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Abstract

Every chemical compound is characterised by a specific type and level of toxicity. Making a comparison and a toxicological ranking of chemicals is therefore a difficult task. In this work we set up a ranking of chemicals based on an adaptation of the multi-criteria method. The various chemical compounds were considered as alternatives, whose evaluation was based on their level and different type of toxicity, considered as different criteria. As in the classic multi-criteria analysis (MCA) methods, each criterion can have a different weight on the overall evaluation, leading to the creation of a dynamic ranking that can vary depending on the priorities. In this technique, chemicals are not included in a class or category, but are assigned a numerical value, representing their overall toxicity. Such information could be useful for further evaluations in various fields. We propose a study focusing on the textile sector: levels of toxic compounds in wastewater (incoming water, untreated and treated wastewater) were first thoroughly evaluated using univariate and multivariate exploratory techniques; then the toxicological impact of approximately one hundred textile factories around the world was evaluated on the basis of the previously developed toxicological ranking of chemicals. Arsenic, cyanide, hexavalent chromium and other heavy metals were the most toxic compounds among the 12 classes of chemicals investigated.

Keywords	Multi-Criteria Analysis; textile industry; water pollution; toxicological assessment; health effect assessment.

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To the Editor of *Environmental Pollution*

Dear Editor,

Please find attached a manuscript entitled "*Multi-criteria ranking of chemicals for toxicological impact of textile industry*".

In this paper we illustrated a new hazard assessment method, based on an adaptation of multi-criteria analysis, which takes into account different type of toxicity and different levels of toxicity at the same time. Pollutants are not included in a class or category, such as in other classifications, but are assigned a numerical value representing their overall toxicity, which can be easily used in further elaborations. In this paper we proposed a case study focused in the textile sector: the potential health impact of textile factories was evaluated based on the concentration of chemicals in wastewater.

I think that this work is perfectly suited for *Environmental Pollution*, since it describes a new technique able to evaluate the health effect of a measured concentration of pollutants, by assessing their global toxicological impact.

We would like you to consider this work for publication.

Sincerely yours,

Elena Gregoris
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elena.gregoris@unive.it

Concentration data

+

Toxicological information

TOXICOLOGICAL INDEX

Ranking of pollutants based on global toxicity

CASE STUDY

Assessment of health impact of textile factories

TITLE

Multi-criteria ranking of chemicals for toxicological impact of textile industry

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Abstract

Every chemical compound is characterised by a specific type and level of toxicity. Making a comparison and a toxicological ranking of chemicals is therefore a difficult task. In this work we set up a ranking of chemicals based on an adaptation of the multi-criteria method. The various chemical compounds were considered as alternatives, whose evaluation was based on their level and different type of toxicity, considered as different criteria. As in the classic multi-criteria analysis (MCA) methods, each criterion can have a different weight on the overall evaluation, leading to the creation of a dynamic ranking that can vary depending on the priorities. In this technique, chemicals are not included in a class or category, but are assigned a numerical value, representing their overall toxicity. Such information could be useful for further evaluations in various fields. We propose a study focusing on the textile sector: levels of toxic compounds in wastewater (incoming water, untreated and treated wastewater) were first thoroughly evaluated using univariate and multivariate exploratory techniques; then the toxicological impact of approximately one hundred textile factories around the world was evaluated on the basis of the previously developed toxicological ranking of chemicals. Arsenic, cyanide, hexavalent chromium and other heavy metals were the most toxic compounds among the 12 classes of chemicals investigated.

Capsule

A dynamic toxicity ranking of chemicals is set up using an adaptation of multi-criteria analysis and it is applied in order to assess the potential health impact of textile factories.

Introduction

Conducting a global toxicological evaluation of chemicals is a considerable challenge, as every chemical is characterised by a specific kind of toxicity (lethal effects, carcinogenicity, etc.), which complicates the comparison. Given the increasing concern regarding the use of chemicals in everyday life and workplaces, several chemical hazard screening methods have been developed in recent years. For example, the US Environmental Protection Agency (EPA) organised the Safer Choice Program in order to help consumers in finding products that perform well and are safer for human health and the environment. In the Safer Chemical Ingredient List by the US Environmental Protection Agency (2016), increasingly safer alternatives of commercial ingredients are marked with a green circle, green half-circle or yellow triangle. A similar classification is given by GreenScreen® For Safer Chemicals (Clean Production Action, 2016), which sets out 4 benchmarks that define progressively safer chemicals. In both cases, the limited number of categories may smooth down significant differences in toxicity among chemicals.

In this work, a toxicological ranking of chemicals has been developed using a specially designed multi-criteria method. Multi-criteria analysis (MCA) is a family of decision-making tools that are often used in strategic environmental assessment procedures to ensure that environmental, societal and economic aspects are integrated and taken into consideration (Convertino et al., 2013; Omo-Irabor et al., 2011; Srivastava et al., 2012; Valle Junior et al., 2015). Typically, MCA quantitatively evaluate alternatives based on their utility value for stakeholders, with respect to previously defined criteria. We adapted MCA in order to create a ranking of chemicals based on the most important types of toxicity. This method goes beyond the simple toxicological evaluation, which is based on a single specific type of toxicology: MCA takes into consideration a potentially unlimited number of factors at the same time, leading to a ranking of compounds based on a global hazard concept. Since every criterion could be assigned a relative weight, this

method leads to the construction of a dynamic ranking of analytes (or general scenarios) that may change with the relative importance of the criteria. This feature makes MCA a very versatile technique, applicable to various fields. Here we propose a case study focused on the textile sector. Available data were not sufficient to achieve a complete overview of the impact of the textile industry worldwide, but were used to illustrate the possible application of a new toxicological evaluation method that could be used in addition to the classical statistical techniques. This method is simple to implement, as it does not require experimental phases; reliable, because the toxicological data are official and provided by universally recognised agencies; and versatile, as it can be used for environmental evaluations in various fields and for different purposes.

Material and Methods

Sampling and analysis

Concentration data was kindly provided by a multinational corporation in the textile sector.

Analysed compounds

Globally, 177 different chemicals, divided in 12 classes of compounds, were analysed. 11 of the 12 classes belong to the priority list established by GreenPeace within the Detox Campaign, an initiative which challenges top textile brands to work with their suppliers to eliminate all hazardous chemicals across the entire supply chain and life-cycle of their products. The priority list includes: alkylphenols (C01), phthalates (C02), brominated and chlorinated flame retardants (C03), azo dyes (C04), organotin compounds (C05), perfluorinated chemicals (C06), chlorobenzenes (C07), chlorinated solvents (C08), chlorophenols (C09), short-chain chlorinated paraffins (C10) and total heavy metals (C11) (Greenpeace International, 2016). For this evaluation, cyanide (C12) was added to the above-mentioned 11 classes, due to its known lethal effect. The complete list of analysed chemicals is reported in the Supplementary Material (Table A.1). Each compound was assigned a Axxyy code, where xx represent the class and yy the arbitrary order of the compound into the class.

Sampling design

Water sampling was performed at 102 textile facilities located in 10 different countries: 48% of the facilities were in China; 14% in Bangladesh; 10% in India and Tunisia; 7% in Turkey, 4% in Egypt and the remaining factories were located in Europe (Romania, Italy, Portugal and Croatia). In some facilities, sampling was conducted twice, leading to a total number of 112 studies. Studies were carried out over the years as follows: 42 studies were performed in 2013; 43 in 2014; and 27 in 2015. For every facility three sampling points were identified, corresponding to three different types of samples: incoming water (IW), untreated wastewater (UWW), and treated wastewater (TWW). According to the monitoring strategy, when all the analytes of a given class were under the limit of detection (LOD) in UWW, samples from IW and TWW would not be analysed for that class. As a consequence, most data relate to UWW, with 141 compounds analysed for each facility on average, 112 studies conducted and 15822 data, followed by IW (60 compounds, 111 studies and 6611 data) and TWW (53 compounds, 65 studies, 3425 data).

Analytical methods

Samples were analysed using different official methods, depending on the laboratory and the country were the analyses were performed. A summary of analytical methods, divided by class, is reported in the Supplementary Material (Table A.2).

Data elaboration

Univariate analysis

Preliminary data elaboration was conducted in order to investigate the overall characteristics of datasets. Since most data were below LOD, a specific assessment approach was developed. Univariate analyses were first performed by focusing on the number and distribution of detected analytes, compared to non-detected analytes; the frequency of detected analytes was evaluated by class, by facility, by country and by type of sample. Subsequently, concentration values in different kinds of samples were evaluated.

Correspondence analysis

Correspondence analysis is a descriptive/exploratory technique designed to analyse simple two-way and multiway tables containing some measure of correspondence between rows and columns. The results are similar in nature to those produced by factor analysis, with the difference that the former use categorical variables. The advantage of correspondence analysis is that values above and below LOD can be included in the same evaluation after an appropriate categorisation. Correspondence analysis was conducted starting from three datasets that contained the concentration values of compounds from IW, UWW and TWW samples. All the values were categorised as follows: ND (not detected) was the category associated to values under LOD; LOW (low concentration) was the category related to values from LOD to one-third of the maximum value; MED (medium concentration) was the category for values ranging from one-third of the maximum value to two-thirds of the maximum value; HIGH (high concentration) was the category associated to values from two-thirds of the maximum value to the maximum value. Datasets were rearranged as matrices with categories as columns and compounds as rows, i. e. every analyte was represented by a profile of frequencies of its values. The resulting table of frequencies was standardised, so that the relative frequencies among all cells amounted to 1. Correspondence analysis was performed using STATISTICA 8.0, using standardisation of coordinates on row profiles.

Multi-criteria analysis (MCA)

Comparing compounds with different kinds of toxicity is not a trivial task. For instance, is a compound more toxic if it has immediate lethal effects or if it is carcinogenic? Is an endocrine disruptor more toxic than a compound that it is toxic for aquatic systems? The relative importance of the different types of toxicity must first be defined. One should also consider that compounds can have different types of toxicity and different values at the same time, which complicates the evaluation. MCA is a structured approach that integrates a wide variety of data to evaluate alternatives and rank them based on their aggregate value with respect to a set of criteria. It also allows one to define the relative importance of each criterion relative to the other (Convertino et al., 2013). These are precisely the most suitable characteristics in order to create a ranking of chemicals based on a global hazard value. MCA is often used to evaluate project priorities, thereby enabling project managers to make comprehensive and well-informed decisions; criteria could potentially include environmental, societal and economic aspects. In this work we applied MCA by choosing chemical compounds as alternatives and different kinds of toxicity as criteria. This approach

consists of three phases: i) criteria identification and selection; ii) calculation of the relative weight of each criterion; iii) comparison of alternatives.

Criteria identification and selection

In order to conduct a global toxicological evaluation, the following kinds of toxicity were identified as criteria: acute toxicity (ACT), carcinogenicity (CG), reproductive toxicity (RPT), acute aquatic toxicity (ACAT) and chronic aquatic toxicity (CHAT). At this stage, the decision-maker usually selects a score from a range of values that expresses the performance of each criterion for every alternative. In this specific study toxicological scores were assigned to each compound on the basis of the above-mentioned 5 kinds of toxicity. The toxicity data were provided by internationally recognised organisations and can be considered standard values. The sources of toxicity data are listed in detail in **Error! Reference source not found.**.

For classes of compounds and for chemicals that can be present in different forms in the environment (i.e. metals), the principle of precaution was followed: for every kind of toxicity, the toxicity of the analyte corresponds to that of the most dangerous compound of the class. In order to obtain a numerical value that describes the toxicity of the compounds, each group and category was converted into a numerical value ranging from 0 (no toxicity) to 1 (maximum toxicity), as shown in Table 2. ACT was expressed by the normalised reciprocal of LD_{50}; UNECE categories were used only when LD_{50} was not available. To the UNECE categories of RPT, we added a further category (CAT*) for specific cases where there is evidence of an adverse effect on reproduction, but the analyte is not classified in any other UNECE category.

Weights of criteria

In MCA, relative weights can be determined by pair-wise comparison, a mathematical technique that determines the relative weights of criteria by dividing the complex decision problem into a series of one-to-one judgements about the significance of each criterion relative to the others (Garfì et al., 2011). For each pair-wise comparison between two criteria, a value from 1/9 (extremely less important) to 9 (extremely more important) is given, 1 being representative of equally important criteria. The comparison values are inserted in a square matrix where the criteria names are used as row and column heads (Table 3). A statistical index (Consistency Ratio, CR) is calculated to check whether the criteria weights are consistent. CR is the ratio between the Consistency Index (CI), as defined in Equation (1), and the Random consistency Index (RI), where RI is obtained by averaging the CIs of many randomly generated pair-wise comparison matrices and is a tabulated value, depending on n.

$$CI = \frac{\lambda_{max} - n}{n - 1} \quad (1)$$

λ_{max} is the largest eigenvalue of the matrix and n is the number of criteria (Srivastava et al., 2012). The smaller the ratio between CI and RI, the lower the probability for matrix values to be generated randomly. When this probability becomes greater than 10% (CR > 0.1), the choices of the comparison values must be reassessed. In this work CR was 0.007, indicating a very high consistency of the matrix.

The final weights of the factors are the components of the main eigenvector calculated from that square matrix (Valle Junior et al., 2015) and are reported in the last column of Table 3. CI and the relative weights were calculated using MATLAB R2015b. Garfì et al. (Garfì et al., 2011) propose an alternative method to obtain an estimation of the relative weights of the criteria under comparison, consisting in operations

which can be processed with a simple spreadsheet. With this method CR was 0.009 and the relative weights were 0.480 (ACT), 0.242 (CG), 0.147 (RPT), 0.081 (ACAT) and 0.051 (CHAT), with a maximum error of 0.5%, compared to the values of Table 3, confirming the validity of this alternative procedure.

Comparison of alternatives

For every analyte, the sum of the toxicological values, each weighted for the importance of its toxicity, corresponds to the analyte global toxicity score (AGTS), which can be considered as an expression of the hazard that characterises the particular analyte.

$$AGTS = \sum_{i=1}^{n} (TV_i \cdot W_i) \cdot 100 \quad (2)$$

where TV is the toxicological value of the analyte with respect to the type of toxicity i; W is the weight of the criterion (or type of toxicity) i and n is the number of criteria. The Equation 2 was applied to all the analytes investigated in this work.

Facilities evaluation

For every facility and for every sampling site (IW, UWW and TWW), a facility global toxicological score (FGTS) was calculated. FGTS is the sum of the concentration of all the analysed compounds, weighted for their toxicity (Equation 3).

$$FGTS = \sum_{j=1}^{m} (C_j \cdot AGTS_j) \cdot 10^{-3} \quad (3)$$

where C_j is the concentration (µg/l) of the analyte j; AGTS is the global toxicity score of the analyte j; and m is the number of analytes. In the calculation of FGTS the following principles were adopted: i) for all the analytes that have a concentration <LOD, the value of half the LOD was considered; ii) in order not to overestimate the toxicity of sites, the concentration of hexavalent chromium was subtracted to the concentration of total chromium; iii) the presence of additional overestimation due to other overlaps (i. e. a class of compounds with its components) was checked; in all the other cases, if a class of compounds was analysed, none of the components of that class were analysed and vice versa. Based on the calculated FGTS, sites were classified into 5 impact categories. For IW and UWW the categories were: minimum impact (from 0 to 12), weak impact (from 12 to 23), medium impact (from 23 to 47), strong impact (from 47 to 93) and extreme impact (from 93 to 360). In the case of TWW, which enter directly into the environment, the 5 impact categories were more restrictive than those used for IW and UWW data evaluation: minimum impact (from 0 to 6.5), weak impact (from 6.5 to 13), medium impact (from 13 to 20), strong impact (from 20 to 50) and extreme impact (from 50 to 100). In addition to these three facility rankings (IW, UWW and TWW), the supplier responsibility (SR) ranking was established by calculating the difference between the concentration in UWW and the concentration in IW, data by data and site by site. When a value in UWW did not have a correspondence in IW, the missing data in IW was substituted with a value <LOD, therefore it was numerically considered as half LOD. This approximation was chosen considering that, as a rule, only cases with UWW <LOD did not have a correspondence in IW, and assuming that the concentration in UWW was usually higher than the concentration in IW. In SR ranking, facilities were classified into 5 responsibility categories, characterised by the same minimum and maximum scores used for IW and UWW.

Results and discussion

General evaluation of datasets

Detected values assessment

As expected, the number of detected analytes was higher in UWW than in the other samples: considering an average facility, 4 compounds (7%) were above LOD in IW, 11 compounds (8%) were above LOD in UWW and 7 compounds (13%) were above LOD in TWW. Similarly, the number of compounds with values <LOD in all studies increased from 112 for UWW to 134 for IW and 140 for TWW, out of the 177 total analysed compounds.

The distribution per class of detected analytes showed a few differences in the three samples (Figure 1a, b and c). The most representative class was C11 across the types of samples (73% of detected values for IW, 59% for UWW and 72% in TWW). The reduction in the percentage of C11 from IW to UWW corresponded to an increment in the other minor classes: specifically, C04 was almost absent in IW and increased by about 65 times in UWW (Figure 1d), reaching 10% of total detected analytes (Figure 1b); for C05, the increase from IW to UWW was not exactly estimable due to the fact that the entire class was totally absent in IW. Details about the analysed and detected compounds per class are reported in the Supplementary Material (Table A.3). C01, C09 and C12 are also noteworthy, as they showed an almost 10-fold increase in the number of detected analytes from IW to UWW.

In TWW (Figure 1c) the percentage of C11 was close to that in IW (Figure 1a) and all the other classes decreased in percentage compared to UWW (Figure 1b). It should also be noted that C04 was reduced by 58% from UWW to TWW (Figure 1e), but this decrease was not enough to compensate for the extreme increment mentioned in the previous paragraph, and indeed C04 remained much higher than in IW (27-fold increase, Figure 1f). The same was observed for C05, which was reduced by 77% from UWW to TWW. Comparing UWW with TWW (Figure 1e), C03 and C06 seem to be completely removed from the wastewater by the treatment process, even if they were present in IW (with a very reduced number of detections). C11 was not only the most represented class on average, but was also detected in almost all the facilities investigated (93% of the investigated facilities in IW, 99% in UWW; Figure A.1 of the Supplementary Material). The second most frequent class was C04, present in two thirds of the sites in UWW. Globally, in UWW, the less frequent class was C03, which was present (with maximum 1 compound out of 21, Table A.3) in only 3% of the facilities. These results could be affected by the differences in the data size among the samples.

Concentration values assessment

By comparing concentration values by classes (Table 4), it was confirmed that C04 and C05 were the most affected by the presence of facilities (increase of median concentration from 0.2 µg/l to 2.5 µg/l for C04 and from under LOD (udl) to 0.2 µg/l for C05, comparing IW with UWW). The median concentration of these classes in TWW (1.6 µg/l for C04 and 0.1 µg/l for C05) was still higher than in IW, confirming that the reduction in the median concentration of these classes, from UWW to TWW (-56% for C04 and -31% for C05), was not enough to compensate for the great increase observed from IW to UWW. C1 and C12, which were characterised by an almost 10-fold increase in the number of detected analytes from IW to UWW, have a stable median concentration.

A data-to-data comparison was conducted in order to identify specific cases that differed from the average trend. Data were compared considering every possible couple of sample types (IW-UWW, UWW-TWW and IW-TWW). As expected, the IW-UWW comparison showed that the majority of data were characterised by a higher concentration in UWW than in IW, but in 2% of cases (142 out of 6595 comparable couples of data) compounds showed the opposite trend. Exceptions were widely distributed among compounds and sites. A similar profile was obtained comparing UWW to TWW: 16% of total data-to-data comparison showed a higher concentration in UWW than in TWW and 5% of comparisons (178 out of 3425 comparable couples of data) showed the opposite behaviour. In this case anomalies were concentrated in a few facilities, where further investigation about the efficiency of the treatment process are needed. The last comparison (IW-TWW) showed 11% of couples with TWW concentration higher than IW concentration, with a few exceptions (4%).

Correspondence analysis

2D plots resulting from the application of correspondence analysis to the three datasets (IW, UWW and TWW) are reported in the Supplementary Material (Figures A.2, A.3 and A.4). In all the plots, near the origin of the graph, a group containing many overlapping analytes was evidenced ("ND" group). It represents all the compounds with all (or most) values <LOD. In IW data (Figure A.2), the compounds that differed the most from the ND group were zinc, manganese and copper. Zinc and manganese were characterised by a greater number of values above LOD, variously distributed among categories; copper profile showed approximately half of the values >LOD. The ND-LOW group was characterised by about 75% of the values <LOD and 20% of values in low concentrations. 2D plot of UWW data (Figure A.3) highlighted 11 compounds that were different from those included in the ND group. They were classified by their profile in ND-LOW, LOW-ND and LOW groups. The ND-LOW group included nonylphenolethoxilates (NPEOs), arsenic and cyanide. Despite the fact that most values for arsenic and cyanide were <LOD, their presence could be alerting, because of their known high toxicity. Lead, antimony and aniline (group LOW-ND) were present in low concentrations in almost 60% of the cases and under the LOD in 40% of the cases. The LOW group included nickel, chromium, zinc, copper and manganese; this category of compounds must be kept under control due to its high prevalence in wastewater (90%). TWW included 4 compounds with most values >LOD, and which must be kept under control: manganese, nickel, copper and zinc. The concentration of manganese was above LOD in 90% of the cases; regarding the average profiles of nickel, copper and zinc (LOW group), about 70% of the values indicated low concentrations and 25% were <LOD. Di-(2-ethyl-hexyl)-phthalate (DEHP), lead, aniline, short-chain chlorinated paraffin (C10-C13), antimony and chromium were classified in the ND-LOW group.

Ranking of analytes

The toxicity ranking of analytes was built using the MCA method described above. The resulting AGTSs are reported in the supplementary information material (Table A.4). Since ACT was indicated as the most important type of toxicity (Table 3), the most toxic analytes extracted from MCA were arsenic and cyanide, which have the strongest lethal acute effect among the investigated compounds, with LD_{50} of 4.7 and 8 mg/kg of body weight, respectively. The third most toxic analyte was hexavalent chromium: it has a lower ACT (52 mg/kg of body weight) compared to other compounds, such as mercury (18 mg/kg of body weight) and pentachlorophenol (27 mg/kg of body weight), but it was considered the most dangerous among them, due to the classification in the highest group for CG (Group 1). Similarly, cadmium and nickel show a lower

ACT than the previously mentioned compounds (LD_{50} of 107 and 186 mg/kg of body weight), but are dangerous for the reproductive system (Category 1B).

Ranking of facilities

UWW ranking of facilities

Regarding UWW, facilities were distributed among the impact categories as follows: 1 facility (in China) was classified as having an extreme impact; 4 facilities (2 in China and 2 in India) had a strong impact; 7 facilities (3 in China, 3 in India and 1 in Tunisia) had a medium impact; 19 facilities had a weak impact and 81 facilities a minimum impact. Specifically, the first facility in the ranking showed a FGTS of 360, significantly above the others (maximum of 92), due to the strong concentration of highly toxic compounds such as nickel (4050 µg/l; n. 5 of the ranking); zinc (6880 µg/l; n. 30 of the ranking), lead (1800 µg/l; n. 10 of the ranking); chromium (2050 µg/l; n. 49 of the ranking) and copper (320 µg/l; n. 29 of the ranking). In general the most toxic facilities were located in Asia, and India and China proved the most important contributors to global toxicity (27% and 20% of global toxicity, respectively). FGTS values decreased from 2013 to 2015.

IW ranking of facilities

For a global evaluation of the responsibility of suppliers, the situation of UWW must be compared to the toxicity in IW. Unexpectedly, one facility having weak impact in UWW, was classified as having an extreme impact in IW. It was characterised by an exceptional concentration of zinc (7709 µg/l; n. 30 of the ranking) and N-Et-FOSA (7709 µg/l; n. 75 of the ranking). The other facilities were categorised in IW ranking having weak (5 facilities) or minimum impact (105 facilities). The country with the highest FGTS is Croatia. The chronological evolution did not indicate a specific trend.

SR ranking of facilities

Since the most polluting facilities in UWW had a minimum impact in IW, the evaluation of SR led to a similar ranking to the one obtained for UWW data, at least in the upper part. Specifically, the facility with extreme impact in UWW was also characterised by extreme supplier responsibility; and 3 suppliers with strong impact in UWW were observed to have a strong responsibility. The other suppliers were classified as having medium responsibility (5 suppliers), weak responsibility (18 suppliers) and minimum responsibility (70 suppliers). Sometimes the concentration of chemicals in IW could be higher than in UWW; as a consequence, 14 suppliers with negative FGTS were classified having a negative responsibility. As expected, the trend reflects the findings for UWW, with India and China as the countries with highest FGTS (33% and 23% of global toxicity, respectively) and a decreasing FGTS over the years. In Figure 2 the average FGTS per country is represented in a map.

TWW ranking of facilities

TWW showed a lower FGTS than UWW, on average. No facility was classified as having an extreme impact; 2 facilities (in China) were categorised as having a strong impact, due to the high contribution of zinc and nickel; one facility (in Bangladesh) had a medium impact and the other facilities showed a weak (10 sites) or minimum impact (52 sites). In contrast to what happened for IW and UWW, the countries with the highest average toxicity score in TWW were Portugal and Croatia, indicating Europe as an important contributor to global toxicity (43% and 38% of global toxicity, for Europe and Asia, respectively). It should be noted that

the evaluation of TWW was conducted using much less data than IW and UWW, therefore any comparison should be made carefully. No chronological trend was observed for TWW toxicological scores.

Conclusions

Every chemical compound is characterised by a characteristic type and level of toxicity. Making a comparison and a toxicological ranking of chemicals is therefore a difficult task. In this work, the MCA method was adapted in order to build a toxicological ranking of chemical compounds: each compound was considered as an alternative, evaluated using its types of toxicity as criteria. Specifically, the investigated compounds belong to 12 classes of compounds largely used in textile industry. Arsenic, cyanide, hexavalent chromium and other heavy metals were the most toxic compounds. The resulting ranking was used to evaluate the toxicological impact of textile facilities around the world. Available data were not sufficient to achieve a complete overview of the toxicological impact of textile industries worldwide, but they were used to illustrate a possible application of MCA as hazard evaluation in manufacturing plants. Concentration of chemicals in wastewater were first assessed using univariate and multivariate techniques; subsequently, each textile facility was assigned a toxicological score, based on the combined information of pollutant global hazard and concentration values in water. The use of IW and UWW in the same facilities allowed us to compare the toxicological levels of water entering and leaving the factory. This gave us an indication of the effect of the plants in terms of potential release of toxic substances into the environment, which reflects the amount of chemicals used in the various production processes; moreover, toxicological scores assigned to TWW gave information about the effective environmental impact of factories. The use of such data yielded the following findings: i) some facilities were identified as critical sites, analysing UWW, due to the high concentrations of highly toxic compounds; ii) China and India were the countries with the highest toxicological scores, on average, considering UWW; iii) since facilities with a high toxicological score in UWW generally had a minimum impact in IW, that high score could be linked to the active processes in the facilities, rather than to the bad quality of IW; iv) Asia and Europe seem to have a comparable average toxicological score, regarding the release of chemicals in the environment.

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363 **Table 1. Data source for each kind of toxicity. LD_{50}: Median lethal dose. UNECE: United Nations Economic Commission for**
364 **Europe; IARC: International Agency for Research on Cancer.**

Toxicity	Data Source
ACT	LD_{50} (oral toxicity on rat, mg/kg of body weight) or UNECE categories or LD_{50} (oral toxicity on mouse, mg/kg of body weight)
CG	IARC groups
RPT	UNECE categories
ACAT	UNECE categories
CHAT	UNECE categories

366 **Table 2. Converted values for categories and groups representative of the different kinds of toxicity.**

ACT		CG		RPT		ACAT		CHAT	
CAT 1	1	**GR 1**	1	**CAT 1A**	1	**CAT 1**	1	**CAT 1**	1
CAT 2	0.1	**GR 2A**	0.1	**CAT 1B**	0.1	**CAT 2**	0.1	**CAT 2**	0.1
CAT 3	0.005	**GR 2B**	0.01	**CAT 2**	0.01	**CAT 3**	0.01	**CAT 3**	0.01
CAT 4	0.001	**GR 3**	0.001	**CAT** *	0.001				
CAT 5	0.0002	**GR 4**	0						

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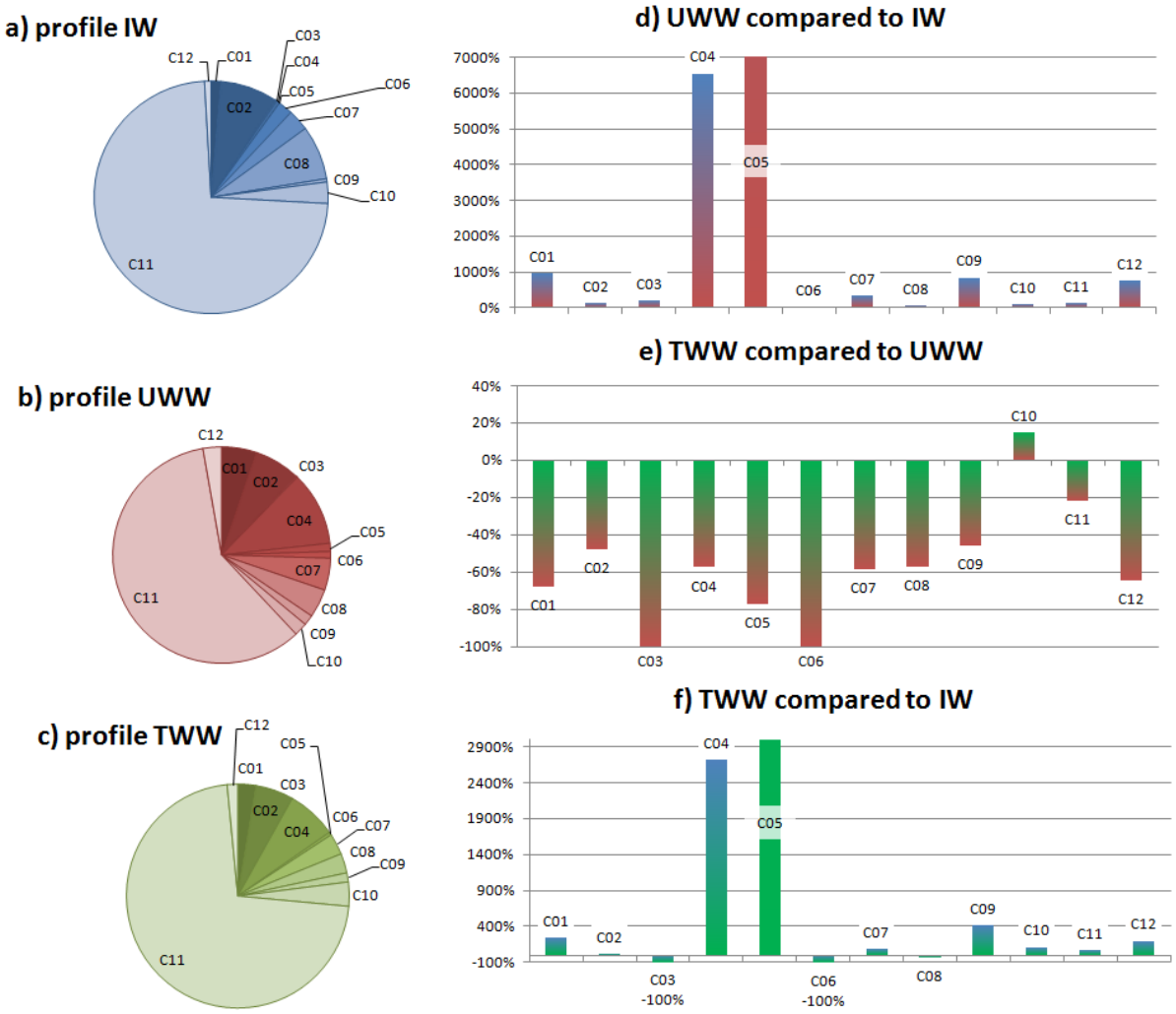
Table 3. Pair-wise comparison between criteria and calculated weight.

	ACT	CG	RPT	ACAT	CHAT		WEIGHT
ACT	1	2	3	7	9	→	0.481
CG	1/2	1	2	3	4	→	0.242
RPT	1/3	1/2	1	2	3	→	0.147
ACAT	1/7	1/3	1/2	1	2	→	0.080
CHAT	1/9	1/4	1/3	1/2	1	→	0.050

Figure 1. Distribution of detected analytes among classes in the three types of samples. a), b) and c) report the profiles of detected analytes among classes in the three types of samples (IW, UWW and TWW). d), e) and f) report a comparison between types of samples: in d), the number of detected analytes in UWW is compared to IW; in e), the number of detected analytes in TWW is compared to UWW; in f), the number of detected analytes in TWW is compared to UWW.



375 **Table 4. Median concentration in IW, UWW and TWW (µg/l). udl: under LOD.**

	IW (µg/l)	UWW (µg/l)	TWW (µg/l)
C01	39	14	14
C02	3.7	5.8	3.5
C03	0.85	0.22	udl
C04	0.20	2.5	1.6
C05	udl	0.17	0.13
C06	5.0	0.05	udl
C07	0.33	0.18	0.44
C08	12	6.0	6.0
C09	0.50	2.3	1.7
C10	21	17	12
C11	6.8	16	11
C12	12	15	6.0

Figure 2. Map representing the average FGTS (SR) per country. Average FGTS are represented by colours (from yellow - low FGTS - to brown - high FGTS). Countries in grey were not investigated in this work. Map was created using Qlik® Sense Desktop.

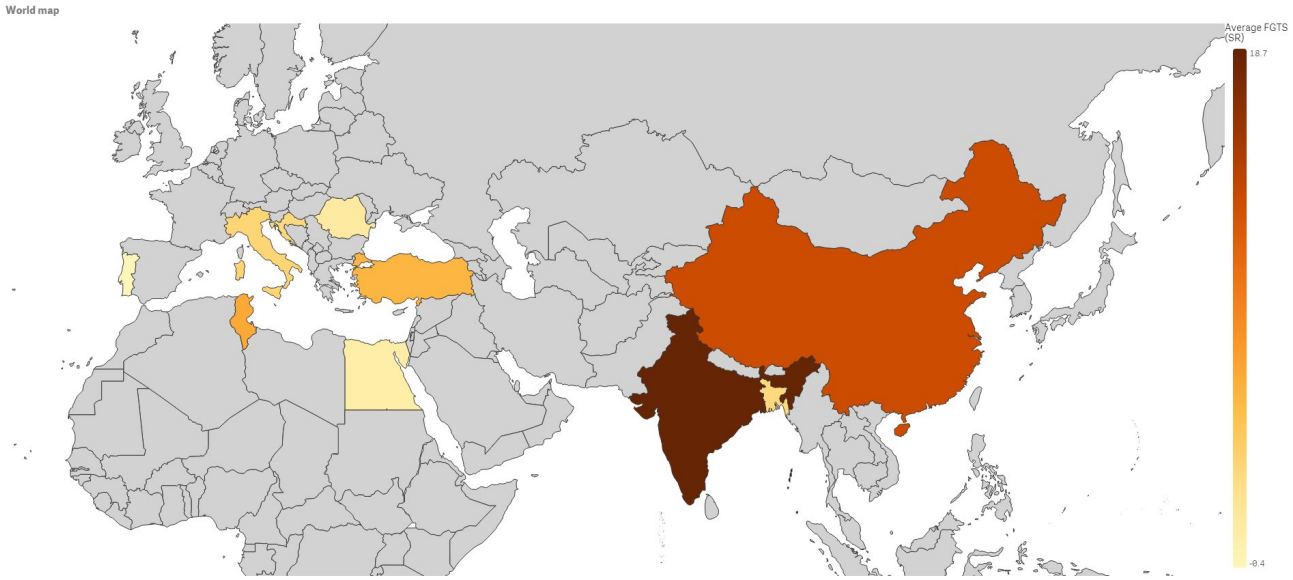
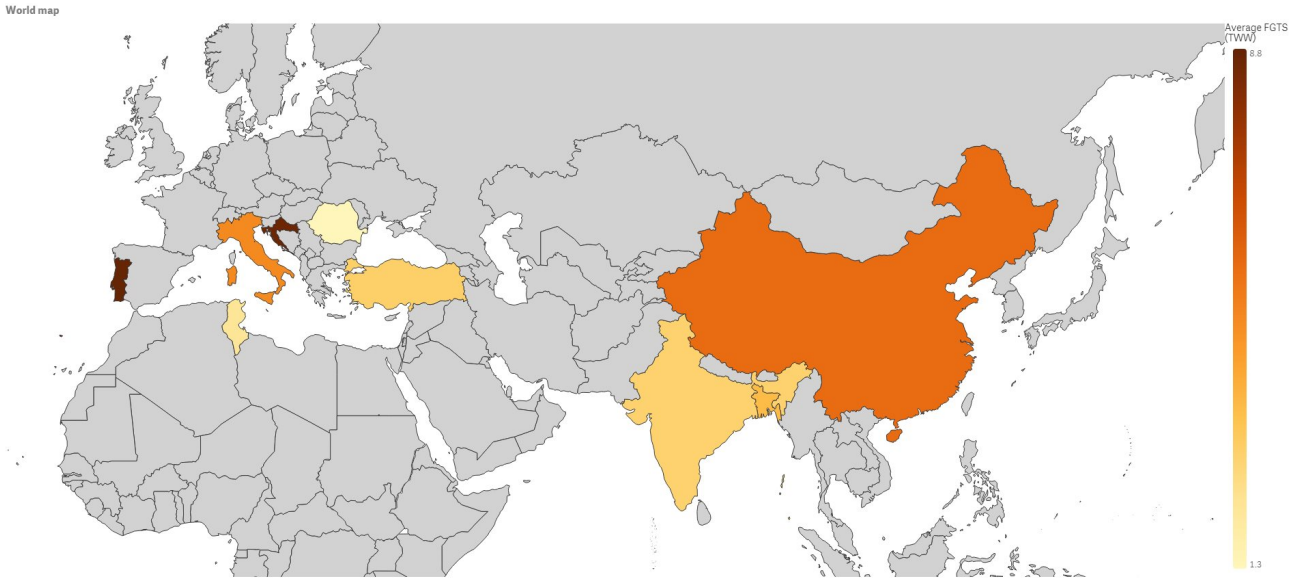


Figure 3. Map representing the average FGTS (TWW) per country. Average FGTS values are represented by colours (from yellow - low FGTS - to brown - high FGTS). Countries in grey were not investigated in this work. The map was created using Qlik® Sense Desktop.



Highlights

- a dynamic toxicity ranking of chemicals is set up using Multi-Criteria Analysis
- chemicals are considered as alternatives and their different toxicity as criteria
- the impact of textile factories using the ranking of chemicals is assessed

SUPPLEMENTARY MATERIAL of

Multi-criteria ranking of chemicals for toxicological impact of textile industry

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Table A.1. Analysed chemical compounds, CAS and internal code for classification (A).

A	CAS	Name
C01 – Alkylphenols		
A0101	1806-26-4,140-66-9	Octylphenols (OPs)
A0102	Various	Octylphenolethoxylates (OPEOs)
A0103	54852-15-3,104-40-5,1173019-62-9	Nonylphenols (NPs)
A0104	Various	Nonylphenolethoxylates (NPEOs)
C02 – Phthalates		
A0201	85-68-7	Benzyl-butyl-phthalate (BBP)
A0202	84-74-2	Di-butyl-phthalate (DBP)
A0203	117-81-7	Di-(2-ethyl-hexyl)-phthalate (DEHP)
A0204	117-84-0	Di-n-octyl-phthalate (DNOP)
A0205	68515-48-0	Di-iso-nonyl-phthalate (DINP)
A0206	26761-40-0	Di-iso-decyl-phthalate (DIDP)
A0207	131-11-3	Di-methyl-phthalate (DMP)
A0208	84-66-2	Di-ethyl-phthalate (DEP)
A0209	131-16-8	Di-n-propyl-phthalate (DPP)
A0210	84-69-5	Di-iso-butyl-phthalate (DIBP)
A0211	84-61-7	Di-cyclo-hexyl-phthalate (DCHP)
A0212	84-75-3	Di-n-hexyl-phthalate (DNHP)
A0213	84-76-4	Di-nonyl-phthalate (DNP)
A0214	27554-26-3	Di-iso-octyl-phthalate (DIOP)
A0215	117-82-8	Bis-(2-methoxy-ethyl)-phthalate (DMEP)
A0216	605-50-5	Di-iso-pentyl-phthalate (DIPP)
A0217	71888-89-6	Di-iso-heptyl-phthalate (DIHP)
A0218	84777-06-0	1,2-Benzene-di-carboxylic acid di-pentyl-esters, branched and linear (DHNUP)
A0219	776297-69-9	N-iso-pentyl-iso-pentyl-phthalate (PIPP)
A0220	3648-20-2	Di-heptyl-phthalate (DHP)
C03 - Brominated and Chlorinated Flame Retardants		
A0301	Various	Polybromodiphenyls (PBBs)
A0302	126-72-7	Tri-(2,3-di-bromo-propyl)-phosphate (TRIS)
A0303	Various	Polybromodiphenyl ethers (PBDEs)
A0304	79-94-7	Tetra-bromo-bisphenol-A (TBBPA)
A0305	5412-25-9	Bis-(2,3-di-bromo-propyl)-phosphate
A0306	3194-55-6	Hexa-bromo-cyclo-dodecan (HBCDD)
A0307	3296-90-0	2,2-Bis(bromomethyl)-1,3-propanediol (BBMP)
A0308	115-96-8	Tris-(2-chloro-ethyl)-phosphate (TCEP)

A	CAS	Name
A0309	13674-87-8	Tris-(1,3-di-chloro-iso-propyl)-phosphate (TDCPP)
A0310	Various	Bromo-diphenyl
A0311	Various	Di-bromo-diphenyl
A0312	Various	Tri-bromo-diphenyl
A0313	Various	Tetra-bromo-diphenyl
A0314	Various	Penta-bromo-diphenyl
A0315	Various	Hexa-bromo-diphenyl
A0316	Various	Hepta-bromo-diphenyl
A0317	Various	Octa-bromo-diphenyl
A0318	Various	Nona-bromo-diphenyl
A0319	13654-09-6	Deca-bromo-diphenyl
A0320	Various	Bromo-diphenyl-ether
A0321	Various	Di-bromo-diphenyl-ether
A0322	Various	Tri-bromo-diphenyl-ether
A0323	Various	Tetra-bromo-diphenyl-ether
A0324	Various	Penta-bromo-diphenyl-ether
A0325	Various	Hexa-bromo-diphenyl-ether
A0326	Various	Hepta-bromo-diphenyl-ether
A0327	Various	Octa-bromo-diphenyl-ether
A0328	Various	Nona-bromo-diphenyl-ether
A0329	1163-19-5	Deca-bromo-diphenyl-ether
A0330	21850-44-2	Tetra-bromo-bisphenol A bis-(di-bromo-propyl-ether) (TBBPA-BDPE)
A0331	13674-84-5	Tris-(2-chloroisopropyl)-phosphate (TCPP)
A0332	Various	Tris-(aziridinyl)-phosphinoxide (TEPA)
C04 - Azo Dyes		
A0401	92-67-1	4-Aminodiphenyl
A0402	92-87-5	Benzidine
A0403	95-69-2	4-Chloro-o-toluidine
A0404	91-59-8	2-Naphthylamine
A0405	97-56-3	o-Aminoazotoluene
A0406	99-55-8	5-Nitro-o-toluidine
A0407	106-47-8	4-Chloroaniline
A0408	615-05-4	2,4-Diaminoanisole
A0409	101-77-9	4,4'-Diaminodiphenylmethane
A0410	91-94-1	3,3'-Dichlorobenzidine
A0411	119-90-4	3,3'-Dimethoxybenzidine
A0412	119-93-7	3,3'-Dimethylbenzidine
A0413	838-88-0	3,3'-Dimethyl-4,4'-diaminodiphenylmethane
A0414	120-71-8	p-Cresidine
A0415	101-14-4	4,4'-Methylene-bis(2-chloroaniline)
A0416	101-80-4	4,4'-Oxydianiline
A0417	139-65-1	4,4'-Thiodianiline
A0418	95-53-4	o-Toluidine
A0419	95-80-7	2,4-Diaminotoluene
A0420	137-17-7	2,4,5-Trimethylaniline
A0421	90-04-0	o-Anisidine
A0422	60-09-3	4-Aminoazobenzene
A0423	95-68-1	2,4-Xylidine
A0424	87-62-7	2,6-Xylidine
A0425	62-53-3	Aniline
A0426	106-50-3	1,4-Phenylenediamine
A0427	95-51-2	2-Chloroaniline

A	CAS	Name
A0428	99-59-2	5-Nitro-o-anisidine
A0429	108-44-1	m-Toluidine
A0430	91-66-7	n,n-Diethylanaline
A0431	103-69-5	n-Ethylaniline
A0432	100-61-8	n-Methylaniline
A0433	106-49-0	p-Toluidine
C05 - Organotin Compounds		
A0501	Various	Monobutyltin (MBT)
A0502	Various	Dibutyltin (DBT)
A0503	Various	Dioctyltin (DOT)
A0504	Various	Tributyltin (TBT)
A0505	Various	Triphenyltin (TPhT)
A0506	Various	Tricyclohexyltin(TCyHT)
A0507	Various	Trioctyltin(TriOT)
A0508	Various	Tripropyltin (TPT)
A0509	Various	Monooctyltin (MOT)
A0510	Various	Tetrabutyltin (TeBT)
C06 - Perfluorinated Chemicals (PFCs)		
A0601	335-67-1	Perfluoro-n-octanoic acid (PFOA)
A0602	2795-39-3 / Various	Perfluorooctane sulphonates (PFOS)
A0603	307-24-4	Perfluoro-n-hexanoic acid (PFHxA)
A0604	3871-99-6	Perfluorohexane sulphonates (PFHxS)
A0605	375-22-4	Perfluorobutyric Acid (PFBA)
A0606	375-73-5	Perfluoro-butane-sulfonic acid
A0607	754-91-6	Perfluoro-octane-sulfon- amide (PFOSA)
A0608	31506-32-8	N-Methyl-Perfluoro-octane-sulfon-amide (N-Me-FOSA)
A0609	4151-50-2	N-Ethyl-Perfluoro-octane-sulfon-amide (N-Et-FOSA)
A0610	24448-09-7	N-Methyl-Perfluoro-octane-sulfon-amido-ethanol (N-Me-FOSE alcohol)
A0611	1691-99-2	N-Ethyl-Perfluoro-octane-sulfon-amido-ethanol (N-Et-FOSE alcohol)
A0612	2706-90-3	Perfluoro-pentanoic acid
A0613	375-85-9	Perfluoro-heptanoic acid
A0614	375-95-1	Perfluoro-nonanoic acid
A0615	335-76-2	Perfluoro-n-decanoic acid (PFDA)
A0616	2058-94-8	Perfluoro-undecanoic acid
A0617	307-55-1	Perfluorododecanoic Acid (PFDoA)
A0618	72629-94-8	Perfluoro-tridecanoic acid
A0619	376-06-7	Perfluoro-tetradecanoic acid
A0620	355-46-4 / 432-50-7	Perfluoro-hexane-sulfonic acid
A0621	375-92-8	Perfluoro-heptane-sulfonic acid
A0622	355-77-3	Perfluor-decane-sulfonic acid
A0623	27619-97-2	1H,1H,2H,2H-Perfluoro-octane-sulphonic acid
A0624	34598-33-9	2H,2H,3H,3H-Perfluoroundecanoic acid (PFUnA)
A0625	172155-07-6	Perfluoro-3-7-dimethyl octane carboxylate
A0626	1546-95-8	7H-Dodecafluoro heptane carboxylate
C07 - Chlorobenzenes		
A0701	108-90-7	Chlorobenzene
A0702	Various	Dichlorobenzenes
A0703	Various	Trichlorobenzenes
A0704	Various	Tetrachlorobenzenes
A0705	608-93-5	Pentachlorobenzene
A0706	118-74-1	Hexachlorobenzene

A	CAS	Name
C08 - Chlorinated Solvents		
A0801	75-09-2	Dichloromethane
A0802	67-66-3	Chloroform
A0803	56-23-5	Carbon tetrachloride
A0804	107-06-2	1,2-dichloroethane
A0805	71-55-6	1,1,1-trichloroethane
A0806	79-00-5	1,1,2-trichloroethane
A0807	630-20-6	1,1,1,2-tetrachloroethane
A0808	79-34-5	1,1,2,2-tetrachloroethane
A0809	76-01-7	Pentachloroethane
A0810	75-35-4	1,1-dichloroethylene
A0811	156-59-2	cis-1,2-Dichloroethylene
A0812	156-60-5	trans-1,2-Dichloroethylene
A0813	79-01-6	Trichloroethylene
A0814	127-18-4	Tetrachloroethylene
C09 - Chlorophenols		
A0901	Various	Monochlorophenols
A0902	Various	Dichlorophenol (DiCP)
A0903	Various	Trichlorophenols (TriCP)
A0904	25167-83-3	Tetrachlorophenols (TeCP)
A0905	87-86-5	Pentachlorophenol (PCP)
A0906	95-57-8	2-Chlorophenol
A0907	108-43-0	3-Chlorophenol
A0908	106-48-9	4-Chlorophenol
A0909	576-24-9	2,3-Dichlorophenol
A0910	95-77-2	3,4-Dichlorophenol
A0911	120-83-2, 583-78-8, 87-65-0, 591-35-5	2,4-Dichlorophenol, 2,5-Dichlorophenol, 2,6-Dichlorophenol, 3,5-Dichlorophenol
A0912	933-78-8	2,3,5-Trichlorophenol
A0913	95-95-4	2,4,5-Trichlorophenol
A0914	88-06-2	2,4,6-Trichlorophenol
A0915	609-19-8, 15950-66-0	3,4,5-Trichlorophenol, 2,3,4-Trichlorophenol
A0916	4901-51-3	2,3,4,5-Tetrachlorophenol
A0917	58-90-2	2,3,4,6-Tetrachlorophenol
A	CAS	Name
A0918	935-95-5	2,3,5,6-Tetrachlorophenol
C10 - Short-Chain Chlorinated Paraffins		
A1001	85535-84-8	Short-chain chlorinated paraffins (C10-C13)
C11 - Total Heavy Metals		
A1101	7440-47-3	Chromium (Cr)
A1102	18540-29-9	Hexavalent Chromium (Cr VI)
A1103	7439-95-4	Manganese (Mn)
A1104	7440-48-4	Cobalt (Co)
A1105	7440-02-0	Nickel (Ni)
A1106	7440-50-8	Copper (Cu)
A1107	7440-66-6	Zinc (Zn)
A1108	7440-38-2	Arsenic (As)
A1109	7440-43-9	Cadmium (Cd)
A1110	7440-36-0	Antimony (Sb)
A1111	7439-97-6	Mercury(Hg)
A1112	7439-92-1	Lead(Pb)
C12 – Cyanide		

A	CAS	Name
A1201	74-90-8	Cyanide

Table A.2. Extraction and analytical methods used for every class of chemicals.

Class	Extraction & analytical methods	Class	Extraction & analytical methods
C01	ASTM D7065 ASTM D5369 U. S. EPA 3540c Dichloromethane or generic solvent extraction GC/MS or LC/MS or LC/MS-MS analysis	**C07**	U. S. EPA 3540c ASTM D5369 U. S. EPA 3510c U. S. EPA 8260B U. S. EPA 8270D Hexane or dichloromethane or generic solvent extraction GC/MS or LC/MS analysis
C02	ASTM D8270 ASTM D5369 U. S. EPA 3510c U. S. EPA 3540c Hexane or dichloromethane or generic solvent extraction GC/MS or HPLC/MS analysis	**C08**	U. S. EPA 8260B U. S. EPA 8270D U. S. EPA 3540c ASTM D5369 Dichloromethane extraction GC/MS or HS-GC/MS or LC/MS analysis
C03	EPA 527 ASTM D5369 U. S. EPA 3510c U. S. EPA 3540c EPA 8321B Hexane or dichloromethane or generic solvent extraction	**C09**	U. S. EPA 3540c ASTM D5369 U. S. EPA 3510c U. S. EPA 8270D Dichloromethane or generic solvent extraction GC/MS or LC/MS analysis
C04	U. S. EPA 3510c ASTM D5369 DIN 38407-16 EN 14362-1 EN 14362-3 Methyl-terbuthyl ether extraction GC/MS or HPLC/DAD or LC/MS analysis	**C10**	ISO 12010 ASTM D5369 U. S. EPA 3540c Hexane or dichloromethane or generic solvent extraction GC/MS or LC/MS analysis
C05	U. S. EPA 3540c ASTM D5369 EN ISO 17353 ISO 23161 Hexane or generic solvent extraction GC/MS or LC/MS analysis	**C11**	U. S. EPA 3015A U. S. EPA 3051A U. S. EPA 3060A U. S. EPA 6020A U. S. EPA 7196A
C06	U. S. EPA 3540c ASTM D5369 Generic solvent extraction GC/MS or LC/MS analysis	**C12**	U. S. EPA 9013 APHA 4500 CN- C:2012 & APHA 4500 CN-E:2012

Table A.3. Analysed (average) and detected compounds (average percentage and maximum) per class, in IW, UWW and TWW.

	IW			UWW			TWW		
Classes	**Anal comp (average)**	**Det comp (average)**	**Det comp (max)**	**Anal comp (average)**	**Det comp (average)**	**Det comp (max)**	**Anal comp (average)**	**Det comp (average)**	**Det comp (max)**
C01	2	2.9%	1	4	14%	2	1	13%	1
C02	7	4.5%	4	18	4.1%	5	6	6.9%	4
C03	3	0.3%	1	21	0.1%	1	2	-	0
C04	19	0.1%	1	29	4.2%	5	17	3.0%	3
C05	2	-	0	10	1.4%	2	3	1.2%	1
C06	3	2.3%	4	21	0.5%	3	2	-	0
C07	2	4.9%	2	6	8.9%	4	2	8.7%	2
C08	5	5.6%	2	12	4.0%	3	4	4.5%	2
C09	2	1.1%	1	8	2.0%	2	2	4.3%	2
C10	0.4	33%	1	1	2.1%	1	0.4	59%	1
C11	12	25%	7	12	55%	10	12	43%	10
C12	1	5.3%	1	1	34%	1	1	14%	1

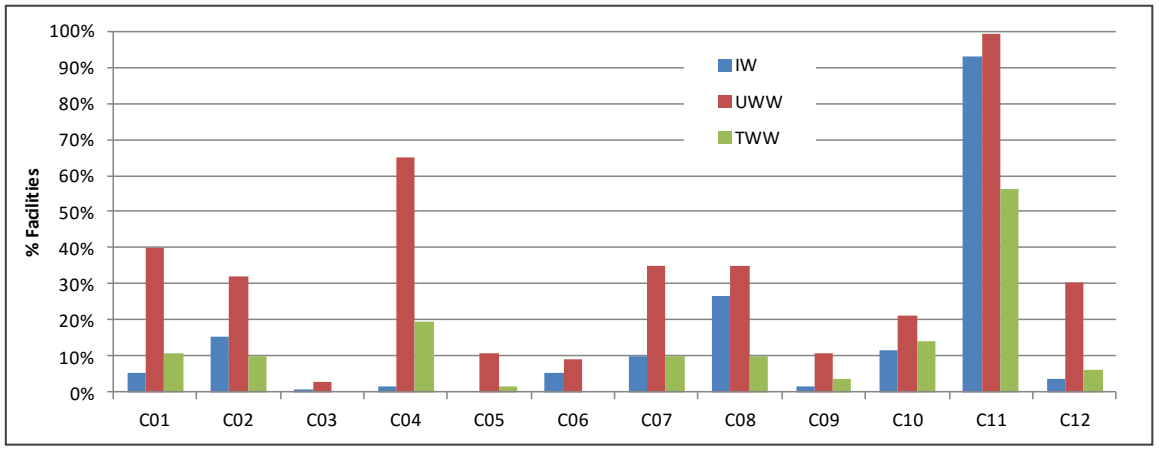

Figure A.1. Frequency of detected class of compounds per facilities, expressed as percentage in IW, UWW and TWW.

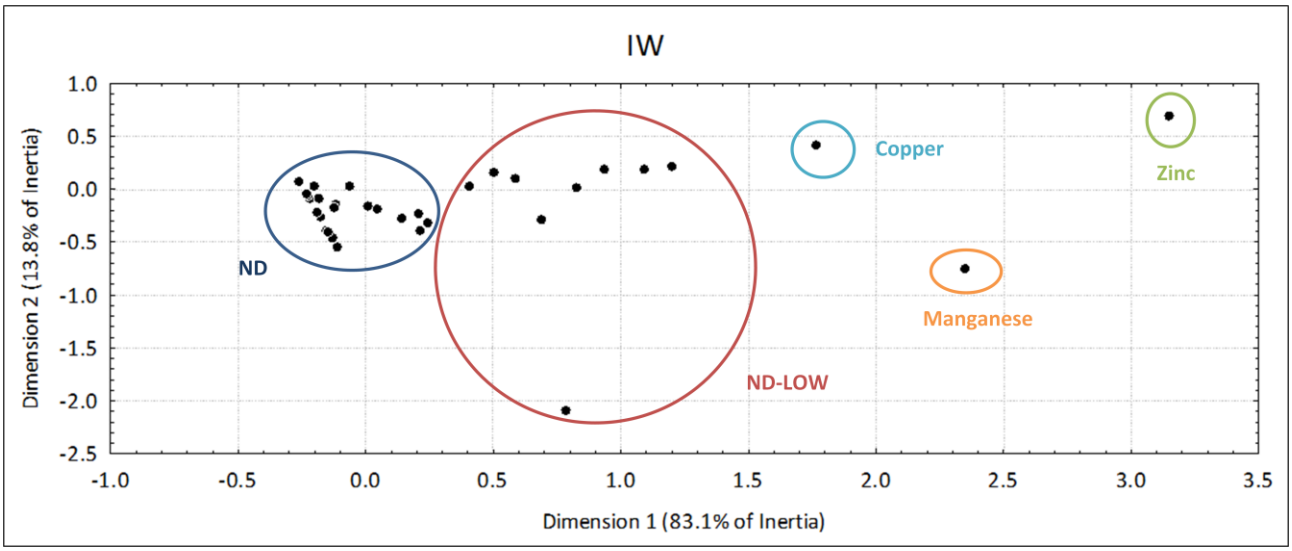

Figure A.2 Correspondence analysis of incoming water (IW) data. 2D plot of row coordinates; Dimensions: 1x2; Input Table (Rows x Columns): 177x4; Standardisation: row profiles.

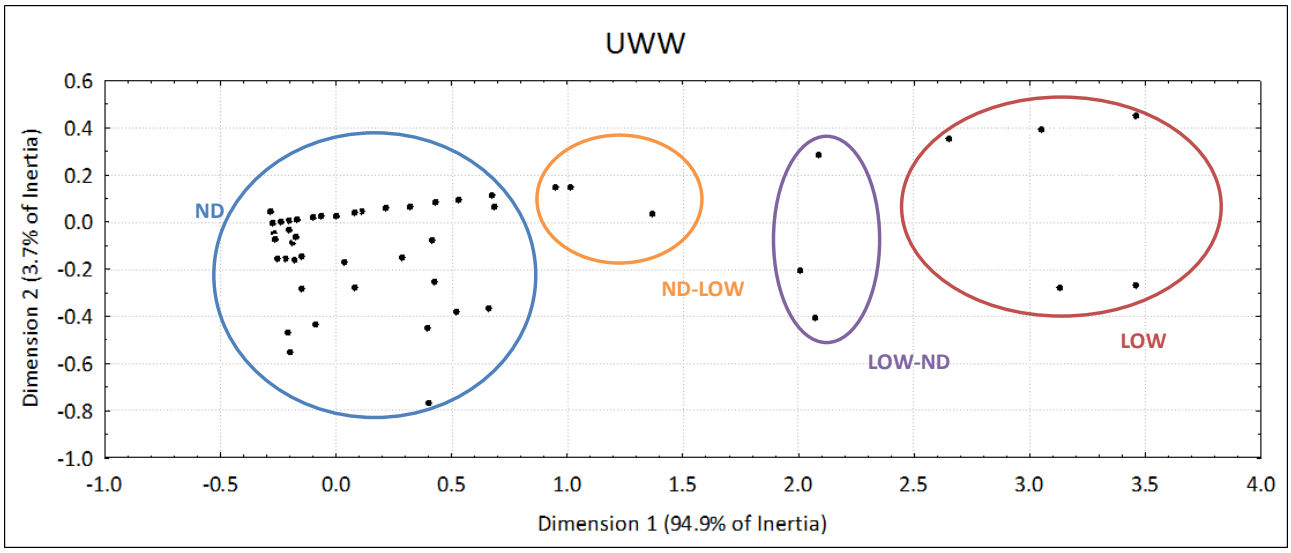

Figure A.3 Correspondence analysis of untreated wastewater (UWW) data. 2D plot of row coordinates; Dimensions: 1x2; Input Table (Rows x Columns): 177x4; Standardisation: row profiles.

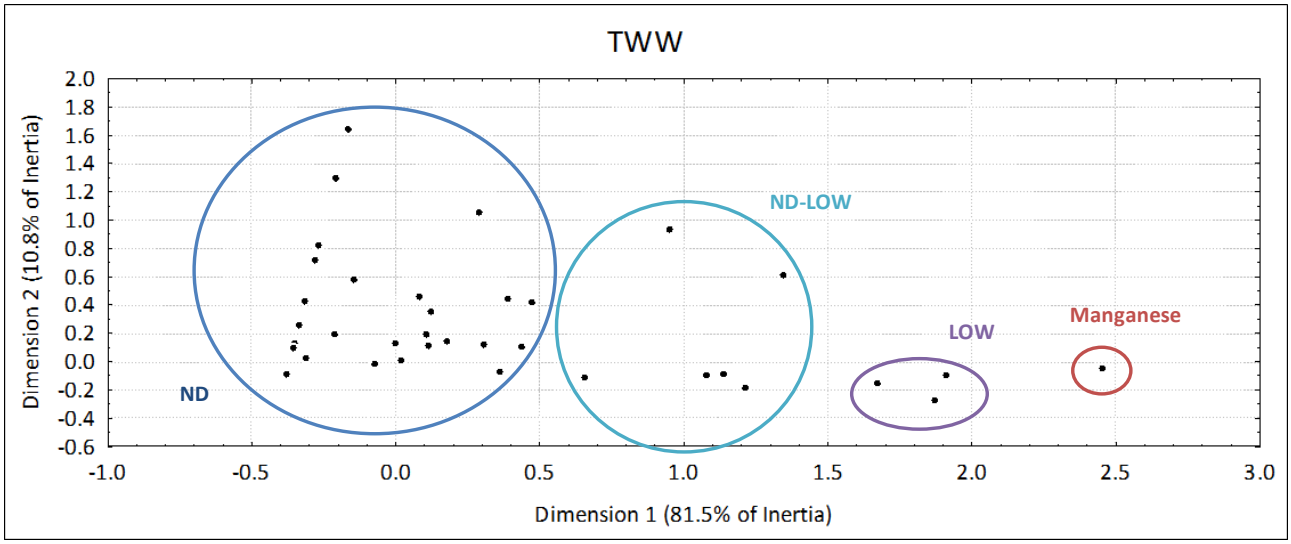

Figure A.4 Correspondence analysis of treated wastewater (TWW) data. 2D plot of row coordinates; Dimensions: 1x2; Input Table (Rows x Columns): 175x4; Standardisation: row profiles.

Table A.4. Ranking of analytes, with internal code for classification (A), based on the analyte global toxicity score (AGTS), % of toxicity with respect to the sum of toxicity of all analytes.

	A	Name	AGTS	%
1	A1108	Arsenic (As)	65	5.0%
2	A1201	Cyanide	61	4.7%
3	A1102	Hexavalent Chromium (Cr VI)	42	3.2%
4	A1109	Cadmium (Cd)	41	3.1%
5	A1105	Nickel (Ni)	40	3.1%
6	A0402	Benzidine	38	2.9%
7	A0415	4,4'-Methylene-bis(2-chloroaniline)	37	2.9%
8	A0410	3,3'-Dichlorobenzidine	37	2.9%
9	A0418	o-Toluidine	33	2.5%
10	A1112	Lead (Pb)	31	2.3%
11	A1111	Mercury (Hg)	27	2.1%
12	A0404	2-Naphthylamine	25	1.9%
13	A0401	4-Aminodiphenyl	25	1.9%
14	A0813	Trichloroethylene	24	1.9%
15	A0905	Pentachlorophenol (PCP)	22	1.7%
16	A0502	Dibutyltin (DBT)	19	1.5%
17	A0301	Polybromodiphenyls (PBBs)	16	1.2%
17	A0311	Di-bromo-diphenyl	16	1.2%
18	A0426	1,4-Phenylenediamine	16	1.2%
19	A1104	Cobalt (Co)	16	1.2%
20	A0403	4-Chloro-o-toluidine	16	1.2%
21	A0416	4,4'-Oxydianiline	16	1.2%
21	A0904	Tetrachlorophenols (TeCP)	16	1.2%
21	A0917	2,3,4,6-Tetrachlorophenol	16	1.2%
22	A0505	Triphenyltin (TPhT)	15	1.2%
23	A0427	2-Chloroaniline	15	1.2%

	A	Name	AGTS	%
23	A0432	n-Methylaniline	15	1.2%
24	A0504	Tributyltin (TBT)	15	1.1%
25	A0201	Benzyl-butyl-phthalate (BBP)	15	1.1%
26	A0210	Di-iso-butyl-phthalate (DIBP)	15	1.1%
27	A0425	Aniline	14	1.1%
28	A0702	Dichlorobenzenes	14	1.1%
29	A1106	Copper (Cu)	14	1.1%
30	A1107	Zinc (Zn)	14	1.1%
31	A0903	Trichlorophenols (TriCP)	14	1.0%
31	A0913	2,4,5-Trichlorophenol	14	1.0%
31	A0914	2,4,6-Trichlorophenol	14	1.0%
32	A0312	Tri-bromo-diphenyl	14	1.0%
32	A0506	Tricyclohexyltin(TCyHT)	14	1.0%
32	A0912	2,3,5-Trichlorophenol	14	1.0%
32	A0915	3,4,5-Trichlorophenol, 2,3,4-Trichlorophenol	14	1.0%
33	A0703	Trichlorobenzenes	13	1.0%
34	A0706	Hexachlorobenzene	13	1.0%
35	A0422	4-Aminoazobenzene	13	1.0%
35	A1001	Short-chain chlorinated paraffins (C10-C13)	13	1.0%
36	A0705	Pentachlorobenzene	13	1.0%
37	A0704	Tetrachlorobenzenes	13	1.0%
38	A0510	Tetrabutyltin (TeBT)	13	1.0%
39	A0103	Nonylphenols (NPs)	13	1.0%
40	A0303	Polybromodiphenyl ethers (PBDEs)	13	1.0%
40	A0320	Bromo-diphenyl-ether	13	1.0%
41	A0206	Di-iso-decyl-phthalate (DIDP)	13	1.0%
42	A0304	Tetra-bromo-bisphenol-A (TBBPA)	13	1.0%
43	A0101	Octylphenols (OPs)	13	1.0%
43	A0306	Hexa-bromo-cyclo-dodecan (HBCDD)	13	1.0%
43	A0508	Tripropyltin (TPT)	13	1.0%
44	A0310	Bromo-diphenyl	11	0.83%
45	A0302	Tri-(2,3-di-bromo-propyl)-phosphate (TRIS)	11	0.82%
46	A0916	2,3,4,5-Tetrachlorophenol	10	0.79%
47	A0202	Di-butyl-phthalate (DBP)	10	0.73%
48	A0216	Di-iso-pentyl-phthalate (DIPP)	9.5	0.73%
48	A0217	Di-iso-heptyl-phthalate (DIHP)	9.5	0.73%
48	A0219	N-iso-pentyl-iso-pentyl-phthalate (PIPP)	9.5	0.73%
49	A1101	Chromium (Cr)	9.1	0.69%
50	A0433	p-Toluidine	8.7	0.67%
51	A0429	m-Toluidine	8.5	0.65%
52	A0419	2,4-Diaminotoluene	7.5	0.58%
53	A0902	Dichlorophenol (DiCP)	5.6	0.43%
53	A0911	2,4-Dichlorophenol, 2,5-Dichlorophenol, 2,6-Dichlorophenol, 3,5-Dichlorophenol	5.6	0.43%

	A	Name	AGTS	%
54	A0615	Perfluoro-n-decanoic acid (PFDA)	4.0	0.30%
55	A0814	Tetrachloroethylene	3.0	0.23%
56	A0423	2,4-Xylidine	2.8	0.21%
57	A0602	Perfluorooctane sulphonates (PFOS)	2.4	0.19%
58	A0431	n-Ethylaniline	2.3	0.17%
58	A0918	2,3,5,6-Tetrachlorophenol	2.3	0.17%
59	A0308	Tris-(2-chloro-ethyl)-phosphate (TCEP)	2.2	0.17%
60	A1103	Manganese (Mn)	2.1	0.16%
61	A0601	Perfluoro-n-octanoic acid (PFOA)	1.9	0.15%
62	A0203	Di-(2-ethyl-hexyl)-phthalate (DEHP)	1.7	0.13%
62	A0204	Di-n-octyl-phthalate (DNOP)	1.7	0.13%
63	A0808	1,1,2,2-tetrachloroethane	1.7	0.13%
64	A0215	Bis-(2-methoxy-ethyl)-phthalate (DMEP)	1.5	0.12%
65	A0212	Di-n-hexyl-phthalate (DNHP)	1.5	0.11%
66	A0412	3,3'-Dimethylbenzidine	1.3	0.10%
67	A0408	2,4-Diaminoanisole	1.2	0.09%
68	A1110	Antimony (Sb)	1.2	0.09%
69	A0810	1,1-dichloroethylene	1.2	0.09%
70	A0424	2,6-Xylidine	1.0	0.08%
71	A0417	4,4'-Thiodianiline	1.0	0.08%
72	A0407	4-Chloroaniline	1.0	0.08%
73	A0104	Nonylphenolethoxylates (NPEOs)	1.0	0.07%
74	A0901	Monochlorophenols	0.92	0.07%
75	A0609	N-Ethyl-Perfluoro-octane-sulfon-amide (N-Et-FOSA)	0.92	0.07%
76	A0907	3-Chlorophenol	0.90	0.07%
77	A0908	4-Chlorophenol	0.86	0.07%
78	A0906	2-Chlorophenol	0.84	0.06%
79	A0309	Tris-(1,3-di-chloro-iso-propyl)-phosphate (TDCPP)	0.82	0.06%
80	A0809	Pentachloroethane	0.77	0.06%
81	A0409	4,4'-Diaminodiphenylmethane	0.75	0.06%
82	A0701	Chlorobenzene	0.71	0.05%
83	A0102	Octylphenolethoxylates (OPEOs)	0.63	0.05%
84	A0804	1,2-dichloroethane	0.59	0.05%
85	A0606	Perfluoro-butane-sulfonic acid	0.53	0.04%
86	A0209	Di-n-propyl-phthalate (DPP)	0.50	0.04%
86	A0430	n,n-Diethylanaline	0.50	0.04%
87	A0802	Chloroform	0.49	0.04%
88	A0313	Tetra-bromo-diphenyl	0.45	0.03%
88	A0314	Penta-bromo-diphenyl	0.45	0.03%
88	A0319	Deca-bromo-diphenyl	0.45	0.03%
88	A0501	Monobutyltin (MBT)	0.45	0.03%
88	A0611	N-Ethyl-Perfluoro-octane-sulfon-amido-ethanol (N-Et-FOSE alcohol)	0.45	0.03%
88	A0613	Perfluoro-heptanoic acid	0.45	0.03%

	A	Name	AGTS	%
88	A0616	Perfluoro-undecanoic acid	0.45	0.03%
88	A0620	Perfluoro-hexane-sulfonic acid	0.45	0.03%
88	A0910	3,4-Dichlorophenol	0.45	0.03%
89	A0421	o-Anisidine	0.44	0.03%
90	A0414	p-Cresidine	0.40	0.03%
91	A0803	Carbon tetrachloride	0.39	0.03%
92	A0307	2,2-Bis(bromomethyl)-1,3-propanediol (BBMP)	0.36	0.03%
93	A0807	1,1,1,2-tetrachloroethane	0.36	0.03%
94	A0411	3,3'-Dimethoxybenzidine	0.36	0.03%
95	A0305	Bis-(2,3-di-bromo-propyl)-phosphate	0.36	0.03%
96	A0806	1,1,2-trichloroethane	0.34	0.03%
97	A0205	Di-iso-nonyl-phthalate (DINP)	0.24	0.02%
97	A0405	o-Aminoazotoluene	0.24	0.02%
97	A0801	Dichloromethane	0.24	0.02%
98	A0812	trans-1,2-Dichloroethylene	0.23	0.02%
99	A0626	7H-Dodecafluoro heptane carboxylate	0.21	0.02%
100	A0331	Tris-(2-chloroisopropyl)-phosphate (TCPP)	0.21	0.02%
101	A0428	5-Nitro-o-anisidine	0.10	0.01%
102	A0909	2,3-Dichlorophenol	0.10	0.01%
103	A0330	Tetra-bromo-bisphenol A bis-(di-bromo-propyl-ether) (TBBPA-BDPE)	0.09	0.01%
104	A0406	5-Nitro-o-toluidine	0.07	0.01%
105	A0811	cis-1,2-Dichloroethylene	0.05	0.004%
106	A0805	1,1,1-trichloroethane	0.05	0.004%
107	A0208	Di-ethyl-phthalate (DEP)	0.04	0.003%
108	A0207	Di-methyl-phthalate (DMP)	0.03	0.002%
109	A0329	Deca-bromo-diphenyl-ether	0.02	0.002%
109	A0420	2,4,5-Trimethylaniline	0.02	0.002%
110	A0507	Trioctyltin(TriOT)	0.01	0.001%
111	A0211	Di-cyclo-hexyl-phthalate (DCHP)	0	0%
111	A0213	Di-nonyl-phthalate (DNP)	0	0%
111	A0214	Di-iso-octyl-phthalate (DIOP)	0	0%
111	A0218	1,2-Benzene-di-carboxylic acid di-pentyl-esters, branched and linear (DHNUP)	0	0%
111	A0220	Di-heptyl-phthalate (DHP)	0	0%
111	A0315	Hexa-bromo-diphenyl	0	0%
111	A0316	Hepta-bromo-diphenyl	0	0%
111	A0317	Octa-bromo-diphenyl	0	0%
111	A0318	Nona-bromo-diphenyl	0	0%
111	A0321	Di-bromo-diphenyl-ether	0	0%
111	A0322	Tri-bromo-diphenyl-ether	0	0%
111	A0323	Tetra-bromo-diphenyl-ether	0	0%
111	A0324	Penta-bromo-diphenyl-ether	0	0%
111	A0325	Hexa-bromo-diphenyl-ether	0	0%
111	A0326	Hepta-bromo-diphenyl-ether	0	0%

	A	Name	AGTS	%
111	A0327	Octa-bromo-diphenyl-ether	0	0%
111	A0328	Nona-bromo-diphenyl-ether	0	0%
111	A0332	Tris-(aziridinyl)-phosphinoxide (TEPA)	0	0%
111	A0413	3,3'-Dimethyl-4,4'-diaminodiphenylmethane	0	0%
111	A0503	Dioctyltin (DOT)	0	0%
111	A0509	Monooctyltin (MOT)	0	0%
111	A0603	Perfluoro-n-hexanoic acid (PFHxA)	0	0%
111	A0604	Perfluorohexane sulphonates (PFHxS)	0	0%
111	A0605	Perfluorobutyric Acid (PFBA)	0	0%
111	A0607	Perfluoro-octane-sulfon- amide (PFOSA)	0	0%
111	A0608	N-Methyl-Perfluoro-octane-sulfon-amide (N-Me-FOSA)	0	0%
111	A0610	N-Methyl-Perfluoro-octane-sulfon-amido-ethanol (N-Me-FOSE alcohol)	0	0%
111	A0612	Perfluoro-pentanoic acid	0	0%
111	A0614	Perfluoro-nonanoic acid	0	0%
111	A0617	Perfluorododecanoic Acid (PFDoA)	0	0%
111	A0618	Perfluoro-tridecanoic acid	0	0%
111	A0619	Perfluoro-tetradecanoic acid	0	0%
111	A0621	Perfluoro-heptane-sulfonic acid	0	0%
111	A0622	Perfluor-decane-sulfonic acid	0	0%
111	A0623	1H,1H,2H,2H-Perfluoro-octane-sulphonic acid	0	0%
111	A0624	2H,2H,3H,3H-Perfluoroundecanoic acid (PFUnA)	0	0%
111	A0625	Perfluoro-3-7-dimethyl octane carboxylate	0	0%