

CHRONECT Workstation MCPD



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Introduction

3-monochloro-1,2-propanediol (3-MCPD), 2-monochloro-1,3-propanediol (2-MCPD) and glycidol belong to the group of production-related contaminants in foodstuffs. MCPD fatty acid esters can be formed during refining at high temperatures in the presence of chloride containing salts. However, refining is a necessary chemical and physical refining process in the production of many oils. It is only through this temperature treatment that undesirable odors and flavorings as well as any traces of toxic compounds such as pesticides, heavy metals or mycotoxins can be removed during further processing.

The analysis of these contaminants is becoming more and more important due to their carcinogenicity. The CHRONECT Workstation MCPD offers a fully automated solution. The automation improves the turnaround time of the analysis and ensures reproducible results.

Methods

The methods for the analysis of MCPD esters can be divided into two groups: direct determination by LC-MS/MS or indirect determination by GC-MS. The direct analysis is very complex due to the large number of esters, since each ester is determined individually by LC-MS. Therefore, the indirect methods have become generally accepted in practice.

In indirect methods the analytes bound to fatty acids are first converted into their respective free form. The release from the fatty acid esters is done by transesterification of MCPD in its free alcohol. The free MCPD is then extracted and derivatized in a further step. Depending on the method, a clean step is then performed to remove the excess derivatizing agent. Then the injection into the GC-MS system takes place.

The CHRONECT Workstation MCPD performs these steps fully automated and simplifies the MCPD analysis for the user by eliminating manual interaction.

There are currently four indirect methods that have been standardized or are in the process of being standardized. These methods are:

- ISO 18363-1 (AOCS Cd 29c-13 or DGF C-VI 18)
- ISO 18363-2 (AOCS Cd 29b-13 or 3-in-1)
- ISO 18363-3 (AOCS Cd 29a-13 or Unilever)
- Draft ISO 18363-4 (Zwagerman – in standardization process)

For the DGF method, Axel Semrau offers a version for automated operation that has been optimized in terms of sample throughput and robustness: DGF Fast and Clean.

For all these methods modules for the CHRONECT Workstation MCPD are available. Thus, the system can be adapted to changing regulatory requirements at any time. Depending on the user's requirements regarding time to first result, sample throughput of the entire system, compatibility with existing GC-MS systems and regulatory requirements in the regional market, the decision for the method used should be made. To meet the different technical requirements of the methods, the CHRONECT Workstation MCPD must be equipped with different hardware options depending on the method used. In general, the use of a Triple Quad GC-MS for MCPD analysis is recommended. This allows all sensitivity requirements to be met. Regarding the analytical performance, e.g. LOQ, LOD, reproducibility, all methods are comparable. For some methods, the "One-Piece-Workflow" makes it possible to measure priority samples promptly. The result of the priority sample will be available after one hour at the longest.

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Table 1: Methods for the determination of MCPD by GC-MS. Values when using two injection units.

Method name	Based on the official method	Based on the official method	One-Piece-Workflow	Special modules	Samples per 24 h	First Sample result after
Unilever	ISO 18363-3	AOCS Cd29a-13	-	Heated Tray at 40 °C	10	18 h
3-in-1	ISO 18363-2	AOCS Cd29b-13	-	Cooled Tray at -22 °C	32	17 h
DGF Fast & Clean	ISO 18363-1	AOCS Cd29c-13	√	-	36	48 min
Zwagerman	Draft ISO 18363-4	-	√	Cooled Tray at 10 °C	36	46 min

System setup

The CHRONECT Workstation MCPD consists of two general components:

CHRONECT Robotic sample robot

The used CHRONECT Robotic sample robot can be equipped with one or two injection units and is available in 120 cm, 160 cm and 200 cm length. The configuration depends on the chosen methods and on the amount of methods, which should run parallel on the system. The entire workflow is controlled by the automation platform CHRONOS. This platform also handles the integration of the GC-MS data system. All common data systems for GC-MS devices can be used.

GC-MS system

The second important component of the CHRONECT Workstation MCPD is the GC-MS system. Here, a Triple Quad GC-MS is preferably used. As a complete system, the workstation can be supplied with an EVOQ GC-TQ MS from Bruker. It is also possible to install the workstation on existing GC-MS systems. All major manufacturers are supported.

The AOCS Cd 29 a-c methods can also be operated with single quadrupole GC-MS systems. However, the achievable sensitivities are lower than with triple quadrupole devices. In some cases, not all sensitivity's for special foods such as infant formula can be reached.

To ensure the stability of the analysis, the CHRONECT Workstation MCPD is supplied

with a specially adapted backflush kit for back-flushing matrix components. This kit is installed into the GC-MS instrument during installation.



Figure 1: CHRONECT Workstation MCPD with Bruker GC-TQ MS.



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Figure 2: CHRONECT Workstation MCPD with Shimadzu GCMS-TQ.



Figure 3: CHRONECT Workstation MCPD with Agilent TQ GC/MS.

Analytical performance

The CHRONECT Workstation MCPD can process edible oils and fats directly. Fats are melted in the system prior to analysis. For compound foods, fat extraction must be performed beforehand. In this case, the starting point for automation is the fat extract. Depending on the method used, the CHRONECT Workstation MCPD with a TQMS reaches a limit of determination of 25 µg/kg in oil. For compound foods the limit of determination depends on the fat content. In fat extract 25 µg/kg is also reached. The use of sample robots with Robotic Tool Change technology ensures that there is no carryover between individual samples. The entire workflow and all consumables are also optimized for the lowest possible blank values.

Commissioning

In order to ensure that the systems operate without any problems, CHRONECT workstations are put into operation in advance. Within the scope of a comprehensive Factory Acceptance Test (FAT), not only the correct technical operation but also the analytical performance is checked. After installation, this test

run is repeated in a Site Acceptance Test (SAT) in the customer laboratory.

In this way the analytical accuracy is proven. The system is ready for use immediately after installation. The concept of FAT/SAT ensures that the systems are directly integrated into the laboratory workflow and are used productively as quickly as possible. Training and maintenance offers ensure the permanent uptime and ensure that the necessary knowledge for the operation of the system is available even in case of personnel changes.

Summary

The CHRONECT Workstation MCPD offers automation for all four current GC-MS methods for the determination of 3-MCPD, 2-MCPD and glycidyl esters. Due to the manufacturer-independent concept it fits into every laboratory environment without the need to learn how to operate new software packages for instrument control and data analysis. The support of all four methods makes it possible to retrofit missing modules and to implement current developments in analytics into an existing system. This offers the user the greatest possible investment security.

The concept of Factory and Site Acceptance Test ensures that the analytical performance is tested and documented directly after installation. This enables the CHRONECT Workstation MCPD to be quickly integrated into the laboratory workflow.

A support team specially trained in MCPD analysis offers users assistance at all times, even with application-related questions. All this makes the CHRONECT Workstation MCPD the ideal system for every laboratory dealing with this analysis.

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Technical data

Specifications	Values
Supported methods	<ul style="list-style-type: none"> • AOCS Cd 29a-13 (Unilever) • AOCS Cd 29b-13 (3-in-1) • AOCS Cd 29c-13 (DGF C-VI 18)* • Methode according to Zwagerman *modified as DGF Fast & Clean and original
Number of samples per day	depending on method and robot, up to 37 samples possible
Robot configurations	<ul style="list-style-type: none"> • width 120 cm, 160 or 200 cm • single or Dual head model (typical model 160 cm DualHead)
Supported GC-MS devices	<ul style="list-style-type: none"> • Bruker EVOQ GC-TQ (also as part of a complete offer) • Shimadzu TQ 8040/8050 series • Agilent 7000 series, Thermo TQ GC-MS
LOQ in fat content	better than 25 µg/kg for TQ GC-MS

The CHRONECT Workstation
MCPD is a development by
Axel Semrau.

Subject to technical changes

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