The Dangerous Substances Directive (76/464/EC) lists 125 compounds that have legislated levels in drinking and surface waters, of which, more than 100 are amenable to GC-TOF-MS.

The compounds grouped here represent a wide range of polarities and types, and include benzenes, chlorobenzene, dichlorobenzene, o,p'-DDT, dieldrin, endrin, endosulfan, endrin aldehyde, heptachlor, heptachlor epoxide, hexachlorocyclohexane, isodrin, lindane, mirex, and oxychlordane.

The extraction method used was selected to minimize matrix effects in the chromatograms. A sample of 50 µL is injected in a typical batch analysis bracketing the drinking and surface water samples.

The chromatography was optimized for selectivity, speed, and separation. Targeted screening results were obtained for three critical pairs, 3- and 4-chlorophenol, E and Z mevinphos and o,p'-DDT and p,p'-DDD, using the DB-17ms column. A majority of the pollutants can be confirmed to within 0.1% using this method in surface waters to a confidence level of 99%

Untargeted results are illustrated in Figure 1. The full spectrum approach provided by TOF also allows untargeted pollutants of interest to be identified with ChromaLynx. An example pollutant in Figure 4 is 4-methylbenzenesulfonamide, which is illustrated in Figure 5. Other examples included naphthalene and 1-methylnaphthalene.

To establish a suitable untargeted screening technique there are a number of parameters that would need to be tested, extract, detect, locate and identify all compounds in the sample. These include the minimal non-selective sample preparation for a wide range of compounds with different polarities; simple high resolution GC separation to minimize matrix interference whilst maintaining resolution of critical pairs; and automated peak detection and deconvolution of all components in the sample.

The limits of detection (LODs) were assessed for confirmation (two exact mass chromatograms per compound) and screening (one exact mass chromatogram per compound). A summary of the LODs is given in Table 2. The LODs were based on the S/N ratio and the peak signal to noise (S/N) ratio of 3:1. The instrumental LODs are based on the average LOD obtained from five replicate injections of 0.5 µg/L of a target compound.

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