ANSWERING THE URGENT CALL FOR CHLORINATED PARAFFIN STANDARDS

^{13}C LABELLED CPs

Chloffin

ISO 17034
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What are chlorinated paraffins?

Chlorinated paraffins (CP) also known as polychlorinated n-alkanes (PCA), are produced as complex mixtures of thousands of isomers of different carbon chain length and chlorination degree.

CPs are subdivided according to their carbon chain length:

- Short chain CPs (SCCPs, C10–13)
- Medium chain CPs (MCCPs, C14–17)
- Long chain CPs (LCCPs, C>17)
- Very long chain CPs (vLCCPs, >C21)

The degree of CP chlorination can vary between 30 and 70 wt%

Where are they used?

CPs are used as high-temperature lubricants in metal-working machinery and as flame retardant plasticizers in vinyl plastics. Less common applications include the use as flame retardants in textiles, rubber, paints, adhesives and as sealants.

What are the concerns?

The total global production remains largely unknown, but is believed to exceed at least two million metric tonnes per year. CPs show resistance to degradation, and some show bioaccumulation and toxic potential. They are suspected to be carcinogenic to humans according to the International Agency for Research on Cancer (IARC).

Short-chain CPs have been prohibited by the Stockholm Convention on Persistent Organic Pollutants (POPs) in the EU since 2017 (Regulation (EC)850/2004) and placed on several monitoring lists such as the EU Water Framework Directive. However, due to their persistence and long-range transport, CPs will be in the environment for decades.

The CHLOFFIN project

In October 2019 the Eurostars CHLOFFIN project was launched to address the lack of suitable standards for CPs. The three year collaboration between Chiron, Vrije Universiteit and European Commission, Joint Research Centre aimed to deliver:

- 40 individual standards of CPs
- 8 ^{13}C labelled individual CPs
- 10 congener mixtures
- 1 matrix Certified Reference Material (CRM)

These RMs are intended for quantification of CPs, as internals standards and for helping distinguish the various congener groups according to carbon chain length and chlorine content.

Analytical challenges

One of the (many) challenges researchers face when determining CPs is the lack of suitable and generally accepted reference materials (RM). Current commercially available individual congener standards (native and labelled) have a chlorine pattern that is different than those found in industrial mixtures and the environment. CP mixture standards are not well-characterised nor purity assessed. The available labelled congener standards aimed for use as internal standard do not ionize on most commonly used detection methods (i.e. ESI and APCI). For longer chained CPs (C>17) standards in general are scarce. This all results in semi-quantitative analysis.

> "The lack of suitable standards for Chlorinated Paraffins has presented significant challenges for their analysis and regulation.

Why are internal standards used?

Quantitation is usually accomplished by measuring the response of an analyte relative to an internal standard (IS). IS are used to compensate for loss of analyte during sample preparation and for variation in mass spectrometric analysis. The assumption is that IS losses will be similar to losses of analyte. If a known quantity of IS is added to the unknown sample prior to any manipulations, the ratio of IS to analyte, remains constant, because the same fraction of each is lost in any operation. (Figure 1).

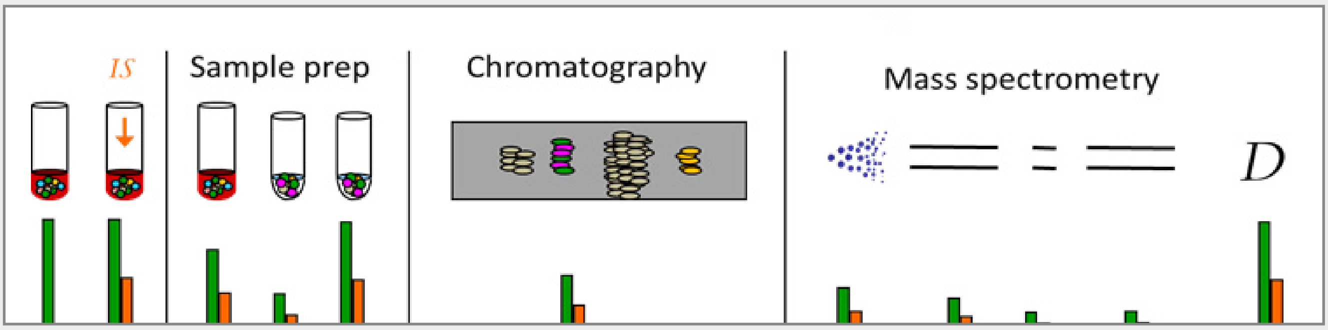

Figure 1: *Loss and fractionation can occur in the sample preparation, during chromatography, and in the mass spectrometer due to ion suppression.*

Different types of internal standard

There are different types of IS including unlabelled, structural analogues or stable isotope labelled internal standards (SILIS). SILIS behave chemically the same as the analyte, but differ in mass (^{2}H, ^{13}C, ^{15}N, ^{18}O). ^{13}C labelled IS are the gold standard choice for analytical chemists using LC-MS due to their correction for ion suppression, high precision, and accuracy.

Available reference materials

Chiron's new range of CHLOFFIN ^{13}C labelled IS for SCCP, MCCP and LCCP are presented here. CHLOFFIN RM are well-characterised, and purity assessed. They have similar chlorine patterns to CPs found in industrial mixtures and ionize on commonly used detection methods. They present an important step forward in the accurate quantification of CPs and harmonization of measurement results.

For a quotation, please contact us today at sales@chiron.no

SCCP ^{13}C internal standards

CLF15356.11-50-IO	1,2,4,5,8,9-Hexachloroundecane-9,10,11-$^{13}C_3$	$C_8{}^{13}C_3H_{18}Cl_6$	50 µg/mL in isooctane	1 mL
CLF15356.11-100-IO	1,2,4,5,8,9-Hexachloroundecane-9,10,11-$^{13}C_3$	$C_8{}^{13}C_3H_{18}Cl_6$	100 µg/mL in isooctane	1 mL
CLF15356.11-50-AN	1,2,4,5,8,9-Hexachloroundecane-9,10,11-$^{13}C_3$	$C_8{}^{13}C_3H_{18}Cl_6$	50 µg/mL in acetonitrile	1 mL
CLF15356.11-100-AN	1,2,4,5,8,9-Hexachloroundecane-9,10,11-$^{13}C_3$	$C_8{}^{13}C_3H_{18}C_{16}$	100 µg/mL in acetonitrile	1 mL
CLF15213.12-50-IO	1,2,5,6,9,10-Hexachlorododecane-10,11,12-$^{13}C_3$	$C_9{}^{13}C_3H_{20}C_{16}$	50 µg/mL in isooctane	1 mL
CLF15213.12-100-IO	1,2,5,6,9,10-Hexachlorododecane-10,11,12-$^{13}C_3$	$C_9{}^{13}C_3H_{20}C_{16}$	100 µg/mL in isooctane	1 mL
CLF15213.12-50-AN	1,2,5,6,9,10-Hexachlorododecane-10,11,12-$^{13}C_3$	$C_9{}^{13}C_3H_{20}C_{16}$	50 µg/mL in acetonitrile	1 mL
CLF15213.12-100-AN	1,2,5,6,9,10-Hexachlorododecane-10,11,12-$^{13}C_3$	$C_9{}^{13}C_3H_{20}C_{16}$	100 µg/mL in acetonitrile	1 mL
CLF15357.13-50-IO	2,3,5,6,10,11-Hexachlorotridecane-11,12,13-$^{13}C_3$	$C_8{}^{13}C_3H_{18}C_{16}$	50 µg/mL in isooctane	1 mL
CLF15357.13-100-IO	2,3,5,6,10,11-Hexachlorotridecane-11,12,13-$^{13}C_3$	$C_8{}^{13}C_3H_{18}C_{16}$	100 µg/mL in isooctane	1 mL
CLF15357.13-50-AN	2,3,5,6,10,11-Hexachlorotridecane-11,12,13-$^{13}C_3$	$C_8{}^{13}C_3H_{18}C_{16}$	50 µg/mL in acetonitrile	1 mL
CLF15357.13-100-AN	2,3,5,6,10,11-Hexachlorotridecane-11,12,13-$^{13}C_3$	$C_8{}^{13}C_3H_{18}C_{16}$	100 µg/mL in acetonitrile	1 mL
CLF15223.13-50-IO	3,4,6,7,10,11-Hexachlorotridecane-11,12,13-$^{13}C_3$	$C_{10}{}^{13}C_3H_{22}C_{16}$	50 µg/mL in isooctane	1 mL
CLF15223.13-100-IO	3,4,6,7,10,11-Hexachlorotridecane-11,12,13-$^{13}C_3$	$C_{10}{}^{13}C_3H_{22}C_{16}$	100 µg/mL in isooctane	1 mL
CLF15223.13-50-AN	3,4,6,7,10,11-Hexachlorotridecane-11,12,13-$^{13}C_3$	$C_{10}{}^{13}C_3H_{22}C_{16}$	50 µg/mL in acetonitrile	1 mL
CLF15223.13-100-AN	3,4,6,7,10,11-Hexachlorotridecane-11,12,13-$^{13}C_3$	$C_{10}{}^{13}C_3H_{22}C_{16}$	100 µg/mL in acetonitrile	1 mL

MCCP ^{13}C Internal Standards

CLF15214.14-50-IO	3,4,7,8,11,12-Hexachlorotetradecane-1,2,3-$^{13}C_3$	$C_{11}{}^{13}C_3H_{24}Cl_6$	50 µg/mL in isooctane	1 mL
CLF15214.14-100-IO	3,4,7,8,11,12-Hexachlorotetradecane-1,2,3-$^{13}C_3$	$C_{11}{}^{13}C_3H_{24}Cl_6$	100 µg/mL in isooctane	1 mL
CLF15214.14-50-AN	3,4,7,8,11,12-Hexachlorotetradecane-1,2,3-$^{13}C_3$	$C_{11}{}^{13}C_3H_{24}Cl_6$	50 µg/mL in acetonitrile	1 mL
CLF15214.14-100-AN	3,4,7,8,11,12-Hexachlorotetradecane-1,2,3-$^{13}C_3$	$C_{11}{}^{13}C_3H_{24}Cl_6$	100 µg/mL in acetonitrile	1 mL
CLF15224.15-50-IO	3,4,7,8,12,13-Hexachloropentadecane-13,14,15-$^{13}C_3$	$C_{12}{}^{13}C_3H_{26}Cl_6$	50 µg/mL in isooctane	1 mL
CLF15224.15-100-IO	3,4,7,8,12,13-Hexachloropentadecane-13,14,15-$^{13}C_3$	$C_{12}{}^{13}C_3H_{26}Cl_6$	100 µg/mL in isooctane	1 mL
CLF15224.15-50-AN	3,4,7,8,12,13-Hexachloropentadecane-13,14,15-$^{13}C_3$	$C_{12}{}^{13}C_3H_{26}Cl_6$	50 µg/mL in acetonitrile	1 mL
CLF15224.15-100-AN	3,4,7,8,12,13-Hexachloropentadecane-13,14,15-$^{13}C_3$	$C_{12}{}^{13}C_3H_{26}Cl_6$	100 µg/mL in acetonitrile	1 mL
CLF15215.16-50-IO	1,2,8,9,13,14-Hexachlorohexadecane-14,15,16-$^{13}C_3$	$C_{13}{}^{13}C_3H_{28}Cl_6$	50 µg/mL in isooctane	1 mL
CLF15215.16-100-IO	1,2,8,9,13,14-Hexachlorohexadecane-14,15,16-$^{13}C_3$	$C_{13}{}^{13}C_3H_{28}Cl_6$	100 µg/mL in isooctane	1 mL
CLF15215.16-50-AN	1,2,8,9,13,14-Hexachlorohexadecane-14,15,16-$^{13}C_3$	$C_{13}{}^{13}C_3H_{28}Cl_6$	50 µg/mL in acetonitrile	1 mL
CLF15215.16-100-AN	1,2,8,9,13,14-Hexachlorohexadecane-14,15,16-$^{13}C_3$	$C_{13}{}^{13}C_3H_{28}Cl_6$	100 µg/mL in acetonitrile	1 mL

LCCP ^{13}C internal standards

CLF15338.21-50-IO	3,4,6,7,9,10,18,19-Octachlorohenicosane-19,20,21-$^{13}C_3$	$C_{18}{}^{13}C_3H_{36}Cl_8$	50 µg/mL in isooctane	1 mL
CLF15338.21-100-IO	3,4,6,7,9,10,18,19-Octachlorohenicosane-19,20,21-$^{13}C_3$	$C_{18}{}^{13}C_3H_{36}Cl_8$	100 µg/mL in isooctane	1 mL
CLF15338.21-50-AN	3,4,6,7,9,10,18,19-Octachlorohenicosane-19,20,21-$^{13}C_3$	$C_{18}{}^{13}C_3H_{36}Cl_8$	50 µg/mL in acetonitrile	1 mL
CLF15338.21-100-AN	3,4,6,7,9,10,18,19-Octachlorohenicosane-19,20,21-$^{13}C_3$	$C_{18}{}^{13}C_3H_{36}Cl_8$	100 µg/mL in acetonitrile	1 mL

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