Supplementary material

Table S1. Type of RW, main characteristics, etc, for the RW analysed in §3.1. The information and data, typical values or ranges thereof for the period May 2017 to April 2018, were on request reported by the DWTPs.

City	Jönköping	Karlstad	Karlskrona	Gothenburg	Luleå	Gävle
Raw water source name	Vättern	Vänern	Lyckebyån	Göta älv	Lule älv	Gävle-Valboåsen
Type	Lake	Lake	Small river 4-13m3/sec	Big river 570m3/sec (+lake)[a]	Big river 500m3/sec	Groundwater from esker ridge
Land use etc.	Forest and agriculture	Forest and agriculture	Forest and some few industries	Agriculture, industries and rel. densely populated	Forest and agriculture, sparsely populated	City (+ seawater intrusion)
Assessment of stability	Stable	Stable	Unstable[b]	Unstable[a]	Relatively stable[c]	Stable
Color 410nm mgPt/L	<5 (-6)	<5	Normally 125-150 (nov/jan 300)	10-33	10-50	<5
Total Organic Carbon mg/L	2.4	na	Normally 15 (nov/jan 26)	4.1-5.6	na	2.3
Fe mg/L	<0.05	<0.05	1,6	0.05-0.24	0.1-0.5	<0.001
Chemical Oxygen Demand Mn mg O2/L	1.0-2	na	28	4.0-6	1-5	1.4-1.7
Turbidity (FNU)	0.18	0.3	2.8	2.5-13	0.5-4	<0.1 FNU
Alkalinity HCO3 mg/L	36	65	7-16	21	11	130-210
Ca mg/L	15	15	6	7.2	3	45-74
Mg mg/L	2.5	2	1.7	1,5-3,5	0.8	3.5-8.9
Hardness °dH	2.6	2.6	1.2	1.4	0.64	7.1-12
Conductivity mS/m	15	14	7	Normally 8-10 (July:8-21)	2.6-5	32-64
Chloride mg/L	10	6	9	Normally 6-11 (July:7-40)	1-4.8	22-64
Na mg/L	7.7	12	6.1	Normally 6.5-9 (July 22)	1-2.6	15-42
pH	7.6	8.2	6.7	7.2-7.5	6.8-7.2	7.7
Sulfat mg/L	18	10	6.5	8	1.8-4	12-41

[a]Gothenburg: Whenever results from analysis of the river water indicate elevated concentrations of bacteria or sea water intrusion (caused by rain or unfavourable wind respectively) the RW source is temporarily switched from river to lake. [b]Karlskrona: An already relatively high level of organic matter increases during winter. [c]Luleå: Relatively stable, although variations occurs due to seasonal variations, e.g. snowmelt runoff and autumn rain.

Table S2. Simplified summary of the purification process for DW production at the DWTPs sampled for the experiment in §3.2. (Due to security reasons a detailed description of the DWTP's purification processes, and main characteristics of the DW quality, cannot be published).

City	Jönköping	Karlstad	Karlskrona
Type of RW	Lake	Lake	River
Artificial infiltration	No	Yes	Yes, after addition of flocculation reagents
Flocculation/coagulation	No	Occasionally	Yes, prior to artificial infiltration
Desinfection	Cl_2	UV	Occasionally NaClO
Carbon filter	No	No	Yes

Table S3. Result of the inter-laboratory exercise described in the introduction. Correct identification is denoted with an X. (Five of the 11 participating laboratories did not have access to advanced instrumentation and did not identify any of the added compounds. These laboratories are excluded from the table.).

Spiked concentration / Laboratory code	D	E	G	H	I	K
Triethylamine 7 mg/L	X					X
Warfarin 2 mg/L	X		X	X	X	X
Acrylamide 1 mg/L		X				
Diflufenican 0,05 mg/L						X
Acetonitrile 80 mg/L				X	X	

Table S4. Analysis of GC-Orbitrap data in §3.5: Number of peaks fulfilling the –Log10 P-value and Log2 Fold Change criteria (i.e. peaks that are significantly higher in the spiked sample compared to the reference sample) depending on the reference sample. Using a reference sample from another city as the spiked sample gave almost twice as many significantly higher peaks in the spiked sample as a reference from the same building.

Reference sample	Number of significantly differentiated peaks
Same building	12
Different building	17
Different city	23

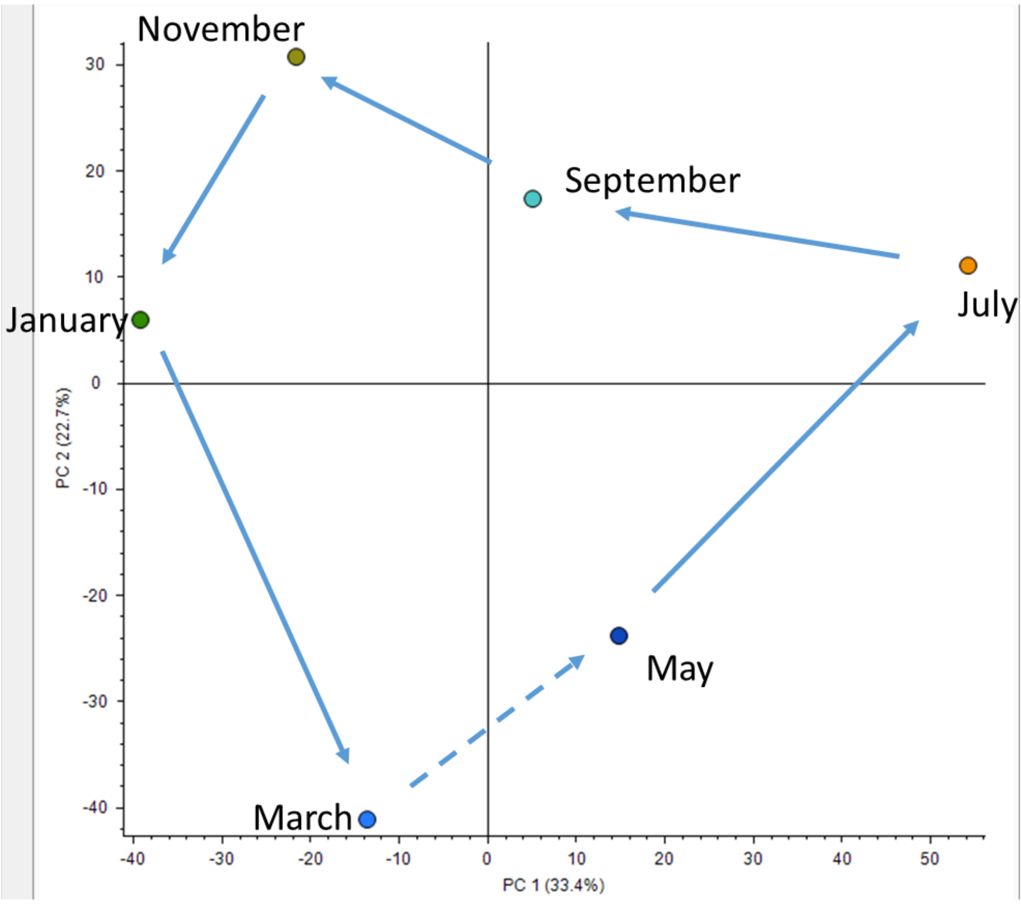

Figure S1. PCA score plot of HRMS-data of RW sampled from a DWTP in Luleå. The samples were collected from May 2017 to March 2018. Arrows represent chronologic order. PC 1 and PC 2 were found to apparently correlate with season, which was in line with information from the DWTP (see text). Percentages bracketed in axis legends are contribution ratios.

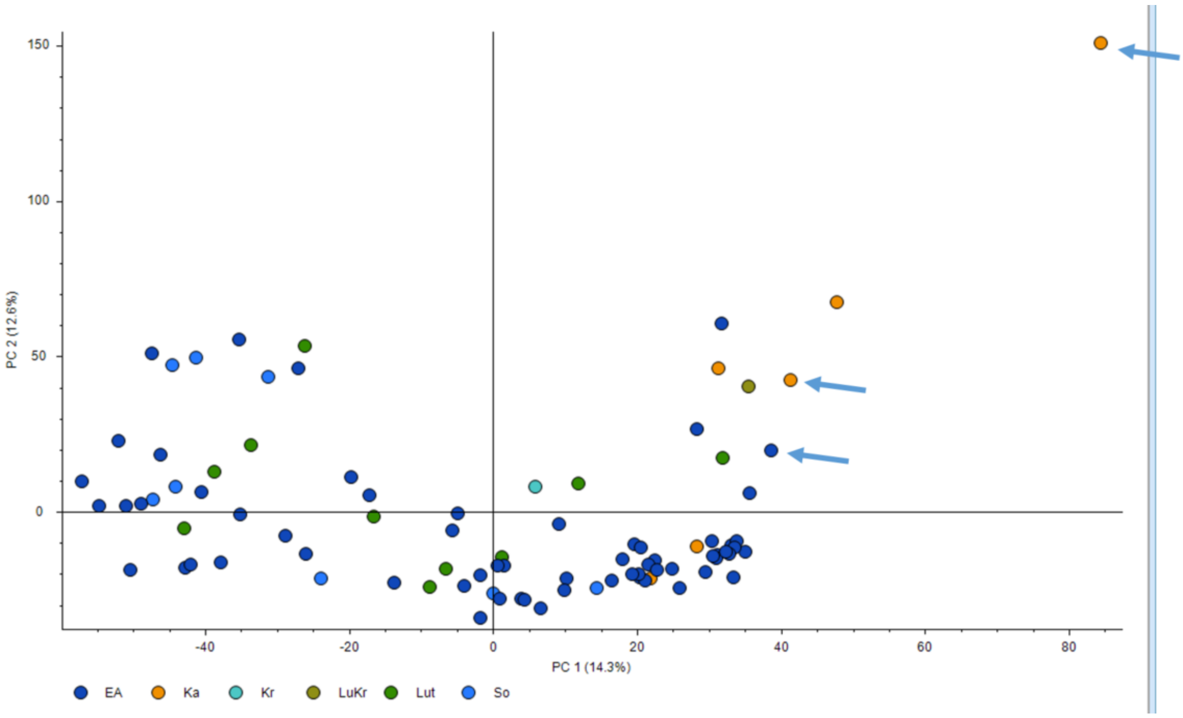

Figure S2. Same score plot as in figure 6, but samples are now labelled according to what chemical – if any – was used for any pre-alkalinisation process step. Ka: Lime, Kr: Chalk, Lut: Lye, So: Sodium bicarbonate, LuKr: a combination of lye and chalk, EA: no pre-alkalinisation applied. The six DWTPs using lime in the pre-alkalinisation step (labelled orange) appear at relatively high PC1 values. Similarly, the three DWTPs using lime in any (later) pH-adjustment step (labelled with arrows) appear at high PC1 values. Thus, there were in total nine indications of use of lime, and six of these indications were found associated with the four DWTPs appearing at the highest PC1 values in the PCA. Percentages bracketed in axis legends are contribution ratios.

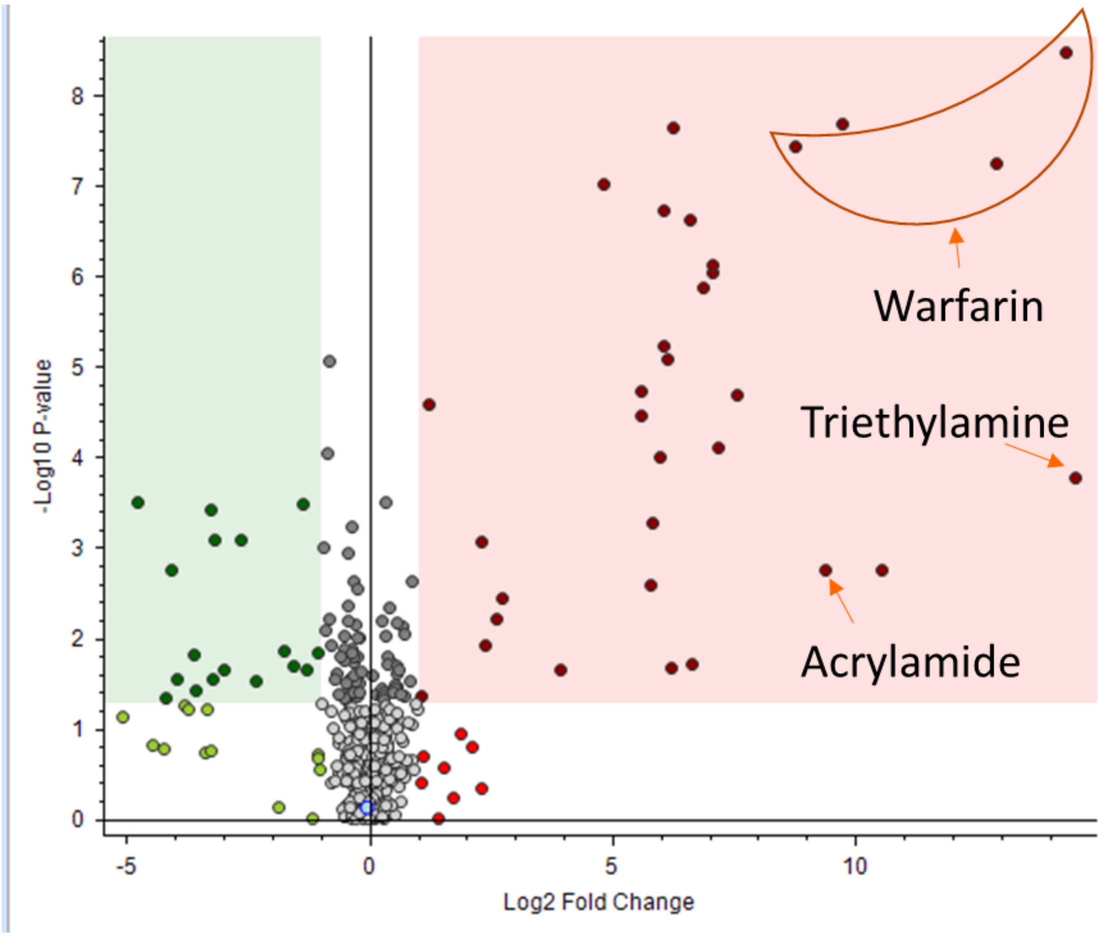

Figure S3. Analysis of LC-Orbitrap data: Differential analysis (volcano plot) used in the follow-up (in §3.5) of the inter-laboratory exercise for revealing the signals from the spiked compounds. For each feature, the fold change (i.e. the ratio between the median peak area of the spiked sample and the median peak area of the reference sample) was calculated (X-axis: Log2 fold change). Both samples (spiked and reference) were analysed in triplicates in order to calculate the level of significance of the fold change (Y-axis: -Log10 P-value).

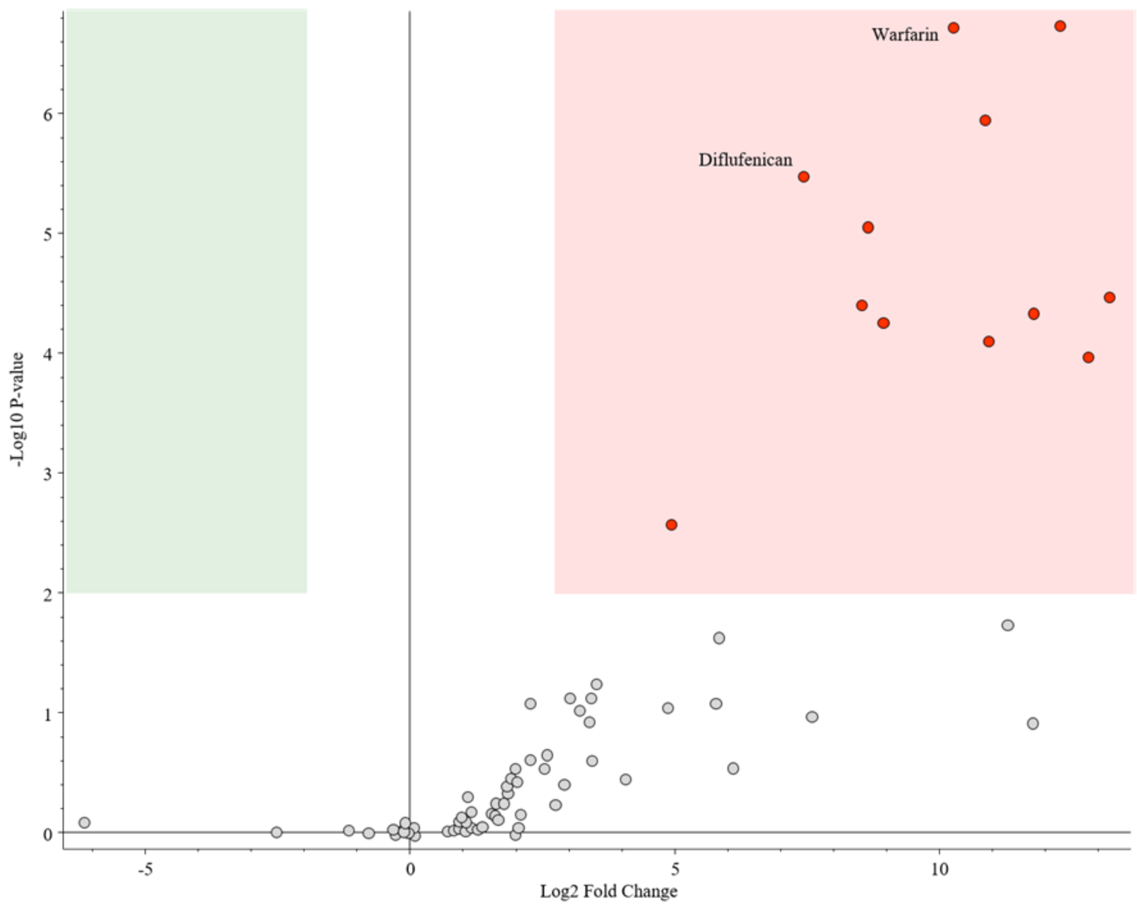

Figure S4. Analysis of GC-Orbitrap data: Differential analysis (volcano plot) used for revealing the signals from the spiked compounds in the exercise described in §3.5. For each compound, the fold change (i.e. the ratio between the median peak area of the spiked sample and the median peak area of the reference sample) was calculated (X-axis: Log2 fold change). The samples were analyzed in triplicates in order to calculate the level of significance of the fold change (Y-axis: -Log10 P-value). The reference sample is DW from the same building as the spiked water.