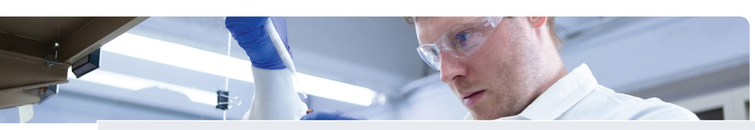



Comprehensive methods for drinking water analysis based on European Directive 2020/2184

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Introduction

Here, standard operating procedures for the analysis of multiple compound classes in drinking water using the SCIEX QTRAP 6500+ and the SCIEX 7500 system have been provided. The documents include full method details such as chemicals and reagents, sample and standard preparation, instrument parameters, a results overview and example chromatograms to ensure easy and repeatable replication of the methods on your instrumentation. Each method has been created with the European drinking water directive 2020/2184 in mind, with the respective limits having been achieved[1].

In the following section, the method highlights have been shown with example XICs (Figures 1 – 6) and other key features discussed.

The methods contain detailed information on how to analyse

- **Acrylamide** using the SCIEX QTRAP 6500+ system or the SCIEX 7500 system
- **Haloacetic acids** using the SCIEX QTRAP 6500+ system or the SCIEX 7500 system
- **Estradiol, ethinyl estradiol, estrone, Bisphenol A, Nonylphenol and Octylphenol** using the SCIEX QTRAP 6500+ system or the SCIEX 7500 system
- **PFAS** using the SCIEX QTRAP 6500+ system or the SCIEX 7500 system
- **Polar pesticides** using the SCIEX QTRAP 6500+ system or the SCIEX 7500 system
- **PPCPs** using the SCIEX QTRAP 6500+ system

Method highlights

Hormones, bisphenol A (BPA) and nonylphenol analysis in drinking water by direct injection using the SCIEX 7500 system

In Figure 1 below, the sensitivity of the SCIEX 7500 system is displayed, with 1 ng/L XICs shown for 4 of the compounds analysed, meeting the EU watch list recommendation when using a large volume injection. This method also combines hormones, BPA and nonylphenol in one analysis, without the need for SPE pre-concentration of samples.

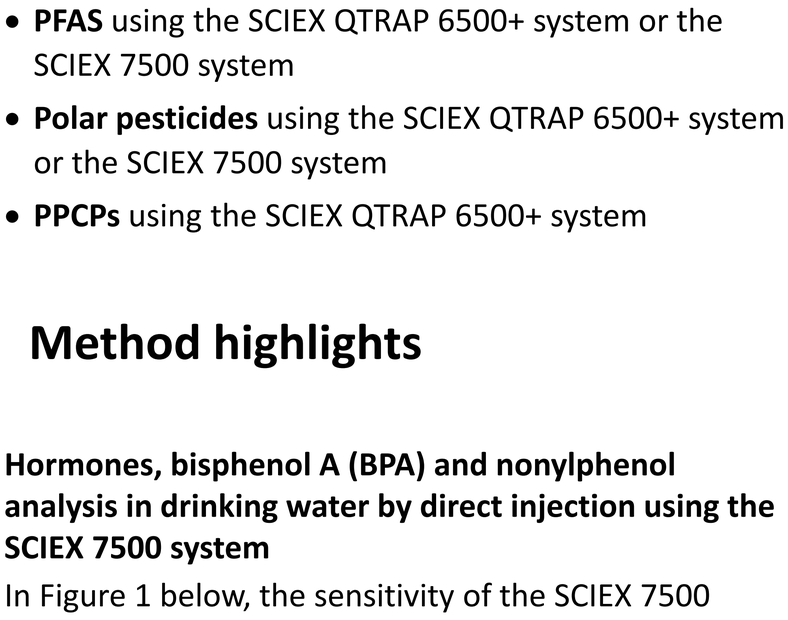

Figure 1. XICs of the steroid hormones analysed along with BPA at 1 ng/L. The images above show the sensitivity achievable when using the SCIEX 7500 system. TOP and bottom XICS indicate quantifier and qualifier.

Acrylamide analysis in drinking water by direct injection using the QTRAP 6500+ LC-MS/MS system and the SCIEX 7500 system

In this example, we demonstrate the importance of column selection and sensitivity improvement with the SCIEX 7500 system. Within the SOPs two columns are mentioned with Figures 2 and 3 highlighting the differences. The recommended column provides increased retention, improving method performance Figure 4 on the other hand shows the sensitivity improvement achieved when using the SCIEX 7500 system.

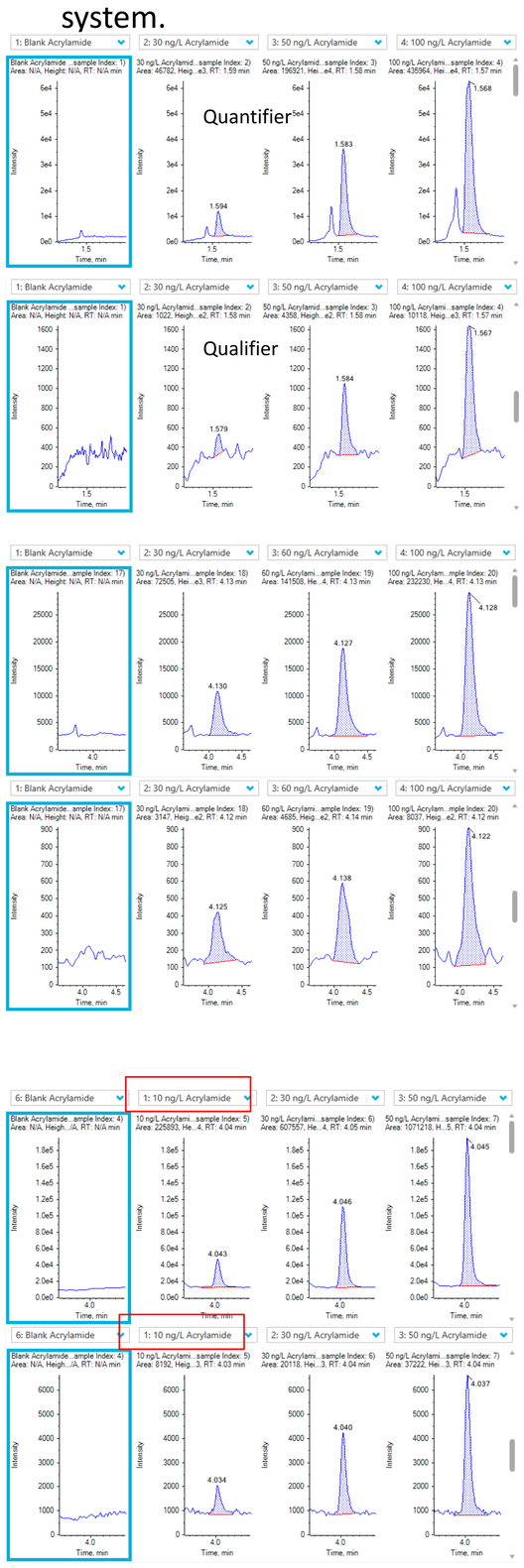

Figure 2. XICs of acrylamide at multiple concentrations for both the quantifier and qualifier transition when using the alternative column and the QTRAP 6500+ system. When using the alternative column, the retention time is only 1.5 minutes meaning that with this set-up the peak is very close to the void volume. In addition, for the qualifier transition, the 30 ng/L peak is barely detectable.

Figure 3. XICs of acrylamide at multiple concentrations for both the quantifier and qualifier transition when using the recommended column and the QTRAP 6500+ system. In comparison to the alternative column, the retention time here is much longer (~4 minutes compared to ~1.5 minutes) meaning that it is well resolved from the void. The sensitivity is also improved with this column, as can be seen at 30 ng/L where both transitions provide a satisfactory peak.

Figure 4. XICs of acrylamide at multiple concentrations for both the quantifier and qualifier transition when using the recommended column and the SCIEX 7500 system. When using the SCIEX 7500 system the sensitivity is improved in comparison to the QTRAP 6500+ system, with XICs shown in the figure of acrylamide at 10 ng/L for both quantifier and qualifier transition which is not possible when using the same method on the QTRAP 6500+ system.

Haloacetic acid analysis in drinking water by direct injection using the QTAP 6500+ LC-MS/MS system and the SCIEX 7500 system

When looking to the current EU regulation for haloacetic acids, the QTRAP 6500+ system can easily achieve the necessary levels of detection. However, the SCIEX 7500 system provides additional sensitivity as can be seen in Figure 5, future proofing your lab for any possible further regulation changes .

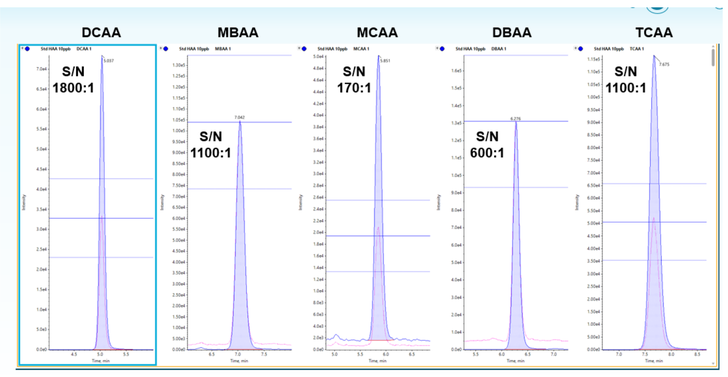

Figure 5. XIC of the SCIEX 7500 system for the analysis of haloacetic acids.

Polar pesticide analysis in drinking water by direct injection using the QTRAP 6500+ LC-MS/MS system and the SCIEX 7500 system

This method shows the importance of the instruments capability to do an MS^3 scan. For glyphosate, the typical second MRM transition provides a high background and lacks sensitivity however, with MS^3 the sensitivity is improved due to increased selectivity. In Figure 6, the comparison is made between the second MRM transition for glyphosate and the MS^3 transition PPCPs and PFAS not mentioned, anything to mention?

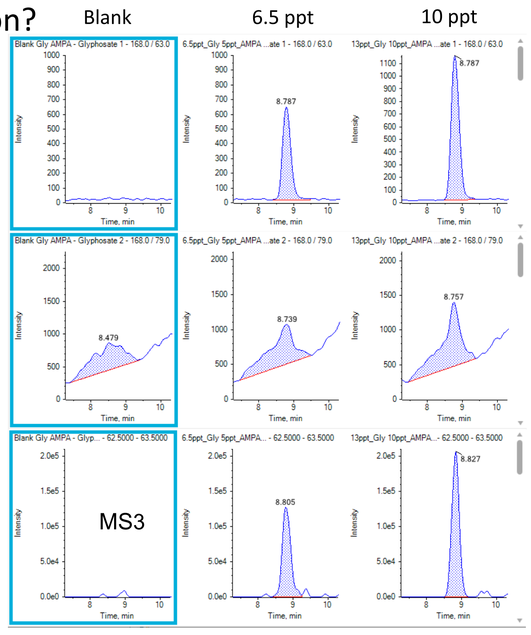

Figure 6. XIC comparisons for 100ng/l glyphosate showing the quantifier and qualifier transition alongside the MS^3 transition, highlighting the increased selectivity shown when using MS^3 in comparison to the qualifier transition, improving the methods sensitivity. Top 1 is MRm quantifier and Top 2 is MRM qualifier:

References

1. DIRECTIVE (EU) 2020/2184 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 16 December 2020 on the quality of water intended for human consumption