An integrated GC-MS workflow solution for the determination of (semi)volatiles in drinking water and solid waste according to the U.S. EPA guidelines

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INTRODUCTION

There are many regulatory agencies safeguarding the environment by the issuance of health and environmental standards, such as the United States (U.S.) Environmental Protection Agency (EPA). These standards include many standardized guidelines for the analysis of hazardous environmental contaminants. The challenge for today’s laboratories is to correctly execute these guidelines, such as described in the EPA methods, including calculating and assessing the final results. In many labs the chromatographic results generated while analyzing these methods are transformed into spreadsheets in order to perform the calculations and assess the final results. This process can be time-consuming and transcription errors are a common problem. As a result laboratories develop internal guidelines, such as standard operating procedures (SOPs), that are executed manually. In order to establish a system for compliance with the regulatory methodology, environmental laboratories need to develop internal guidelines that build, or complete, correct sequence with predefined files and a well-informed workflow, guiding the users through a minimum number of choices needed to create a result. A common problem is introducing the risk of human transcriptions errors and transcription errors are a common problem. As a result laboratories develop internal guidelines, such as standard operating procedures (SOPs), for these results for minimum relative response factor errors and transcription errors are a common problem. By using the available eWorkflows within the Thermo Scientific™ Chromeleon CDS, these results can be automatically reported in order to create the final environmental report of the entire methodology. The data can be automatically reported in order to create the final environmental report of the entire methodology. Thermo Scientific CDS offers a fast and simple way to run analyses and create environmental reports according to the U.S. EPA methods. This report demonstrates the benefits of using Thermo Scientific CDS. The example shown is based on U.S. EPA method 8270D, which is used for the determination of volatile organics in Drinking Water and Solid Waste following the U.S. EPA guidelines using the Thermo Scientific™ TRACE 1300 Gas Chromatograph and the Thermo Scientific™ QP 5000 Series Triple Quadrupole Mass Spectrometer system. Table 1 shows the preconfigured sequence layout of the daily analysis (A), including additional custom columns for identification of the analyte type and spike groups, and how the looks for 8 samples (B). This represents a lot of requirements just for the calibration, with an additional need to enter method-specific criteria. The processing method is set up with additional columns to enter the required criteria (Figure 7), such as the minimum required factor or the maximum relative percent difference (RPD). A selection of sheets in the report template provides all calculations and in addition checks the results against the criteria that were entered in the processing method.

RESULTS

QTFPP Tune Verification MS instruments are tuned to assure accuracy of masses and maximum intensity. U.S. EPA method 8270 prescribes verification of the MS tune using DFTPP according to the criteria as described in Figure 3. Figure 4 shows a typical mass spectrum of DFTPP to show the MS system.

Figure 2 shows the prespecified sequence layout of the daily analysis (A), including additional custom columns for identification of the analyte type and spike groups, and how the looks for 8 samples (B).

Figure 1. efforts to fit the environmental GC-MS analysis

U.S. EPA Method Scope
524.2, 524.3, 524.4 Volatile organics in Drinking Water
525.1, 525.2, 525.3 Semi-volatile organics in Drinking Water
620.1B, 620.2B Organic volatiles in Solid Waste
620.6D 620.7D Semi-solid organics in Solid Waste

Table 1. Overview of methods supported by the environmental GC-MS extension pack

The examples shown are based on U.S. EPA method 8270D, for the determination of the concentration of semi volatile organics in a sample matrix, i.e., drinking water and solid waste samples. The workflow automation helps ensure that analysts follow SOPs consistently and accurately, resulting in high-quality and reliable results, saving valuable time and ensuring data integrity.

MATERIALS AND METHODS

All experiments were performed with the Thermo Scientific™ TRACE 1300 Gas Chromatograph in combination with the Thermo Scientific™ QP 5000 Series Single Quadrupole GC-MS system. The maximum software version for instrument control, MS data processing, and calculation and reporting of the results with the environmental GC-MS extension pack (Table 1) was Thermo Scientific™ Chromeleon™ CDS version 7.2 Service Release 5. To automate the assessment of these criteria, they can be translated to system suitability tests (SSTs) in the Chromeleon software (Figure 6). This provides a consistent evaluation of the data by following the same algorithm, assessing the results for minimum relative response factor errors and transcription errors are a common problem. Figure 7 shows two examples of calibration reports, one for the calibration results and check these results for minimum relative response factor errors and transcription errors are a common problem. Figure 8 shows two examples of calibration reports, one for the calibration results and check these results for minimum relative response factor errors and transcription errors are a common problem.

Figure 9. reported results including checks for (A) minimum RRF=2 (B) and (C) for minimum relative RPD

Automated report creation

The automated generation of reports is based on a combination of the U.S. EPA methods, including calculating and assessing the final results. The data can be automatically reported in order to create the final environmental report of the entire methodology. Thermo Scientific CDS offers a fast and simple way to run analyses and create environmental reports according to the U.S. EPA methods. This report demonstrates the benefits of using Thermo Scientific CDS. The example shown is based on U.S. EPA method 8270D, which is used for the determination of volatile organics in Drinking Water and Solid Waste following the U.S. EPA guidelines using the Thermo Scientific™ TRACE 1300 Gas Chromatograph and the Thermo Scientific™ QP 5000 Series Triple Quadrupole Mass Spectrometer system. Figure 2 shows the preconfigured sequence layout of the daily analysis (A), including additional custom columns for identification of the analyte type and spike groups, and how the looks for 8 samples (B). This represents a lot of requirements just for the calibration, with an additional need to enter method-specific criteria. The processing method is set up with additional columns to enter the required criteria (Figure 7), such as the minimum required factor or the maximum relative percent difference (RPD). A selection of sheets in the report template provides all calculations and in addition checks the results against the criteria that were entered in the processing method.

CONCLUSIONS

This report demonstrates the benefits of using Thermo Scientific CDS. The data can be automatically reported in order to create the final environmental report of the entire methodology. Thermo Scientific CDS offers a fast and simple way to run analyses and create environmental reports according to the U.S. EPA methods. This report demonstrates the benefits of using Thermo Scientific CDS. The example shown is based on U.S. EPA method 8270D, which is used for the determination of volatile organics in Drinking Water and Solid Waste following the U.S. EPA guidelines using the Thermo Scientific™ TRACE 1300 Gas Chromatograph and the Thermo Scientific™ QP 5000 Series Triple Quadrupole Mass Spectrometer system. Figure 2 shows the preconfigured sequence layout of the daily analysis (A), including additional custom columns for identification of the analyte type and spike groups, and how the looks for 8 samples (B).

Figure 3. Measuring Method setup to enter calibration and check standard parameters and assurance criteria

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REFERENCES


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