# New Standards for Chlorinated Paraffins – Eurostars CHLOFFIN Project

Poster ID: 3.07P.6


**Solveig Valderhaug,[1,2] Alexey Gorovoi,[1] Louise M. van Mourik,[3] Marina Ricci,[4] Sicco Brandsma,[3] Jenny Button,[1] Jacob de Boer,[3] Huiling Liu[1] and Jon E. Johansen[1]**

[1] Chiron AS, Stiklestadveien 1, N-7041 Trondheim, Norway

[2] Department of Chemistry, Norwegian University of Science and Technology (NTNU), 7491 Trondheim, Norway

[3] Department of Environment and Health (E&H), Vrije Universiteit, 1081HV, Amsterdam, the Netherlands

[4] European Commission, Joint Research Centre, Geel, Belgium

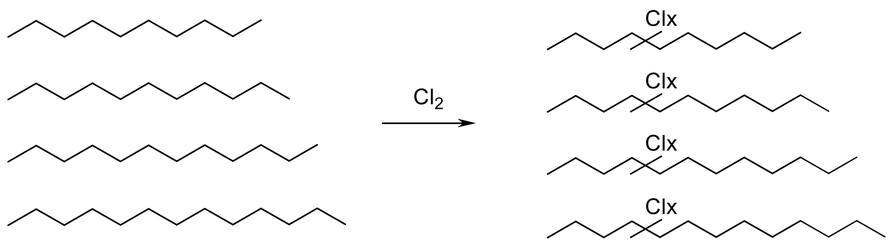

## Introduction:

- **CHLOFFIN project** (oct.2019 - oct.2022) is a collaboration between Chiron AS, the European Commission Joint Research Center (JRC) and the Vrije Universiteit of Amsterdam.
- The ultimate project goal is to develop reference materials for chlorinated paraffins (CPs) that are well-characterized for quantification.
- CPs are high production volume chemicals (> 3 million tonnes / yr) with persistent, bioaccumulative and toxic potential. Therefore it is important to monitor CPs, yet, no generally accepted and well characterized reference materials are commercially available to enable accurate analysis.
- The CHLOFFIN project will help expand the library of reference materials for CPs, including well-characterized single congener compounds and more complex mixtures similar to the industrial mixtures.

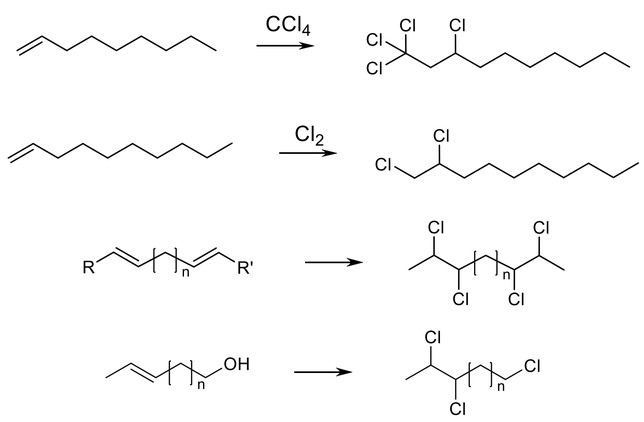
* For more information about analytical methods and certification, see poster ID: 3.07P.3

## Materials and Methods:

1. **The industrial mixtures are produced by direct chlorination, which afford complex product mixtures with low positional selectivity.**




2. **The synthesis of single regioisomers include chlorination of alkenes and conversion of alcohols.**

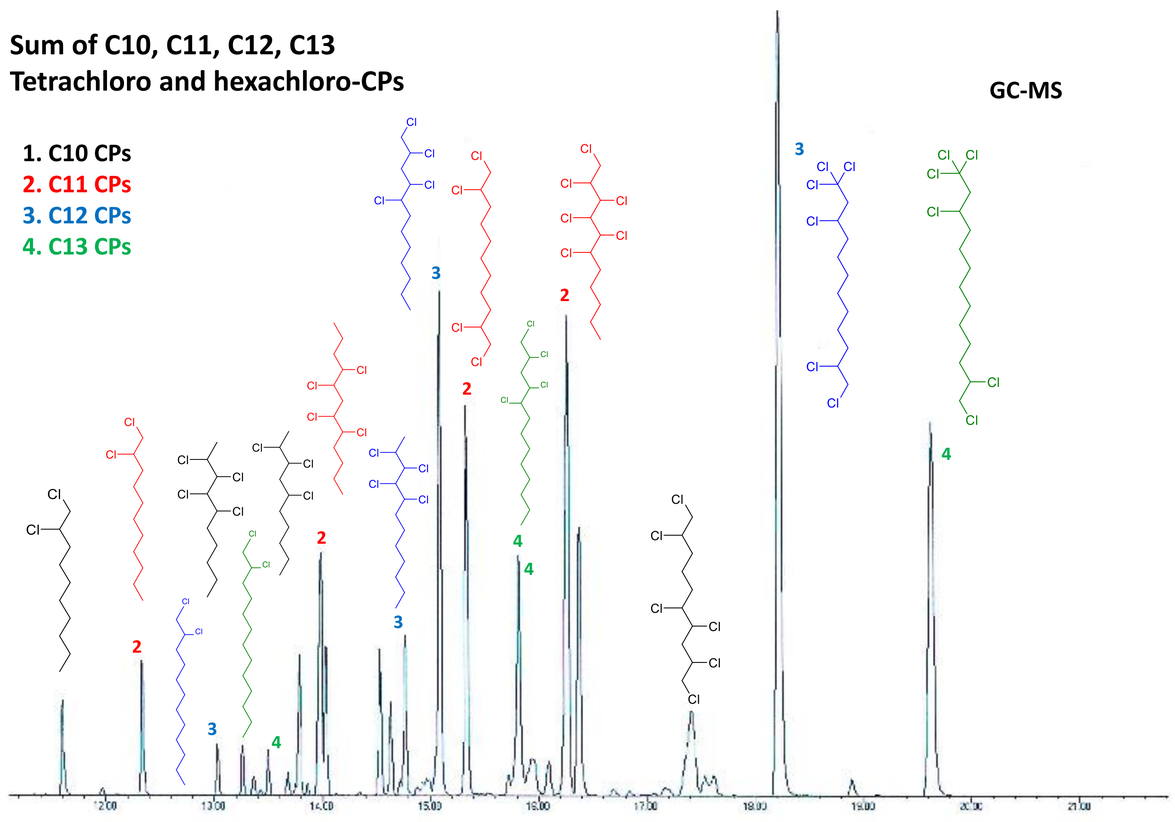



3. **Prepare reference material as a mixture of well-defined CP congeners.**

**Sum of C10, C11, C12, C13**
**Tetrachloro and hexachloro-CPs**

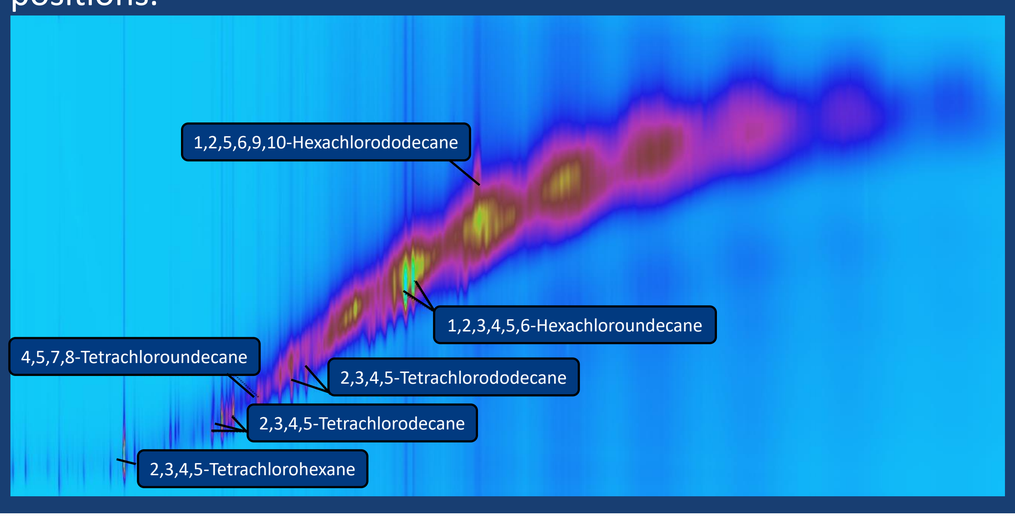
**GC-MS**

**1. C10 CPs**
**2. C11 CPs**
**3. C12 CPs**
**4. C13 CPs**

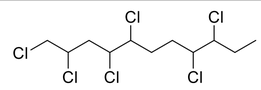
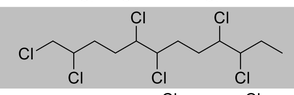
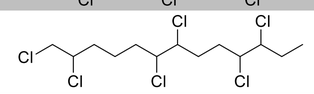
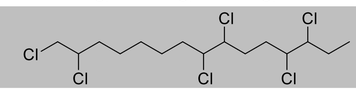
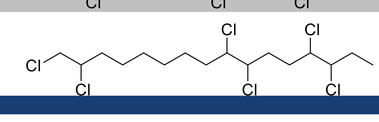


## Results and Discussions:

- A total of 5 new single CP congeners have been synthesized.
- These range from C11-16 with 6 chlorines attached in specific positions.
- With the recent synthetic approach, a variety of single CP congeners can be achieved by altering the chain lengths, amount of double bonds and positions.




- The synthesized single CP congeners are evaluated by comprehensive two-dimensional gas chromatography to establish if their chlorine arrangements are similar to the industrial mixtures.
- CHLOFFIN will also produce CP mixtures similar to industrial products and $^{13}$C-labelled CPs as internal standards.

| New CHLOFFIN Products | Structure |
|---|---|
| 1,2,4,5,8,9-Hexachloroundecane |  |
| 1,2,5,6,9,10-Hexachlorododecane |  |
| 1,2,6,7,10,11-Hexachlorotridecane |  |
| 1,2,8,9,12,13-Hexachloropentadecane |  |
| 1,2,9,10,13,14-Hexachlorohexadecane |  |

## Conclusion:

- CHLOFFIN is working to fill the gap of suitable standards for the analysis of CPs.
- By the combined expertise of the parties involved, the library of CP standards will be expanded and evaluated.
- On-going work includes the production of new single compounds, mixtures as reference materials and $^{13}$C-labelled internal standards.


This project has received funding from the Eurostar-2 joint programme with co-funding from the European Union Horizon 2020 research and innovation programme

www.chloffin.eu