256	73(3)	6(0)
Aldrin	164	2250	162(7)	4(0)
Trifluralin	153	2213	81(4)	12(1)
1,1,2-Trichloroethene	145	1755	17(1)	0(0)
1,2-Dichloroethane	142	2101	17(1)	0(0)
1,2,4-Trichlorobenzene	130	1028	9(1)	0(0)
4,4'- DDD	129	1441	911(63)	12(1)

Chemical Name	No. Cases[a]			
	Quantified	Non-Detects	LOQ>CRT[b]	LOQ>ART[b]
Fluoranthene	976	67	67(100)	12(18)
Metalaxyl	127	831	10(1)	0(0)
2,4'-DDT	125	863	863(100)	12(1)
1,2,3-Trichlorbenzene	116	899	0(0)	0(0)
Fluorene	110	524	1(0)	0(0)
Propyzamide	103	849	0(0)	0(0)
Pirimicarb	100	527	388(74)	10(2)
4,4'- DDE	95	1491	116(8)	4(0)
Heptachlor	94	1075	49(5)	10(1)
Chlorfenvinfos	90	2049	2048(100)	588(29)
2-Methylnaphthalene	88	180	0(0)	0(0)
Endosulfan I	88	1859	440(24)	58(3)
Carbon tetrachloride	87	1957	21(1)	0(0)
Prometryn	86	770	0(0)	0(0)
Dimethoate	85	997	10(1)	0(0)
Acenaphthene	83	349	15(4)	0(0)
2,6-dichlorobenzamide	82	490	0(0)	0(0)
Hexachlorobutadiene	81	2048	128(6)	78(4)
Acetochlor	77	295	0(0)	0(0)
PCB 28	75	422	1(0)	1(0)
Ethofumesate	74	814	0(0)	0(0)
o-Xylene	72	151	0(0)	0(0)
Pentachlorobenzene	72	1719	4(0)	4(0)
Cyanide	71	73	73(100)	0(0)
Ethylbenzene	70	321	0(0)	0(0)
Chloridazon	67	466	0(0)	0(0)
1,1,1-Trichloroethane	63	1068	0(0)	0(0)
Parathion-ethyl	63	864	782(91)	14(2)
Pendimethalin	62	1044	8(1)	0(0)
Propazine	60	629	14(2)	8(1)
Di-(n-butyl) phthalate	58	48	20(42)	0(0)
Dibutyltin	58	500	0(0)	0(0)
Methoxychlor	58	385	0(0)	0(0)
Propiconazole	58	398	10(3)	0(0)
Dichlorvos	56	1020	1019(100)	560(55)
d-Hexachlorocyclohexane	54	641	0(0)	0(0)
Heptachloro Epoxide B	53	262	0(0)	0(0)
Desisopropylatrazine	51	902	0(0)	0(0)
PCB 118	49	8	8(100)	5(62)
2-naphthalenol	42	95	0(0)	0(0)
Terbutryn	42	160	23(14)	6(4)
1,1-Dichloroethene	38	561	0(0)	0(0)
Dicamba	37	707	0(0)	0(0)
Dichlorprop	37	414	0(0)	0(0)
4-Octylphenol	36	462	0(0)	0(0)
Bromodichloromethane	36	99	0(0)	0(0)
Ziram	36	46	46(100)	0(0)
1,2-Dichlorobenzene	35	674	1(0)	0(0)
Acephthylene	32	594	9(2)	0(0)
Dichlobenil	32	720	0(0)	0(0)
4-Nonylphenol	31	1065	143(13)	0(0)
Endosulfan	31	168	49(29)	0(0)
Pentabromoethylbenzene	31	18	18(100)	0(0)

Chemical Name	No. Cases[a]			
	Quantified	Non-Detects	LOQ>CRT[b]	LOQ>ART[b]
Fluoranthene	976	67	67(100)	12(18)
Styrene	31	188	0(0)	0(0)
1,1-Dichloroethane	30	595	0(0)	0(0)
Malathion	30	1246	1225(98)	168(13)
Trichlorofluoromethane	30	51	0(0)	0(0)
1,1,2-Trichloroethane	29	241	0(0)	0(0)
1,3-Dichlorobenzene	29	240	6(2)	0(0)
Lenacil	29	597	0(0)	0(0)
4-Chlorotoluene	28	751	14(2)	0(0)
Bromacil	27	976	0(0)	0(0)
Metribuzin	27	812	0(0)	0(0)
Permethrin	27	600	600(100)	41(7)
Hexazinone	26	530	0(0)	0(0)
Monochlorobenzene	26	234	0(0)	0(0)
PCB 153	26	30	30(100)	1(3)
PCB 126	25	0	0(0)	0(0)
PCB 138	25	12	12(100)	1(8)
1,2-Dibromoethane	24	691	0(0)	0(0)
Methyl parathion	24	1014	869(86)	16(2)
Bisphenol-a	23	10	0(0)	0(0)
Desmedipham	23	24	1(4)	0(0)
Trans-1,2-Dichloroethylene	23	444	0(0)	0(0)
2-Chloroethylphosphonic Acid	21	82	0(0)	0(0)
2,3,4,5-Tetrachlorophenol	20	209	0(0)	0(0)
2,4,6-tri-tert-Butylphenol	20	5	5(100)	0(0)
Clopyralid	20	677	0(0)	0(0)
Dicofol	20	0	0(0)	0(0)
Phenitrothion	20	1239	1141(92)	10(1)
1,2-Dichloroethene	19	78	0(0)	0(0)
Dichlorodifluoromethane	18	36	0(0)	0(0)
2,4,5-Trichlorophenoxyacetic acid	17	769	0(0)	0(0)
Fenpropimorph	17	545	0(0)	0(0)
Methamidophos	17	0	0(0)	0(0)
PCB 101	17	3	3(100)	1(33)
Chlordane	16	0	0(0)	0(0)
Metamitron	16	691	0(0)	0(0)
PCB 52	16	1	1(100)	1(100)
Xylene	16	145	0(0)	0(0)
PCB 180	15	2	2(100)	1(50)
2,4-Dichlorophenol	14	49	17(35)	17(35)
Cis-1,2-Dichloroethylene	13	18	0(0)	0(0)
Terbumeton	13	618	0(0)	0(0)
Vinylchloride	13	60	7(12)	0(0)
Ametryne	12	406	12(3)	0(0)
1-Methylnaphthalene	11	93	0(0)	0(0)
2,4,6-Trichlorophenol	11	23	0(0)	0(0)
2,4'-DB	11	124	0(0)	0(0)
Desmetryn	11	485	0(0)	0(0)
4-Nonylphenol, branched	10	38	18(47)	11(29)
Benfluralin	10	0	0(0)	0(0)
Hexachlorocyclohexane	10	201	0(0)	0(0)
PCB 77	10	130	130(100)	0(0)
2,4'-DDD	9	85	54(64)	0(0)

Chemical Name	No. Cases[a]			
	Quantified	Non-Detects	LOQ>CRT[b]	LOQ>ART[b]
Fluoranthene	976	67	67(100)	12(18)
Butyl benzyl phthalate	9	20	20(100)	20(100)
Demeton-S-Methyl	9	611	501(82)	0(0)
Fluquincozole	9	0	0(0)	0(0)
MCPB	9	38	0(0)	0(0)
Methomyl	9	448	383(85)	0(0)
MTBE	9	25	0(0)	0(0)
Prometon	9	398	0(0)	0(0)
2,4'-DDE	8	89	22(25)	0(0)
Bromoxynil	8	308	0(0)	0(0)
Demeton-S-methylsulfon	8	0	0(0)	0(0)
PCB 169	8	82	82(100)	0(0)
Phosalone	8	312	312(100)	19(6)
Chlorsulfuron	7	0	0(0)	0(0)
Formaldehyde	7	53	29(55)	0(0)
Ioxynil	7	254	0(0)	0(0)
Pentachloronitrobenzene	7	392	0(0)	0(0)
Cyanazine	6	460	0(0)	0(0)
Dipropyl phthalate	6	62	0(0)	0(0)
Fenoprop	6	8	0(0)	0(0)
Deisopropyldeethylatrazine	5	0	0(0)	0(0)
EDTA	5	0	0(0)	0(0)
2,4-Dinitrotoluol	4	110	19(17)	0(0)
4-Bromophenyl phenyl ether	4	40	19(48)	0(0)
Kepon	4	377	0(0)	0(0)
4-Chloro-3-Methylphenol	3	10	0(0)	0(0)
PCB 194	3	316	316(100)	0(0)
Pentachloroanisole	3	6	0(0)	0(0)
Tebufenozide	3	442	0(0)	0(0)
Trans-nonachlor	3	0	0(0)	0(0)
4-Nitrophenol	2	78	0(0)	0(0)
Desethylterbutylazine	2	39	0(0)	0(0)
Dimethyl phthalate	2	167	0(0)	0(0)
Hydroxysimazine	2	92	0(0)	0(0)
Iodofenphos	2	455	453(100)	0(0)
Metsulfuronmethyl	2	0	0(0)	0(0)
Nitrilotriacetic acid	2	0	0(0)	0(0)
Nitrofen	2	203	0(0)	0(0)
Pyridate	2	562	0(0)	0(0)
Terbufos	2	570	570(100)	179(31)
2-Methylphenol	1	0	0(0)	0(0)
2,3-Dimethylphenol	1	0	0(0)	0(0)
2,6-Dichlorophenol	1	15	0(0)	0(0)
Dinitro-o-Cresol	1	7	0(0)	0(0)
Dinoseb	1	8	0(0)	0(0)
Dipentyl phthalate	1	67	0(0)	0(0)
Hexachlorocyclopentadiene	1	19	19(100)	19(100)
m-Xylene	1	14	0(0)	0(0)
Omethoate	1	256	256(100)	0(0)
PBDE 28	1	72	0(0)	0(0)
PCB 105	1	0	0(0)	0(0)
PCB 157	1	0	0(0)	0(0)
1,1,1,3-Tetrachloropropane	0	153	0(0)	0(0)

Chemical Name	No. Cases[a]			
	Quantified	Non-Detects	LOQ>CRT[b]	LOQ>ART[b]
Fluoranthene	976	67	67(100)	12(18)
2,3,4,6-Tetrachlorophenol	0	8	0(0)	0(0)
2,4,5-Trichlorophenol	0	14	4(29)	0(0)
2,4,6-Trinitrotoluene	0	13	0(0)	0(0)
2,5-Dimethylphenol	0	1	0(0)	0(0)
4-Chloro-2-Methylphenol	0	3	0(0)	0(0)
4-Methylphenol	0	218	0(0)	0(0)
Acrylonitrile	0	1	1(100)	1(100)
Captan	0	566	0(0)	0(0)
Chlorthiamid	0	279	0(0)	0(0)
Dalapon	0	3	0(0)	0(0)
Di-ethyl phthalate	0	20	0(0)	0(0)
Ethylenethiourea	0	1	0(0)	0(0)
Fezaquin	0	295	295(100)	0(0)
p-Xylene	0	25	0(0)	0(0)
Secbumeton	0	16	0(0)	0(0)
Thiram	0	53	53(100)	0(0)

[a] Sites from Spain were omitted, because the LOQ was not considered reliable.
[b] The percentage of sites which had LOQ > ART or LOQ > CRT was calculated as: (No. sites LOQ > ART OR No. sites LOQ > CRT / No. sites non-detects)x100

Table S3: Community studies reporting effects from pesticides for the cases exceeding the levels of 1/10 and 1/1,000 of the LC50 values for the analyzed organism groups.

Threshold	Chemical group	MoA[a]	Organism groups	Total no. of cases	No. (%) of affected cases [d]	LoE[e]	Source
1/10 -10 LC50	Insecticides	AChEI	Fish	22	9 (41)	About as likely as not	(15)
			Invertebrates	97	71 (73)	Likely	(15)
			Algae and macrophytes	25	5 (20)	Unlikely	(15)
		SCI	Fish	15	7 (47)	About as likely as not	(15)
			Invertebrates	99	75 (76)	Likely	(15)
			Algae and macrophytes	23	8 (35)	About as likely as not	(15)
	Herbicides	PSI	Fish	11	4 (36)	About as likely as not	(40)
			Invertebrates	32	16 (50)	More likely than not	(40)
			Algae and macrophytes	52	40 (77)	Likely	(40)
		GI	Fish	ns[b]	ns[b]	ns[b]	(40)
			Invertebrates	8	3 (38)	About as likely as not	(40)
			Algae and macrophytes	10	3 (30)	About as likely as not	(40)
1/10-1 LC50	Pesticides		Invertebrates	8	8 (100)	Very likely	(5)
>1/10 LC50	Overall chemical		Fish	48[c]	20 (42)	About as likely as not	
			Invertebrates	228[c]	162 (71)	Likely	
			Algae and macrophytes	110[c]	56 (51)	More likely than not	
1/1,000 LC50	Pesticides		Invertebrates	45	32 (71)	Likely	(5)

[a] Modes of actions groups: Acetylcholinesterase Inhibitor (AChEI) includes organophosphates and carbamates, which interrupt the transmission of nerve impulses by inhibition of the enzyme acetylcholinesterase. Sodium Channel Inhibitor (SCI) includes synthetic pyrethroids, which lead to paralysis by interfering with the sodium channels of the nervous system. Photosynthesis Inhibitors (PSI) includes triazines/triazinones and the urea compounds, which by interfering with the photosynthesis lead to disrupted plant growth. Growth Inhibitors (GI) includes all products that have no direct photosynthesis-inhibiting effects.

[b] ns - No study available

[c] Total number of cases is calculated as the sum of total number of cases for each chemical group and mode of action. For fish and algae: the sum of total no. cases for (i) Insecticides with AChEI, (ii) Insecticides with SCI, (iii) Herbicides with PSI, and (iv) Herbicides with GI. For invertebrates: the sum of total no. of cases for (i) Insecticides with AChEI, (ii) Insecticides with SCI, (iii) Herbicides with PSI, (iv) Herbicides with GI and (v) Pesticides for the level 1/10-1 of the LC50.

[d] Percentage of affected cases is calculated as ((Number of affected cases/Total number of cases)x100). Effects for the micro-/mesocosm reviews (15, 40) ranged from slight, short-term (less than 8 weeks) effects, to pronounced, long-term (longer than 8 weeks) effects. All cases exhibiting at least slight acute effects for concentrations higher than the 1/10 of the LC50 were considered as affected cases. The exposure range was between 1/10 and 10 times the LC50 values. For the meta-analysis on the effects of pesticides on invertebrate communities (5)all sites exhibiting a statistically significant decline in the abundance of the sensitive invertebrate species when compared with both thresholds levels(1/10- of the LC50 and 1/1,000-1/10 of the LC50) were considered as affected cases.

[e] Likelihood of effects classified based on the affected cases and divided into (i) unlikely (<33 %), (ii) more likely than not (>50 %), (iii) About as likely as not (33-66 %), (iv) likely (>66%) and (v) very likely (>90 %). Terminology is based on the guidelines for uncertainty treatment, which is used from the intergovernmental panel on climate change (41).

Table S4: Number of sites for which the chemical concentration exceeds the CRT (chronic risk threshold) and the ART (acute risk threshold) for each organism group represented by the fish *P. promelas* (PP), the invertebrate *D. magna* (DM), and the algae *P. subcapitata* (PS).

	Concentration exceeding ART/CRT (Type of data) [a]		
Chemical	**No. sites PP**	**No. sites DM**	**No. sites PS**
4,4'- DDE	8/9(P/1)	9/21(P/4)	8/8(P/1)
4,4'- DDT	7/8(E)	10/52(E)	-
2,4,6-tri-tert-Butylphenol	5/9(E)	3/17(P/4)	-
Hexachlorobenzene	4/4(P/2)	9/44(E)	5/4(E)
4,4'- DDD	4/4(P/1)	9/24(E)	3/1(P/2)
B-Hexachlorocyclohexane	3/3(P/4)	0/3(P/4)	0/0(B)
Endrin	26/71(E)	0/1(E)	0/0(P/2)
g-Hexachlorocyclohexane	20/51(E)	0/38(E)	0/0(B)
Atrazine	2/3(E)	0/7(E)	72/73(E)
Endosulfan	2/17(E)	0/0(E)	0/0(E)
Tributyltin	15/21(E)	15/363(E)	15/18(E)
Cyanide	13/22(E)	3/82(E)	-
Ziram	11/20(E)	1/24(E)	1/2(E)
Benzo[a]pyrene	1/9(E)	12/759(E)	1/1(E)
Hexachlorobutadiene	1/7(E)	0/7(E)	1/0(P/2)
PCB 194	1/2(E)	1/3(E)	-
Endosulfan I	1/17(E)	0/1(P/4)	1/1(P/2)
Aldrin	1/1(E)	1/5(E)	1/1(P/3)
Chlordane	1/1(E)	1/1(E)	-
Hexachlorocyclohexane	1/1(E)	0/1(P/4)	0/0(B)
Hexachlorocyclopentadiene	1/1(E)	1/1(E)	1/1(P/4)
Dichloromethane	1/0(E)	1/1(E)	0/0(B)
Pentachlorophenol	0/6(P/4)	0/7(E)	0/0(E)
PCB 180	0/2(P/3)	0/3(P/4)	-
2-naphthalenol	0/2(E)	0/6(E)	0/0(E)
4-Nonylphenol	0/1(E)	0/5(E)	0/0(E)
Chlorpyrifos	0/1(E)	146/235(E)	0/0(P/3)
Methoxychlor	0/1(E)	0/1(E)	0/0(P/1)
PCB 153	0/1(E)	0/4(E)	-
Permethrin	0/1(E)	13/27(E)	-
Pyrene	0/1(E)	0/15(E)	-
1,2,3-Trichlorbenzene	0/0(P/4)	0/1(E)	0/0(E)
2,4'-DDT	0/0(P/3)	0/21(P/4)	-
4-Octylphenol	0/0(P/3)	0/1(P/4)	0/0(P/3)
Anthracene	0/0(P/3)	0/6(E)	0/0(P/3)
Dipentyl phthalate	0/0(P/3)	0/1(P/4)	0/0(P/3)
Phenanthrene	0/0(P/3)	0/5(E)	0/0(E)
2,4'-DDD	0/0(P/1)	0/8(P/4)	0/0(B)

Chemical	Concentration exceeding ART/CRT (Type of data) [a]		
	No. sites PP	No. sites DM	No. sites PS
Chlorfenvinfos	0/0(P/1)	69/112(E)	0/0(B)
Demeton-S-Methyl	0/0(P/1)	0/9(E)	0/0(B)
Dibutyltin	0/0(P/1)	0/12(E)	0/0(P/3)
Iodofenphos	0/0(P/1)	0/1(E)	-
Isoproturon	0/0(P/1)	0/12(E)	25/51(E)
Lenacil	0/0(P/1)	0/0(E)	1/3(E)
Linuron	0/0(P/1)	0/1(E)	2/1(E)
Metazachlor	0/0(P/1)	0/0(E)	1/6(E)
Pendimethalin	0/0(P/1)	0/0(E)	1/1(E)
Terbutylazine	0/0(P/1)	0/0(E)	24/31(E)
4-Nonylphenol, branched	0/0(E)	0/1(P/4)	0/0(E)
Alachlor	0/0(E)	0/0(E)	10/14(E)
Bromacil	0/0(E)	0/0(E)	1/1(E)
Butyl benzyl phthalate	0/0(E)	0/1(E)	0/1(E)
Carbofuran	0/0(E)	11/114(E)	0/0(E)
Di-(n-butyl) phthalate	0/0(E)	0/1(E)	0/0(E)
Dichlorvos	0/0(E)	21/56(E)	0/0(E)
Diuron	0/0(E)	0/0(E)	230/345(E)
Heptachlor	0/0(E)	0/8(E)	0/0(E)
Malathion	0/0(E)	7/29(E)	0/0(E)
Methomyl	0/0(E)	1/3(E)	0/0(E)
Methyl parathion	0/0(E)	0/17(E)	0/0(E)
Metolachlor	0/0(E)	0/0(E)	2/7(E)
Para-tert-octylphenol	0/0(E)	0/23(E)	0/0(P/4)
Parathion-ethyl	0/0(E)	1/22(E)	0/0(P/2)
PCB 52	0/0(E)	0/1(E)	-
Pentachloroanisole	0/0(E)	0/1(E)	0/0(P/3)
Phenitrothion	0/0(E)	1/12(E)	0/0(E)
Phosalone	0/0(E)	0/8(E)	0/0(E)
Pirimicarb	0/0(E)	0/4(E)	0/0(E)
Terbufos	0/0(E)	2/2(E)	0/0(B)
Toluene	0/0(E)	0/1(E)	0/0(E)
Trichloromethane	0/0(E)	0/2(E)	0/0(B)
Benz[a]anthracene	-	0/9(E)	-
Fluoranthene	-	4/30(E)	-
Omethoate	-	0/1(E)	-
Pentabromoethylbenzene	-	11/31(P/4)	-

[a] Type of data: **E**: Experimental toxicity data from literature, **B**: Baseline toxicity data estimated from the octanol/water partitioning coefficient, **P**: Predicted toxicity data from read across together with the level of reliability (1: low ; 2: moderate ; 3: high and 4: very high). Toxicity values were removed when they lay outside of the model domain ($1 < \log K_{ow} < 6$) for the baseline prediction (**D**), or when they exceed water solubility by a factor of 10 (**WS**).

Table S5: Number of sites monitored for each river basin (RB) and number of sites with land use (LU) for each river basin.

River basin	Area(km²)	No sites RB	LU	River basin	Area(km²)	No sites RB	LU
Danube	803554	569	343	Sicily	25684	10	-
Loire	156765	388	37	Northumbria	8499	9	-
Rhone	128355	360	103	UK South East	8288	9	-
Po Basin	73341	279	-	Schlei/Trave	6154	8	-
Adour-Garonne	116740	247	52	Venta	21915	8	-
Seine	94356	206	19	Cavado, Ave and Leca	3358	7	-
Middle Appenines	36192	193	-	Andalusia Atlantic Basins	68010	6	-
Rhine	186325	168	32	East Aegean	60875	6	-
Northern Appenines	38477	149	-	Galician Coast	13081	6	-
Internal Basins of Catalonia	16433	106	-	Kokemäenjoki	68628	6	-
Ebro	86012	84	1	Lielupe	17800	6	-
Minho and Lima	40829	75	-	Warnow/Peene	13631	6	-
Elbe	147527	73	1	Algarve Basins	3836	5	-
Eastern Alps	37179	70	-	Daugava	82793	5	-
Scheldt	36904	65	12	Ems	16315	5	-
Douro	97713	60	-	Central Macedonia	31811	4	-
Meuse	34238	58	9	Guadiana	66989	4	-
GB North Western	12375	53	-	Kymijoki-Gulf of Finland	50867	4	-
Scotland	67803	47	-	Vidaa-Krusaa	5718	4	-
Tagus and Western Basins	83120	42	-	Vistula	206058	4	-
Jucar	42959	41	-	Black Sea	20974	3	-
Shannon	18317	41	-	Eastern Sterea Ellada	12201	3	-
Andalusia	17958	35	-	North Adriatic	3852	3	-
Southern Appenines	67496	32	-	SE South West	29032	3	-
Neagh Bann	7920	30	-	NO West Bay	37529	3	-
Basque County internal basins	2267	29	-	Western Macedonia	19761	3	-
IE South Eastern	12859	29	-	Dee	2142	2	-
IE Western	12220	28	-	Gauja	14381	2	-
IE South Western	11363	27	-	Vouga, Mondego and Lis	11596	2	-
UK South West	17631	27	-	Eastern Peloponnese	8408	1	-
Corsica	8694	22	8	Epirus	15294	1	-
Cyprus	9248	22	-	Finnmark	48528	1	-
UK North Eastern	3067	17	-	Glomma	47429	1	-
Western Wales	12213	17	-	Nordland	38369	1	-
Humber	25415	16	-	Northern Peloponnese	7383	1	-
Weser	47291	16	-	Oulujoki-Iijoki	64731	1	-
IE Eastern	6275	14	-	Sado and Mira	10072	1	-
Segura	18905	13	-	Skagerrak and Kattegat	75986	1	-
Severn	21068	13	-	South Baltic	54753	1	-
Ucker	134390	13	-	Thessalia	13133	1	-
UK North West	11370	12	-	Troendelag	35297	1	-
Anglian	25093	11	-	Vuoksi	283356	1	-
Solway Tweed	15218	11	-	NO West	32815	1	-
Thames	15811	11	-	West Aegean	21584	1	-
Nemunas	100082	10	-	Western Peloponnese	7235	1	-
Serchio	1439	10	-				

Table S6: Land use type and their respective categories.

Category	Type of land use
Natural vegetation	Scrub and/or herbaceous vegetation areas
	Open spaces with little or no vegetation
	Forested areas
Anthropogenically influenced areas	Arable land
	Permanent crops
	Heterogeneous agricultural areas
	Urban areas

Table S7: Number of sites with ecological and chemical information. Thresholds comprise chronic risk threshold (CRT) and acute risk threshold (ART). Number of sites exceeding the risk thresholds, number of sites in high (H) and good (G) status which exceed the risk thresholds, as well as the total number of sites analyzed are given for each organism group.

		No. of sites		
Species	**Threshold Classes**	**Exceeding**	**Exceeding (H+G)**	**Total**
Fish	>CRT	87	50	
	CRT-ART	3	1	
	<ART	5	1	**95**
Invertebrates	>CRT	15	8	
	CRT-ART	155	67	
	<ART	21	5	**191**
Diatoms	>CRT	87	53	
	CRT-ART	17	11	
	<ART	32	19	**136**

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