

ANSWERING THE URGENT CALL FOR CHLORINATED PARAFFIN STANDARDS



NATIVE INDIVIDUAL CONGENERS

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:

- Very short chain CPs (vSCCPs, C6–9)
- 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.

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 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 Native individual congener standards of CPs

8 ¹³C labelled individual congener standards of CPs

10 Single chain mixtures

1 Matrix Certified Reference Material (CRM)

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

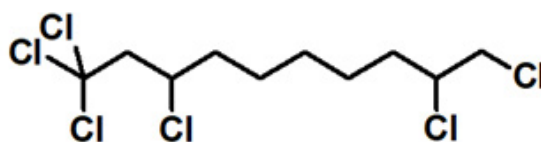




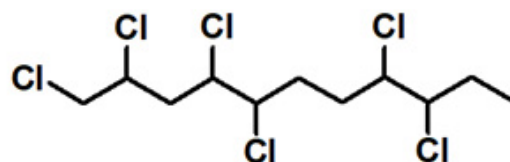
A new generation of reference materials

For ease of differentiation, Chiron have divided the available CP reference materials into three generations. The 1st generation products were developed by Chiron in the early 2000's, and some are recommended as internal standards in the ISO 12010 method for water quality determination, due to their absence in commercial products and different elution. The 2nd generation have one or two chlorines at the end of the chain and are only a minor constituent in commercial mixes. The 3rd generation products – produced through the CHLOFFIN project – are well-characterised, and purity assessed. They have similar chlorine patterns to CPs found in industrial mixtures and ionize on commonly used detection methods. These 3rd generation standards are useful in the quantification of CPs as well as helping in distinguishing the various congener groups according to carbon chain length and chlorine content. They present an important step forward in the accurate quantification of CPs and harmonization of measurement results.

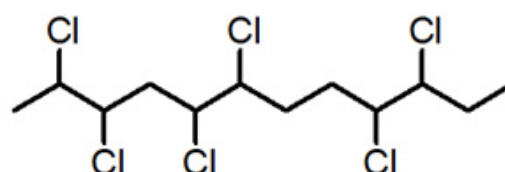
1st Generation: 3+ terminal and geminal chlorines > Not seen in commercial products



2nd Generation: 1 or 2 terminal chlorines > Minor constituent of commercial products



3rd Generation: No terminal chlorines > Major constituent of commercial products




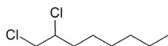
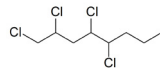
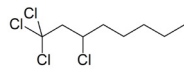
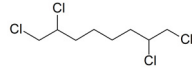
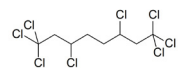
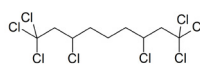
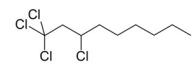
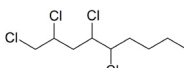
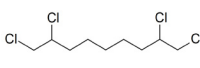
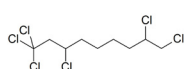
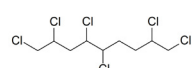
Available reference materials

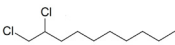
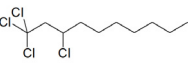
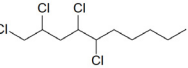
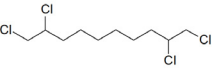
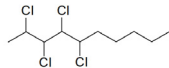
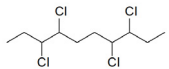
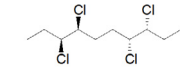
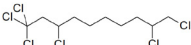
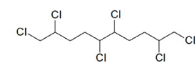
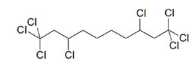
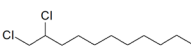
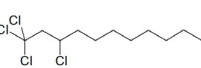
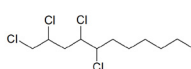
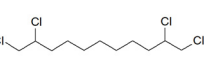
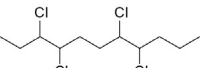
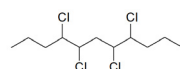
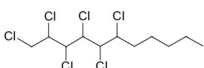
Chiron's complete range of CHLOFFIN individual congener standards are presented here.

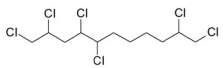
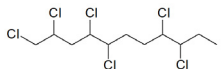
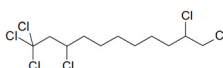
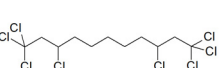
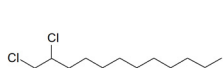
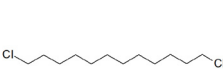


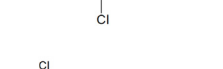

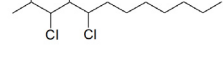
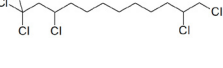
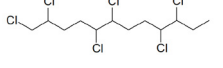
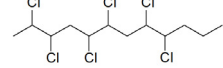
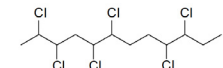
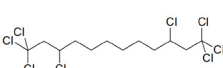
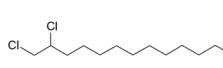
Individual SCCPs, MCCPs and LCCPs have been prepared by chemical synthesis. The synthesis routes were designed to deliver individual CPs with defined chlorine position and number. The chemical structure is identified by NMR and MS techniques; The chemical purity is established by one or several of the following GC-based methods: GC-FID/MS, GC-MS-MS, high resolution GC-MS and GC-GC-MS.

Chiron's 3rd generation reference materials will enable more accurate CP measurements and are superior to the technical mixtures, which have historically been used as reference materials.

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

Generation	Chiron No.	Name	%Wt Cl	Mol. Formula	Structure	CAS
C6-C9 CPs (vSCCPs):						
3 rd	CLF12287.6	2,3,4,5-Tetrachlorohexane, stereoisomers mix	63.32	C ₆ H ₁₀ Cl ₄		N/A
2 nd	CLF1664.8	1,2-Dichlorooctane	38.72	C ₈ H ₁₆ Cl ₂		21948-46-9
2 nd	CLF13254.8	1,2,4,5-Tetrachlorooctane	58.27	C ₈ H ₁₄ Cl ₄		N/A
1 st	CLF1660.8	1,1,1,3-Tetrachlorooctane	58.27	C ₈ H ₁₄ Cl ₄		18088-13-6
2 nd	CLF1672.8	1,2,7,8-Tetrachlorooctane	58.27	C ₈ H ₁₄ Cl ₄		865306-19-0
1 st	CLF1656.8	1,1,1,3,6,8,8,8-Octachlorooctane	97.87	C ₈ H ₁₀ Cl ₈		61856-19-7
2 nd	CLF1665.9	1,2-Dichlorononane	35.93	C ₉ H ₁₈ Cl ₂		56375-96-3
1 st	CLF1661.9	1,1,1,3-Tetrachlorononane	53.30	C ₉ H ₁₆ Cl ₄		1070-27-5
2 nd	CLF13396.9	1,2,4,5-Tetrachlorononane	53.30	C ₉ H ₁₆ Cl ₄		N/A
2 nd	CLF1673.9	1,2,8,9-Tetrachlorononane	53.30	C ₉ H ₁₆ Cl ₄		865306-20-3
1 st	CLF1658.9	1,1,1,3,8,9-Hexachlorononane	63.51	C ₉ H ₁₄ Cl ₆		865306-21-4
2 nd	CLF13898.9	1,2,4,5,8,9-Hexachlorononane	63.51	C ₉ H ₁₄ Cl ₆		N/A

Generation	Chiron No.	Name	%Wt Cl	Mol. Formula	Structure	CAS
C10-C13 CPs (SCCPs):						
2 nd	CLF1666.10	1,2-Dichlorodecane	33.58	C ₁₀ H ₂₀ Cl ₂		34619-32-4
1 st	CLF1662.10	1,1,3-Tetrachlorodecane	50.64	C ₁₀ H ₁₈ Cl ₄		51755-60-3
2 nd	CLF13255.10	1,2,4,5-Tetrachlorodecane, stereoisomers mix	50.64	C ₁₀ H ₁₈ Cl ₄		N/A
2 nd	CLF1671.10	1,2,9,10-Tetrachlorodecane	50.64	C ₁₀ H ₁₈ Cl ₄		205646-11-3
3 rd	CLF12590.10	2,3,4,5-Tetrachlorodecane, stereoisomers mix	50.64	C ₁₀ H ₁₈ Cl ₄		N/A
3 rd	CLF14965.10	3,4,7,8-Tetrachlorodecane, isomer mixture	50.64	C ₁₀ H ₁₈ Cl ₄		N/A
3 rd	CLF15252.10	(3R,4R,7S,8S)-rel-3,4,7,8-Tetrachlorodecane	50.64	C ₁₀ H ₁₈ Cl ₄		N/A
1 st	CLF1659.10	1,1,3,9,10-Hexachlorodecane	61.97	C ₁₀ H ₁₆ Cl ₆		601523-26-6
2 nd	CLF12284.10	1,2,5,6,9,10-Hexachlorodecane	61.97	C ₁₀ H ₁₆ Cl ₆		189350-94-5
1 st	CLF1622.10	1,1,3,8,10,10-Octachlorodecane	67.88	C ₁₀ H ₁₄ Cl ₈		601523-23-3
2 nd	CLF1667.11	1,2-Dichloroundecane	31.49	C ₁₁ H ₂₂ Cl ₂		81246-86-8
1 st	CLF1649.11	1,1,3-Tetrachloroundecane	48.22	C ₁₁ H ₂₀ Cl ₄		56686-55-6
2 nd	CLF13397.11	1,2,4,5-Tetrachloroundecane	48.22	C ₁₁ H ₂₀ Cl ₄		N/A
2 nd	CLF1674.11	1,2,10,11-Tetrachloroundecane	48.22	C ₁₁ H ₂₀ Cl ₄		210049-49-3
3 rd	CLF15181.11	3,4,7,8-Tetrachloroundecane, stereoisomers mix	48.22	C ₁₁ H ₂₀ Cl ₄		N/A
3 rd	CLF12728.11	4,5,7,8-Tetrachloroundecane, stereoisomers mix	48.22	C ₁₁ H ₂₀ Cl ₄		N/A
2 nd	CLF12285.11	1,2,3,4,5,6-Hexachloroundecane, stereoisomers mix	58.60	C ₁₁ H ₁₈ Cl ₆		N/A

Generation	Chiron No.	Name	%Wt Cl	Mol. Formula	Structure	CAS
C10-C13 CPs (SCCPs):						
2 nd	CLF13900.11	1,2,4,5,9,10-Hexachloroundecane, stereoisomers mix	58.60	C ₁₁ H ₁₈ Cl ₆		N/A
2 nd	CLF14069.11	1,2,4,5,8,9-Hexachloroundecane	58.60	C ₁₁ H ₁₈ Cl ₆		N/A
1 st	CLF1650.11	1,1,1,3,10,11-Hexachloroundecane	58.60	C ₁₁ H ₁₈ Cl ₆		601523-28-8
1 st	CLF1623.11	1,1,1,3,9,11,11-Octachloroundecane	65.67	C ₁₁ H ₁₆ Cl ₈		601523-25-5
2 nd	CLF1668.12	1,2-Dichlorododecane	29.64	C ₁₂ H ₂₄ Cl ₂		75121-23-2
2 nd	CLF1663.12	1,12-Dichlorododecane	29.64	C ₁₂ H ₂₄ Cl ₂		3922-28-9
1 st	CLF1651.12	1,1,1,3-Tetrachlorododecane	46.03	C ₁₂ H ₂₂ Cl ₄		14983-60-9
2 nd	CLF13398.12	1,2,4,5-Tetrachlorododecane	46.03	C ₁₂ H ₂₂ Cl ₄		N/A
2 nd	CLF1675.12	1,2,11,12-Tetrachlorododecane	46.03	C ₁₂ H ₂₂ Cl ₄		210115-98-3
3 rd	CLF12425.12	2,3,4,5-Tetrachlorododecane, stereoisomers mix	46.03	C ₁₂ H ₂₂ Cl ₄		N/A
1 st	CLF1652.12	1,1,1,3,11,12-Hexachlorododecane	56.42	C ₁₂ H ₂₀ Cl ₆		865306-22-5
2 nd	CLF14072.12	1,2,5,6,9,10-Hexachlorododecane	56.42	C ₁₂ H ₂₀ Cl ₆		N/A
3 rd	CLF14495.12	2,3,5,6,8,9-Hexachlorododecane	56.42	C ₁₂ H ₂₀ Cl ₆		N/A
3 rd	CLF15009.12	2,3,5,6,9,10-Hexachlorododecane; stereoisomers mix	56.42	C ₁₂ H ₂₀ Cl ₆		N/A
1 st	CLF1624.12	1,1,1,3,10,12,12,12-Octachlorododecane	63.60	C ₁₂ H ₁₈ Cl ₈		601523-21-1
2 nd	CLF1669.13	1,2-Dichlorotridecane	28.00	C ₁₃ H ₂₆ Cl ₂		701920-72-1
1 st	CLF1653.13	1,1,1,3-Tetrachlorotridecane	44.02	C ₁₃ H ₂₄ Cl ₄		67095-50-5

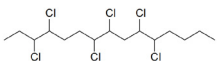

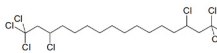
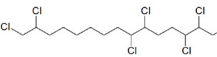
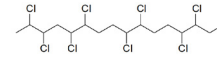
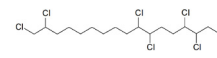
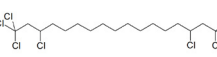
Generation	Chiron No.	Name	%Wt Cl	Mol. Formula	Structure	CAS
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C10-C13 CPs (SCCPs):

2 nd	CLF13399.13	1,2,4,5-Tetrachlorotridecane	44.02	C ₁₃ H ₂₄ Cl ₄		N/A
1 st	CLF1654.13	1,1,1,3,12,13-Hexachlorotridecane	54.40	C ₁₃ H ₂₂ Cl ₆		865306-23-6
3 rd	CLF14496.13	2,3,6,7,10,11-Hexachlorotridecane	54.40	C ₁₃ H ₂₂ Cl ₆		N/A
2 nd	CLF15222.13	1,2,4,5,8,9-Hexachlorotridecane	54.40	C ₁₃ H ₂₂ Cl ₆		N/A
2 nd	CLF14131.13	1,2,6,7,10,11-Hexachlorotridecane	54.40	C ₁₃ H ₂₂ Cl ₆		N/A
1 st	CLF1625.13	1,1,1,3,11,13,13,13-Octachlorotridecane	61.67	C ₁₃ H ₂₀ Cl ₈		865306-24-7

C14-C17 CPs (MCCPs):

2 nd	CLF1670.14	1,2-Dichlorotetradecane	26.53	C ₁₄ H ₂₈ Cl ₂		701920-83-4
1 st	CLF1676.14	1,1,1,3-Tetrachlorotetradecane	42.18	C ₁₄ H ₂₆ Cl ₄		865306-25-8
2 nd	CLF13256.14	1,2,4,5-Tetrachlorotetradecane	42.18	C ₁₄ H ₂₆ Cl ₄		N/A
2 nd	CLF1677.14	1,2,13,14-Tetrachlorotetradecane	42.18	C ₁₄ H ₂₆ Cl ₄		221155-23-3
2 nd	CLF14132.14	1,2,7,8,11,12-Hexachlorotetradecane	52.51	C ₁₄ H ₂₄ Cl ₆		N/A
3 rd	CLF14796.14	3,4,7,8,11,12-Hexachlorotetradecane, stereoisomer mix	52.51	C ₁₄ H ₂₄ Cl ₆		N/A
1 st	CLF1678.14	1,1,1,3,12,14,14,14-Octachlorotetradecane	59.84	C ₁₄ H ₂₂ Cl ₈		865306-26-9
2 nd	CLF14068.14	1,2,5,6,9,10,13,14-Octachlorotetradecane	59.84	C ₁₄ H ₂₂ Cl ₈		N/A
1 st	CLF8506.15	1,1,1,3,14,15-Hexachloropentadecane	50.76	C ₁₅ H ₂₆ Cl ₆		N/A
2 nd	CLF14133.15	1,2,8,9,12,13-Hexachloropentadecane, stereoisomers mix	50.76	C ₁₅ H ₂₆ Cl ₆		N/A
2 nd	CLF14475.15	1,2,8,9,12,13-Hexachloropentadecane, stereoisomers mix, cryst.	50.76	C ₁₅ H ₂₆ Cl ₆		N/A
3 rd	CLF14741.15	3,4,7,8,12,13-Hexachloropentadecane, stereoisomers mix	50.76	C ₁₅ H ₂₆ Cl ₆		N/A

Generation	Chiron No.	Name	%Wt Cl	Mol. Formula	Structure	CAS
C14-C17 CPs (MCCPs):						
3 rd	CLF14497.16	3,4,7,8,10,11-Hexachloropentadecane, stereoisomers mix cryst.	50.76	C ₁₅ H ₂₆ Cl ₆		N/A
2 nd	CLF13596.16	1-Chlorohexadecane	13.59	C ₁₆ H ₃₃ Cl		4860-03-1
1 st	CLF8507.16	1,1,3,14,16,16-Octachlorohexadecane	56.50	C ₁₆ H ₂₆ Cl ₈		N/A
2 nd	CLF14134.16	1,2,9,10,13,14-Hexachlorohexadecane, stereoisomers mix	49.11	C ₁₆ H ₂₈ Cl ₆		N/A
3 rd	CLF14423.16	2,3,5,6,9,10,13,14-Octachlorohexadecane	56.50	C ₁₆ H ₂₆ Cl ₈		N/A
2 nd	CLF14135.17	1,2,10,11,14,15-Hexachloroheptadecane, stereoisomers mix	47.57	C ₁₇ H ₃₀ Cl ₆		N/A
1 st	CLF8508.17	1,1,3,15,17,17-Octachloroheptadecane	54.96	C ₁₇ H ₂₈ Cl ₈		N/A

C18+ CPs (LCCPs):

2 nd	CLF2051.18	1-Chlorooctadecane	12.27	C ₁₈ H ₃₆ Cl ₂		3386-33-2
2 nd	CLF14136.18	1,2,11,12,15,16-Hexachlorooctadecane, stereoisomers mix	46.12	C ₁₈ H ₃₂ Cl ₆		N/A
3 rd	CLF14071.18	3,4,6,7,9,10,18-Heptachlorooctadecane	50.07	C ₁₈ H ₃₁ Cl ₇		N/A
1 st	CLF8509.18	1,1,3,16,18,18-Octachlorooctadecane	53.51	C ₁₈ H ₃₀ Cl ₈		N/A
2 nd	CLF14070.18	1,2,9,10,12,13,15,16-Octachlorooctadecane	53.51	C ₁₈ H ₃₀ Cl ₈		N/A
1 st	CLF8510.19	1,1,3,17,19,19-Octachlorononadecane	52.13	C ₁₉ H ₃₂ Cl ₈		N/A
1 st	CLF8511.20	1,1,3,18,20,20-Octachloroeicosane	50.82	C ₂₀ H ₃₄ Cl ₈		N/A



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