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Detection Identification Quantification of Chlorinated Paraffins

Bo Yuan

Department of Environmental Science, Stockholm University, Sweden

Virtual discussion meeting on chlorinated paraffins, VU AMSTERDAM, 27 August 2020

Analytica Chimica Acta 1074 (2019) 16–32

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journal homepage: www.elsevier.com/locate/aca

Review

Methods for trace analysis of short-, medium-, and long-chain chlorinated paraffins: Critical review and recommendations

Bo Yuan [a], Derek Muir [b], Matthew MacLeod [a, *]

[a] Department of Environmental Science and Analytical Chemistry, Stockholm University, Stockholm, Sweden
[b] Environment and Climate Change Canada, Burlington, ON, Canada

Erratum

Page 26, eq. (4) should be:

Concentration (SCCPs)
= RF (m/z 327) × Signal (m/z 327) + RF (m/z 423) × Signal (m/z 423) + additional term

S. Geiß et al. / *Microchemical Journal* 119 (2015) 30–39

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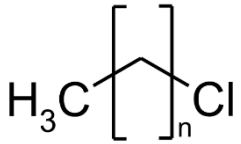
“CPs”



"CPs"

n = 1

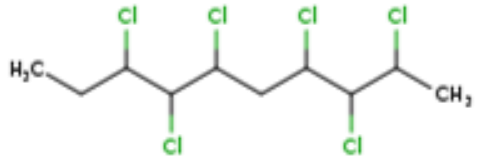
vSCCPs SCCPs MCCPs LCCPs

n = 4

Homologue $C_xH_{2x+2-z}Cl_z$

n = ~700

Postional isomer

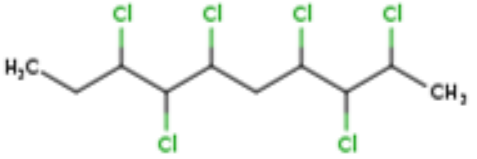


n = ~10,000 –

Composition of CPs

Category		Chain length, x=	$C_xH_{2x+2-z}Cl_z$, z =	Total number of positional isomers*
"CPs"	vSCCPs	6	1-6	35
		7	1-7	71
		8	1-8	135
		9	1-9	271
	SCCPs	10	1-10	527
		11	1-11	1 055
		12	1-12	2 079
		13	1-13	4 159
	MCCPs	14	1-14	8 255
		15	1-15	16 511
		16	1-16	32 895
		17	1-17	65 791
	LCCPs	18	1-18	131 327
		19	1-19	262 655
		20	1-20	524 799
		21	1-21	1 049 599
		22	1-22	2 098 175
		23	1-23	4 196 351
		24	1-24	8 390 655
		25	1-25	16 781 311
		26	1-26	33 558 527
		27	1-27	67 117 055
		28	1-28	134 225 919
		29	1-29	268 451 839
		30	1-30	536 887 295

*assuming no more than one chlorine atom bound to any carbon atom



Anal. Chem. (1997) 69, 2762-2771
Environ. Sci. Technol. 2020, 54, 7, 4356–4366
Environ. Sci. Technol. Lett. 2020, 7, 7, 496–503

Positional isomer

Category		Chain length, x=	$C_xH_{2x+2-z}Cl_z$, z =	Total number of positional isomers*
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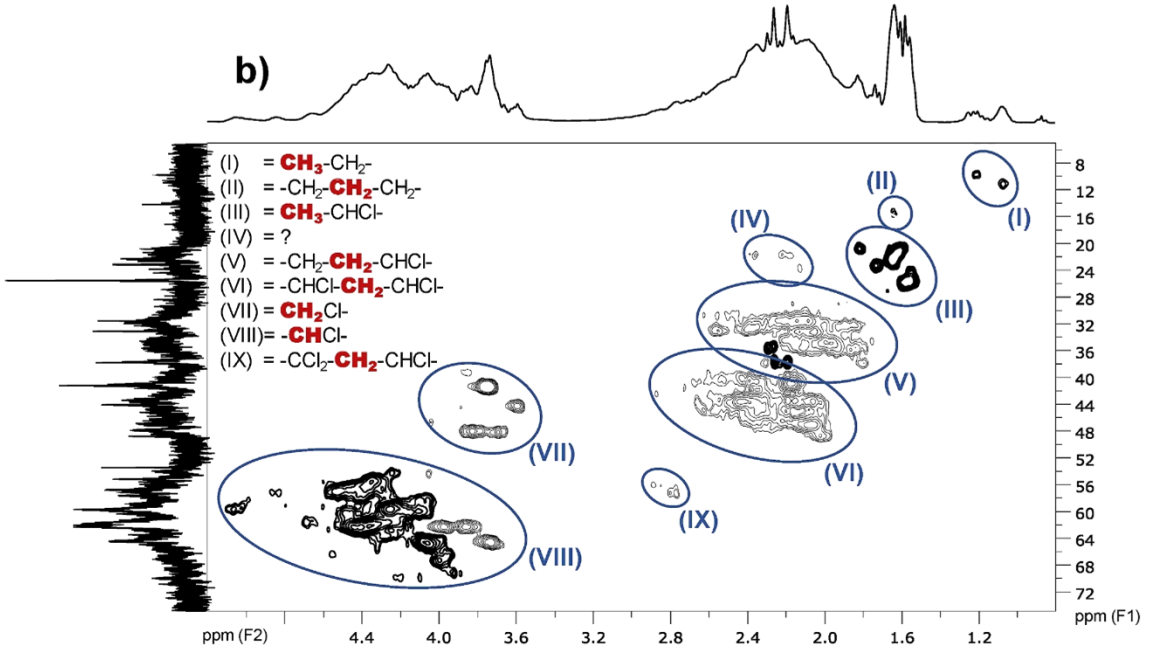
		27	1-27	67 117 055
		28	1-28	134 225 919
		29	1-29	268 451 839
		30	1-30	536 887 295

HSQC-NMR spectrum of C_{11}-CPs 62.6% Cl



MS: C_xCl_z, z>x

NMR: $-CCl_2-$ and $CHCl_2-$

Chemosphere (2019) 69, 2762-2771
Environ. Sci. Technol. 2017, 51, 15, 10633-10641

Positional isomer

Category		Chain length, x=	$C_xH_{2x+2-z}Cl_z$, z =	Total number of positional isomers*
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		27	1-27	67 117 055
		28	1-28	134 225 919
		29	1-29	268 451 839
		30	1-30	536 887 295

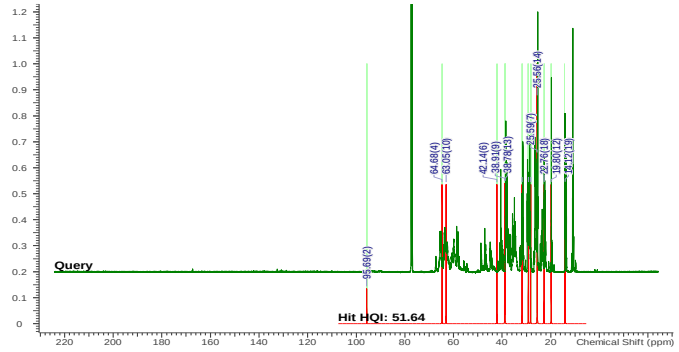
Chain length, x=	$C_xH_{2x+2-z}Cl_z$ z =	Total number of positional isomers**
14	1-12	**~800 000**

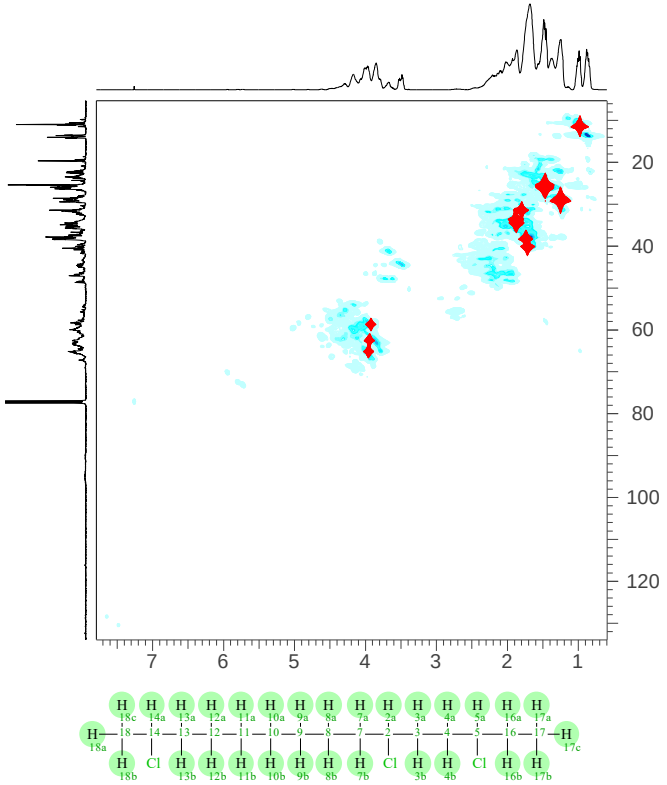
*assuming no more than one chlorine atom bound to any carbon atom

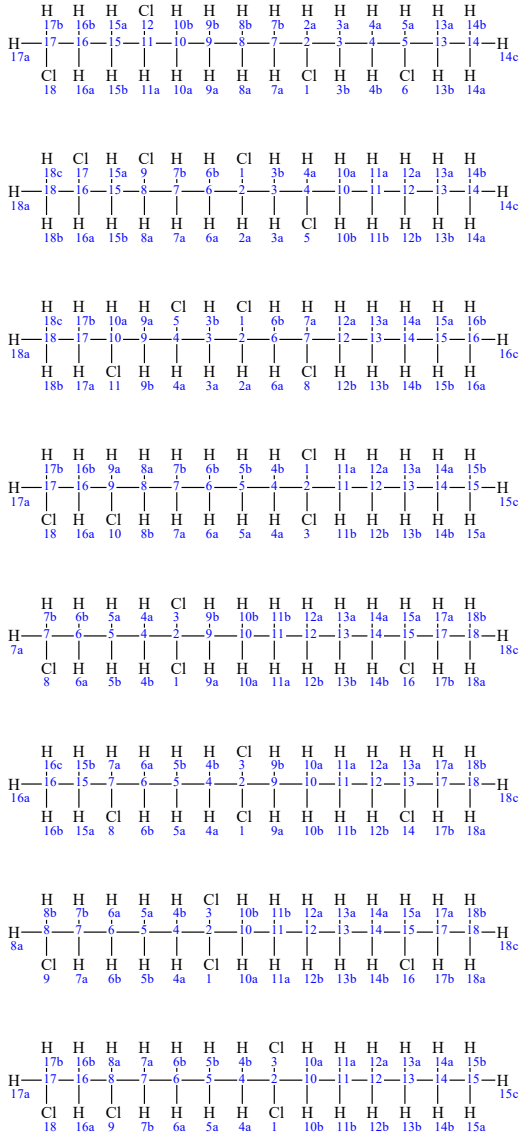
**taking $-CCl_2-$ into account

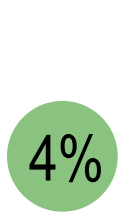
Anal. Chem. (1997) 69, 2762-2771
Environ. Sci. Technol. 2020, 54, 7, 4356–4366
Environ. Sci. Technol. Lett. 2020, 7, 7, 496–503

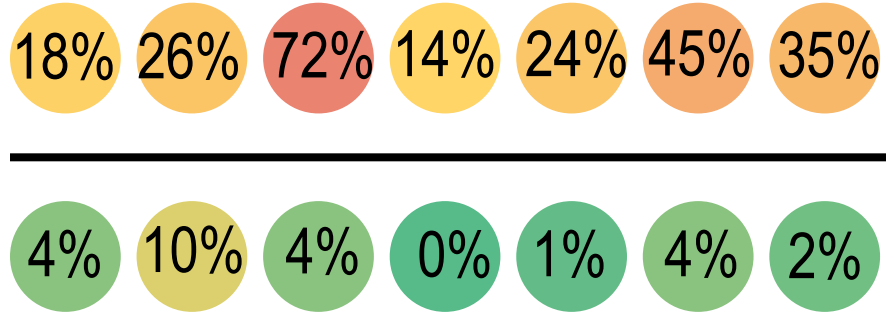
Positional selectivity











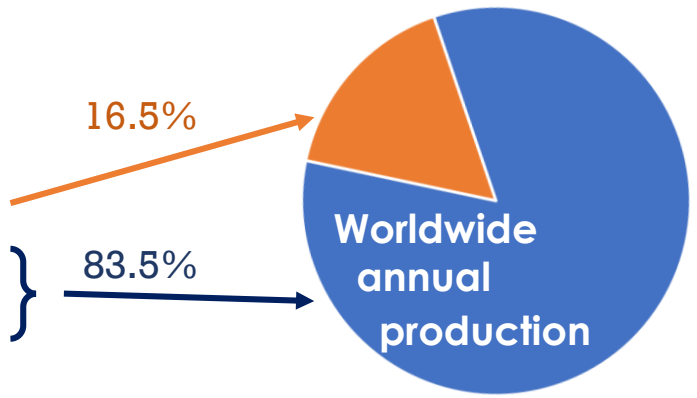
Experimental log K_{OW} (C_{15} 50 %Cl)	6.65
Predicted log K_{OW}	**6.77**
Predicted log K_{OW} based on assumed isomer composition	7.78

Environ. Sci. Technol. Lett. 2020, 7, 7, 496–503
Environ. Sci. Technol. 2011, 45, 2842–2849

Trace measurements

Category		chain length range	homologue
"CPs"	vSCCPs	6 ≤ x ≤ 9	~30 C_xCl_z
	SCCPs	10 ≤ x ≤ 13	~50 C_xCl_z
	MCCPs	14 ≤ x ≤ 17	~70 C_xCl_z
	LCCPs	18 ≤ x	~600 C_xCl_z

CPs vS/S/M/LCCPs C_x C_xCl_z



U.S. EPA (2015)
Environment Canada (2016)
Environ. Int. (2019) 130, 104955
Sci. Tot. Environ. (2016) 573, 1132-1146

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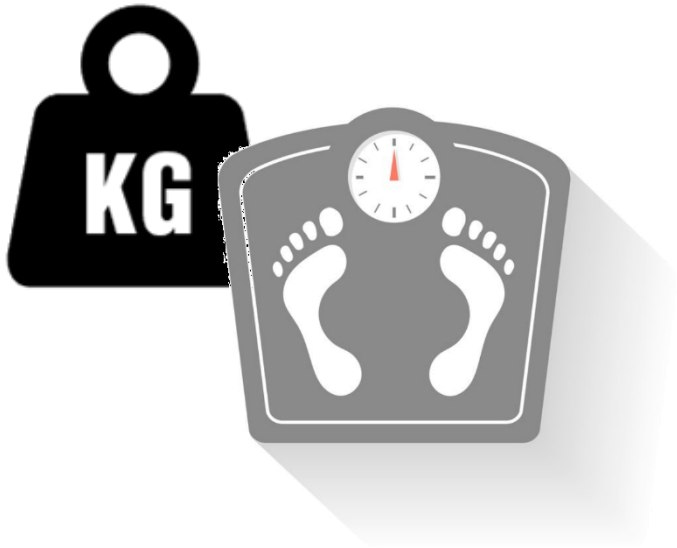
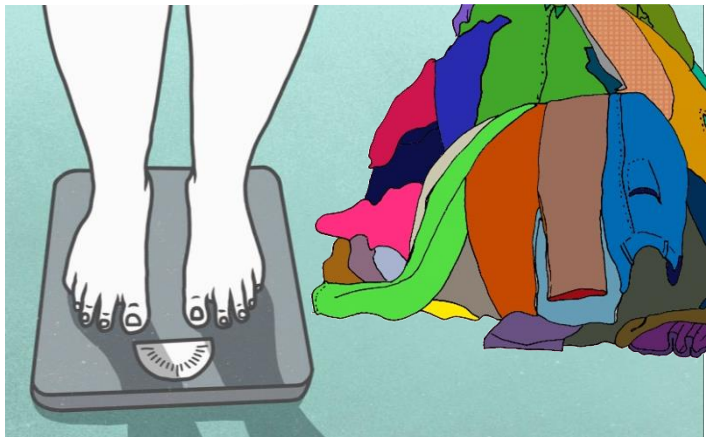
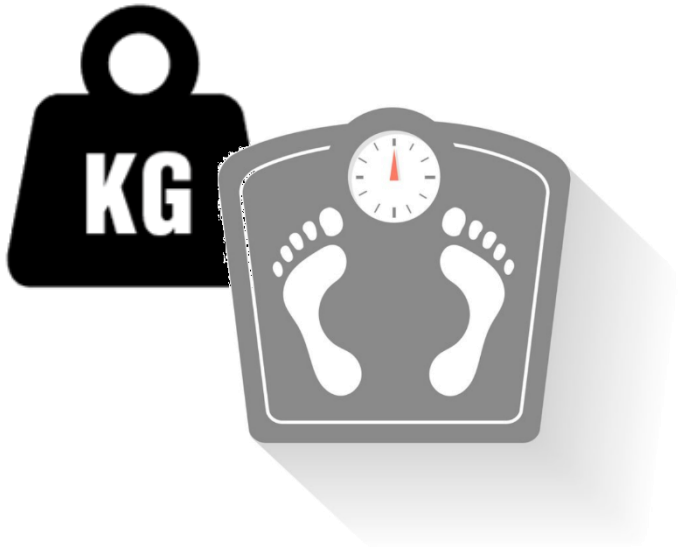
Detection	Identification	Quantification



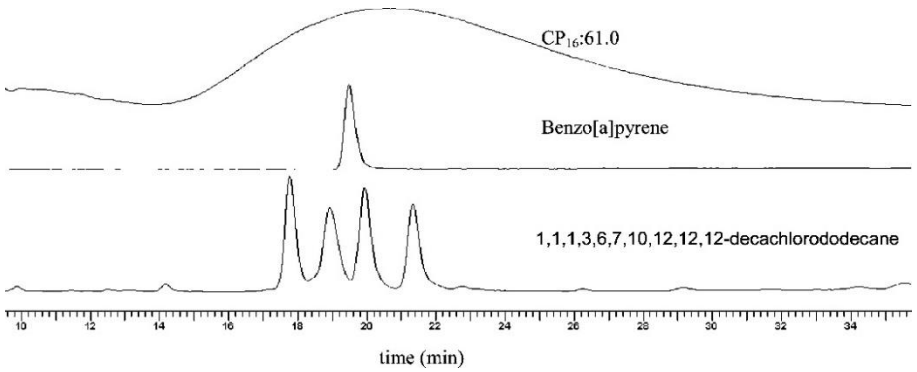


Detection: instrumentation

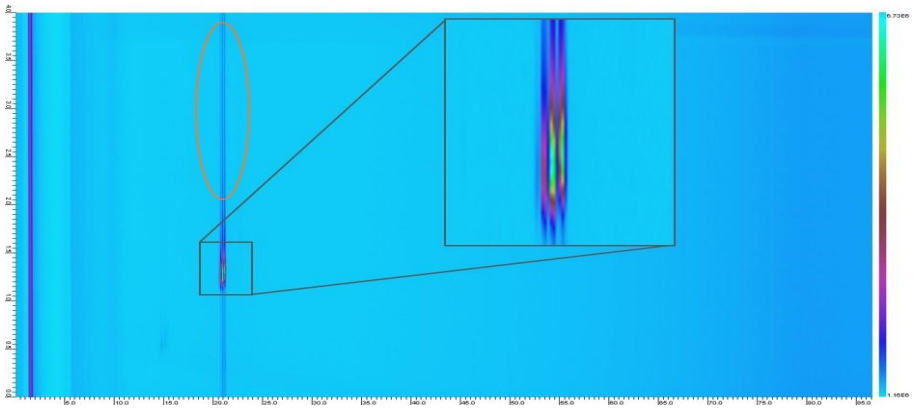


- GC-MS
- LC-MS

Chromatographic separation



HPLC chromatogram of 1,1,1,3,6,7,10,12,12,12-decachlorododecane, with four diastereomers.



GC×GC-μECD chromatogram of 2,5,6,9-Tetrachlorodecane, with three isomers.

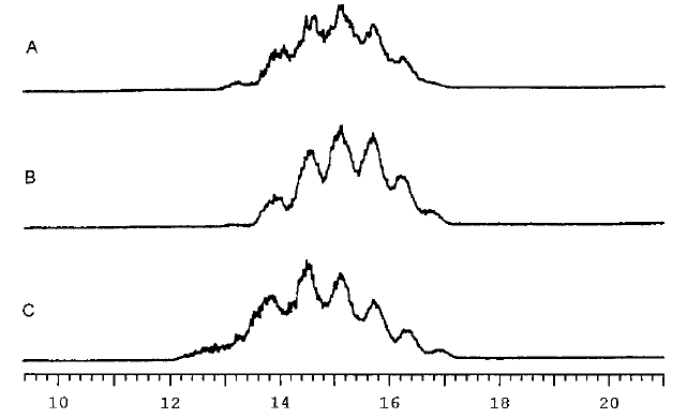
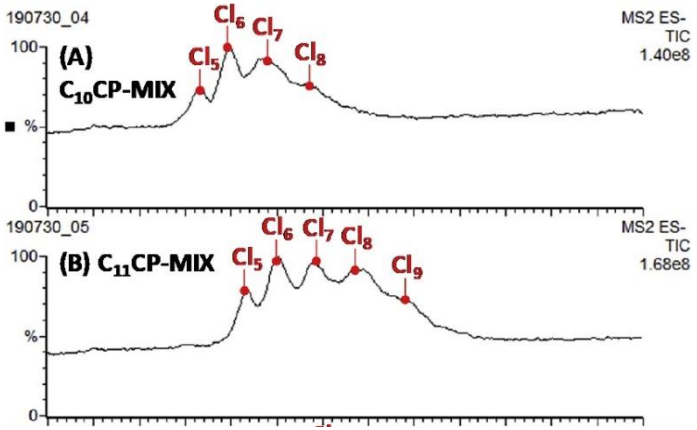


Figure 2. GC/ECNI-MS total ion chromatograms of CP11:66.5 (A), CP12:62 (B), and CP13:47 (C).



UHPLC chromatogram (ZORBAX SB-CN RRHD) of Cx mixture

Environ. Sci. Technol. 2011, 45, 2842–2849 *J. Chromatogr. A* 2020, 1610, 460550 *Anal. Chem*. 1999, 71, 20, 4498-4505 *Chemosphere*. 2020, 244, 125531

GC-ECNI-MS

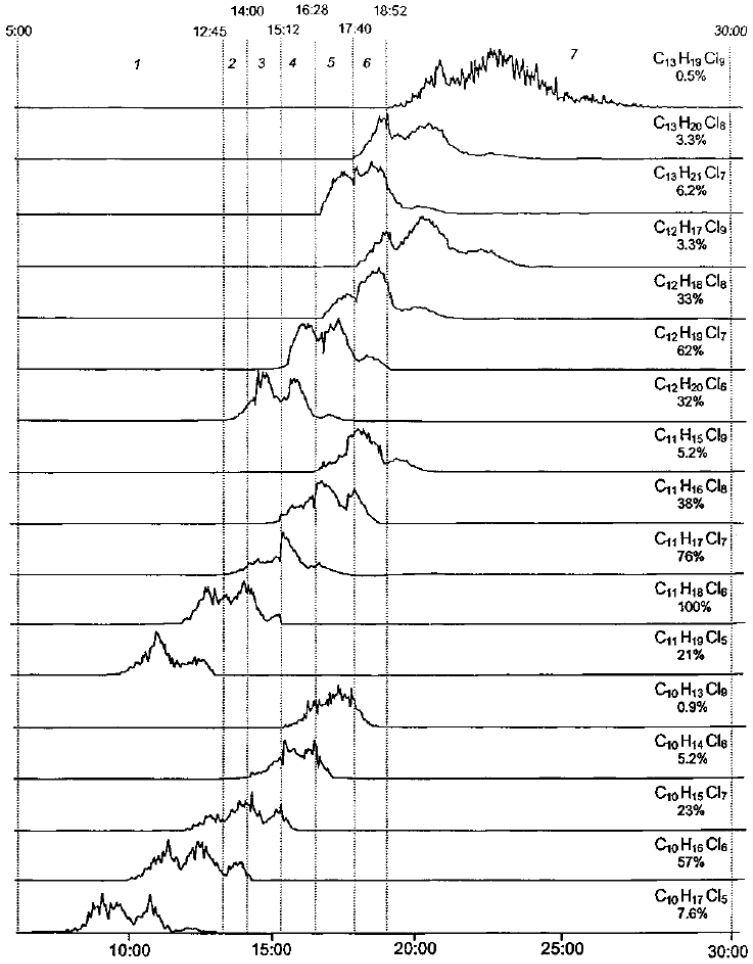


Figure 3. HRGC/ECNI-HRMS elution profiles of monitored ions in PCA-60 aligned to show the seven time windows used.

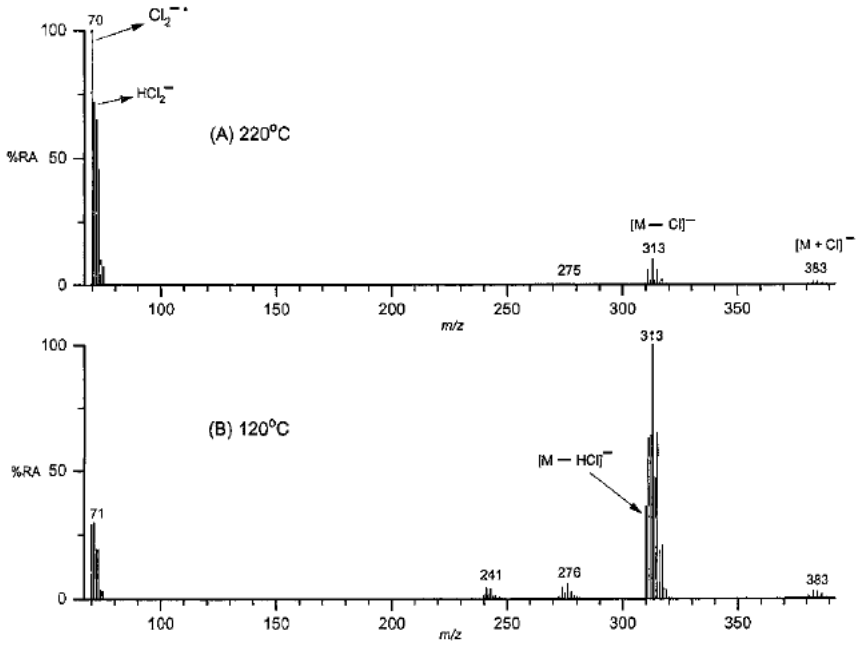


Figure 2. ECNI mass spectra of 1,2,5,6,9,10-hexachloro-*n*-decane at ion source temperatures of (a) 220 and (b) 120 °C.

[M – Cl]⁻

[M – HCl]⁻

[M + Cl]⁻

[M – HCl – Cl]⁻

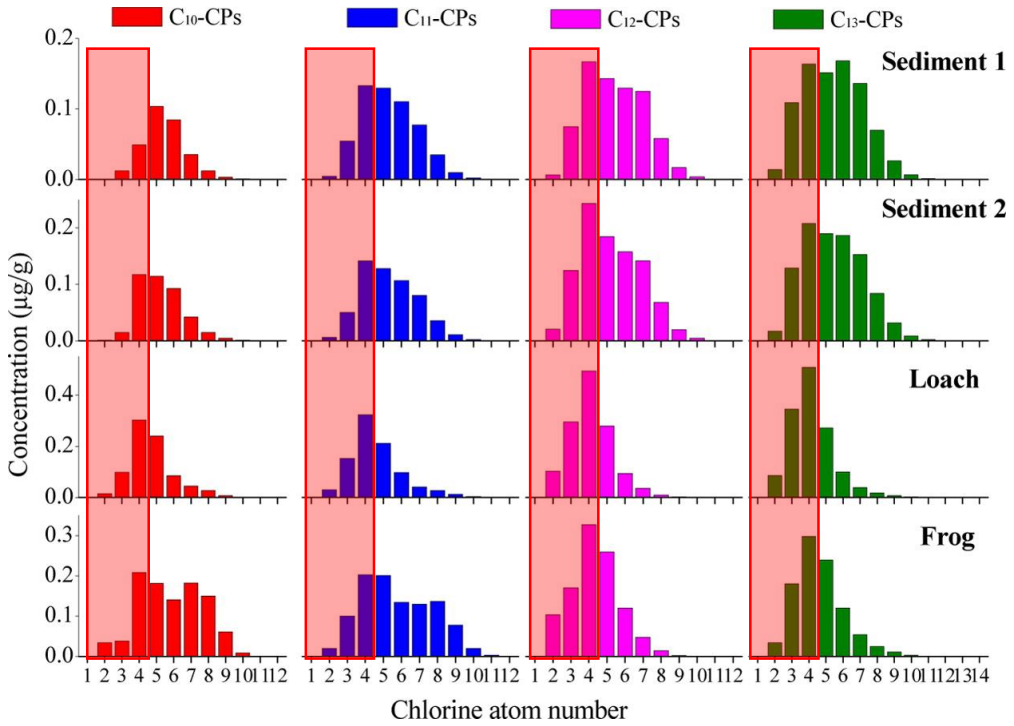
[M – 2Cl]⁻…

- not suitable for the analysis of longer-chain CPs because of their low volatility
- poor ionization efficiency for homologues with $Cl_{<5}$

Anal. Chem., 1997, 69 (14), 2762-2771 *Environ. Sci. Technol. Lett.* 2018, 5, 12, 708–717 *Chemosphere*. 2015, 136, 259-272

GC-ECNI-MS

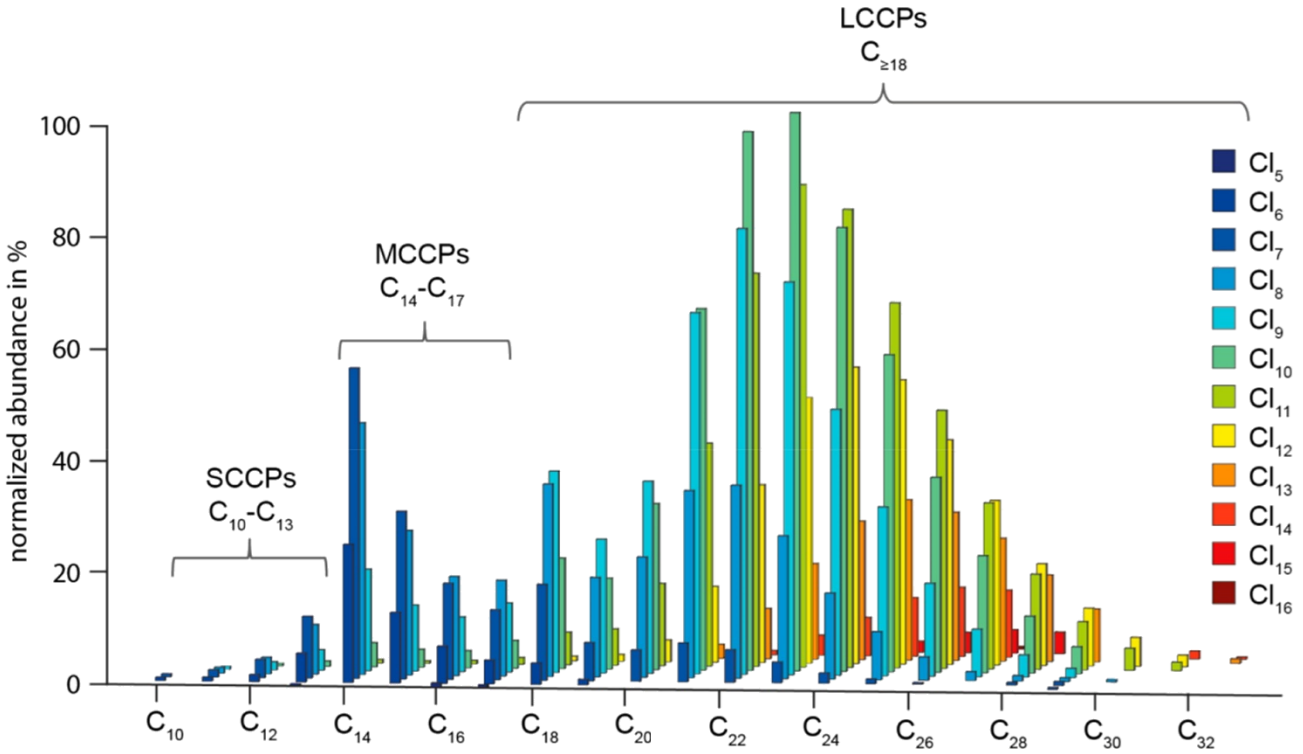
- poor ionization efficiency for homologues with $Cl_{<5}$
- about **30% – 60%** of SCCPs in environmental samples are invisible with this method



sediment, loach, frog (China)

Environ. Sci. Technol. 2016, 50, 7, 3746–3753

- not suitable for the analysis of longer-chain CPs because of their low volatility



top sediment, Rhône River (France)

Environ. Sci. Technol. Lett. 2018, 5, 12, 708–717

Chemosphere. 2015, 136, 259-272

LC-ESI/APCI-MS

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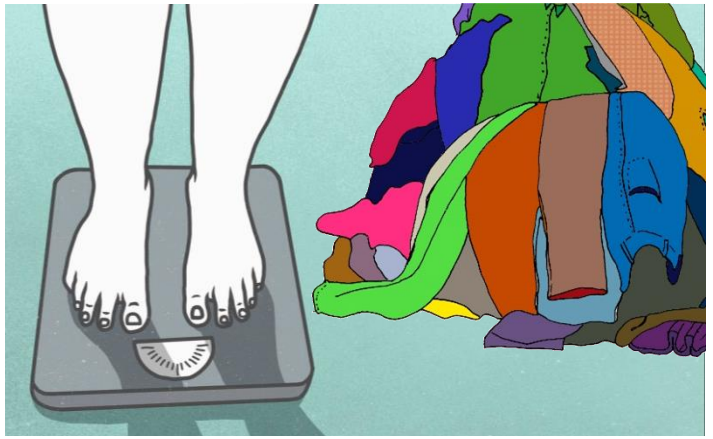
Instrument	Reagent	Target ions	Reference
LC-APCI-MS	chloroform	$[M+Cl]^-$	Rapid Commun. Mass Spectrom. **2004**, 18
LC-APCI-MS	dichloromethane	$[M+Cl]^-$	Anal. Chem. **2015**, 87, 2852-2860
LC-APCI-MS	bromoform	$[M+Br]^-$	Environ. Sci. Technol. Lett. **2018**, 5, 6, 348–353
LC-APCI-MS	dibromomethane	$[M+Br]^-$	Environ. Sci. Technol. **2019**, 53, 18, 10835–10844
LC-ESI-MS	–	$[M-H]^-$	J. Chromatogr. A. **2019**, 1593, 102–109
LC-ESI-MS	dichloromethane	$[M+Cl]^-$	Environ. Sci. Technol. **2017**, 51, 3346-3354
LC-ESI-MS	ammonium chloride	$[M+Cl]^-$	Environ. Pollut. **2019**, 255, 1133032
LC-ESI-MS	ammonium bromide	$[M+Br]^-$	Environ. Pollut. **2019**, 255, 1133032
LC-ESI-MS	ammonium formate	$[M+HCOO]^-$	Environ. Pollut. **2019**, 255, 1133032
LC-ESI-MS	ammonium acetate	$[M+CH_3COO]^-$	Anal. Chim. Acta. **2016**, 936, 130-138
LC-ESI-MSMS	ammonium acetate	$[M+CH_3COO]^-$ $\rightarrow [M-H]^-/[CH_3COO]^-$	Chemosphere. **2020**, 244, 125531

Identification: are the instrumental signal only from target CPs?



Are the instrumental signal only from target CPs?

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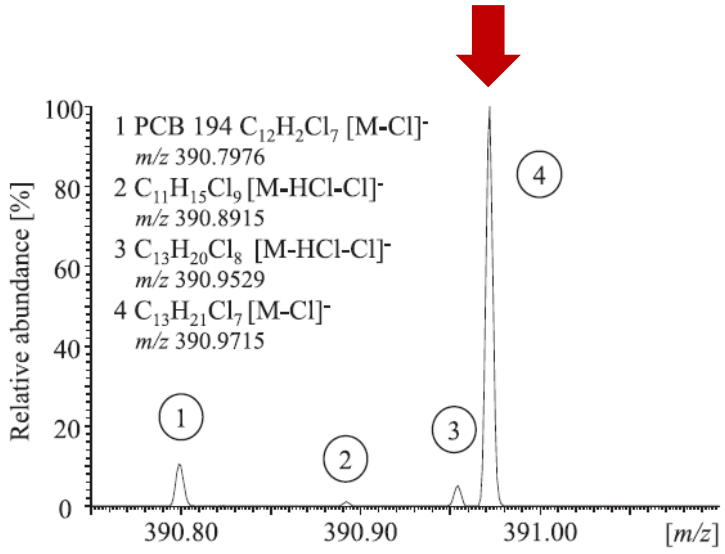
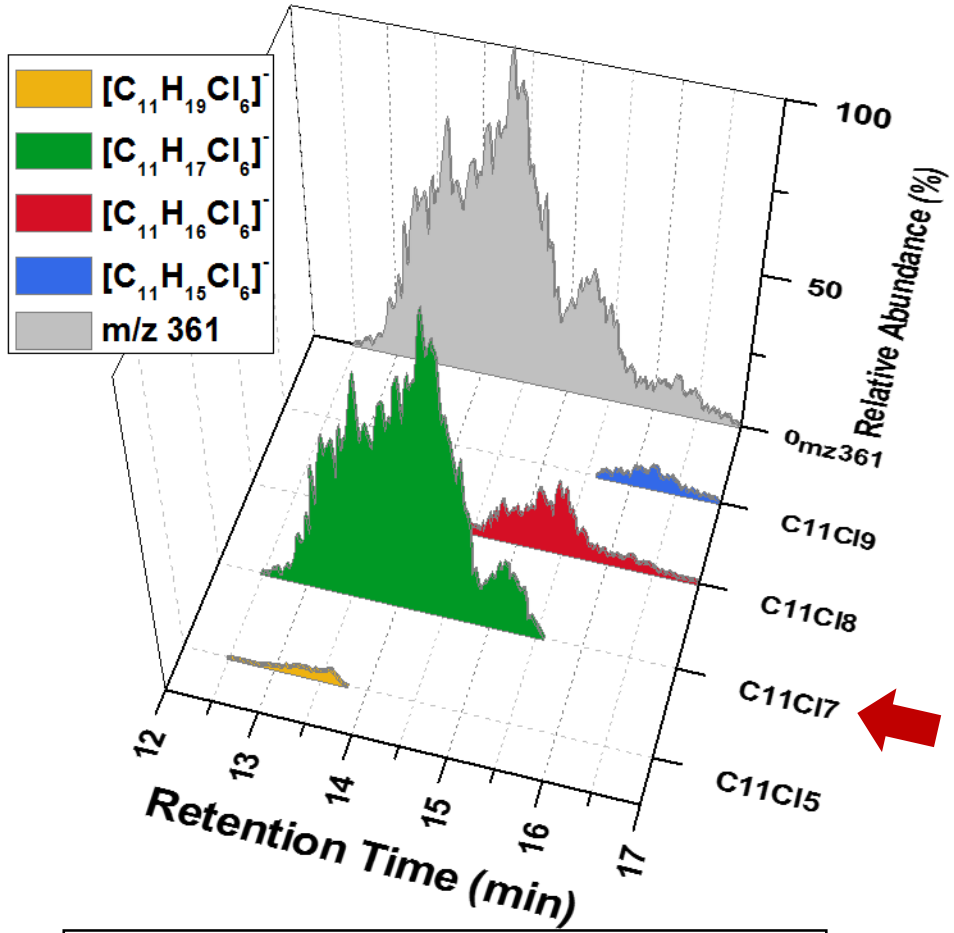
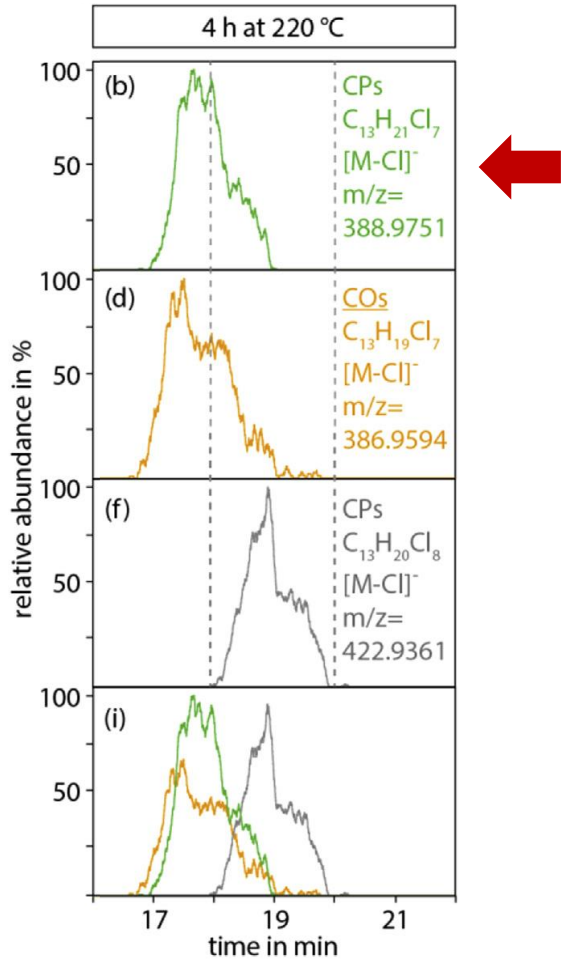
Target CP homologue signal



Mass spectrum, GC-Orbitrap-MS



GC chromatogram, GC-sector-MS



chlorinated (di)olefins

Journal of Chromatography A, 1539 (2018) 53–61

Environmental Science & Technology, 51 (2017) 10633-10641

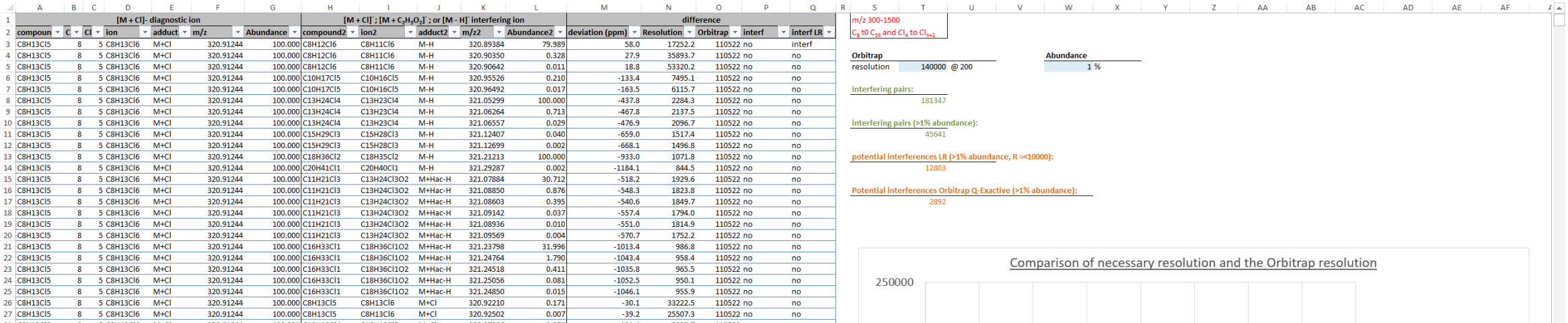
Trends in Analytical Chemistry 106 (2018) 116–124

MS resolution

Category	Chemical formula	Ion formation	One isotope	m/z	Isotopic abundance	Resolution
SCCPs	$C_{11}H_{15}Cl_9$	$[M\text{-}Cl]^-$	m+4	430.8623	27.6%	–
	$C_{11}H_{14}Cl_{10}$	$[M\text{-}HCl\text{-}Cl]^-$	m+6	430.8437	17.6%	23000
	$C_{13}H_{22}Cl_6$	$[M+Cl]^-$	m+8	430.9423	4.5%	5400
	$C_{13}H_{20}Cl_8$	$[M\text{-}Cl]^-$	m+10	430.9237	0.9%	7000
MCCPs	$C_{16}H_{27}Cl_7$	$[M\text{-}Cl]^-$	m+2	431.0214	30.4%	2700
	$C_{16}H_{26}Cl_8$	$[M\text{-}HCl\text{-}Cl]^-$	m+4	431.0029	24.3%	3100
LCCPs	$C_{18}H_{34}Cl_4$	$[M+Cl]^-$	m+6	431.1015	6.7%	1800
	$C_{18}H_{32}Cl_6$	$[M\text{-}Cl]^-$	m+8	431.0829	1.1%	2000
	$C_{21}H_{39}Cl_5$	$[M\text{-}Cl]^-$	m+0	431.1806	26.1%	1400
	$C_{21}H_{38}Cl_6$	$[M\text{-}HCl\text{-}Cl]^-$	m+2	431.1621	33.4%	1400
PCB194-205	$C_{12}H_2Cl_8$	$[M\text{-}H]^-$	m+6	430.7498	17.5%	3800

- To resolve SCCPs, MCCPs, and LCCPs from each other requires a HRMS with a mass resolution of >7000
- To resolve individual C_xCl_z requires a mass resolution > 20 000
- HRMS + MS spectrum deconvolution
- PCBs, chlordane, phthalates, etc.

Journal of Chromatography A. 2020, 1619, 460927



[M + Cl]- diagnostic ion							[M + Cl]⁻; [M + $C_2H_3O_2$]⁻; or [M - H]⁻ interfering ion					difference				
compoun	C	Cl	ion	adduct	m/z	Abundance	compound2	ion2	adduct2	m/z2	Abundance2	deviation (ppm)	Resolution	Orbitrap	interf	interf LR
C8H13Cl5	8	5	C8H13Cl6	M+Cl	320.91244	100.000	C8H12Cl6	C8H11Cl6	M-H	320.89384	79.989	58.0	17252.2	110522	no	interf
C8H13Cl5	8	5	C8H13Cl6	M+Cl	320.91244	100.000	C8H12Cl6	C8H11Cl6	M-H	320.90350	0.328	27.9	35893.7	110522	no	no
C8H13Cl5	8	5	C8H13Cl6	M+Cl	320.91244	100.000	C8H12Cl6	C8H11Cl6	M-H	320.90642	0.011	18.8	53320.2	110522	no	no
C8H13Cl5	8	5	C8H13Cl6	M+Cl	320.91244	100.000	C10H17Cl5	C10H16Cl5	M-H	320.95526	0.210	-133.4	7495.1	110522	no	no
C8H13Cl5	8	5	C8H13Cl6	M+Cl	320.91244	100.000	C10H17Cl5	C10H16Cl5	M-H	320.96492	0.017	-163.5	6115.7	110522	no	no
C8H13Cl5	8	5	C8H13Cl6	M+Cl	320.91244	100.000	C13H24Cl4	C13H23Cl4	M-H	321.05299	100.000	-437.8	2284.3	110522	no	no
C8H13Cl5	8	5	C8H13Cl6	M+Cl	320.91244	100.000	C13H24Cl4	C13H23Cl4	M-H	321.06264	0.713	-467.8	2137.5	110522	no	no
C8H13Cl5	8	5	C8H13Cl6	M+Cl	320.91244	100.000	C13H24Cl4	C13H23Cl4	M-H	321.06557	0.029	-476.9	2096.7	110522	no	no
C8H13Cl5	8	5	C8H13Cl6	M+Cl	320.91244	100.000	C15H29Cl3	C15H28Cl3	M-H	321.12407	0.040	-659.0	1517.4	110522	no	no
C8H13Cl5	8	5	C8H13Cl6	M+Cl	320.91244	100.000	C15H29Cl3	C15H28Cl3	M-H	321.12699	0.002	-668.1	1496.8	110522	no	no
C8H13Cl5	8	5	C8H13Cl6	M+Cl	320.91244	100.000	C18H36Cl2	C18H35Cl2	M-H	321.21213	100.000	-933.0	1071.8	110522	no	no
C8H13Cl5	8	5	C8H13Cl6	M+Cl	320.91244	100.000	C20H41Cl1	C20H40Cl1	M-H	321.29287	0.002	-1184.1	844.5	110522	no	no
C8H13Cl5	8	5	C8H13Cl6	M+Cl	320.91244	100.000	C11H21Cl3	C13H24Cl3O2	M+Hac-H	321.07884	30.712	-518.2	1929.6	110522	no	no
C8H13Cl5	8	5	C8H13Cl6	M+Cl	320.91244	100.000	C11H21Cl3	C13H24Cl3O2	M+Hac-H	321.08850	0.876	-548.3	1823.8	110522	no	no
C8H13Cl5	8	5	C8H13Cl6	M+Cl	320.91244	100.000	C11H21Cl3	C13H24Cl3O2	M+Hac-H	321.08603	0.395	-540.6	1849.7	110522	no	no
C8H13Cl5	8	5	C8H13Cl6	M+Cl	320.91244	100.000	C11H21Cl3	C13H24Cl3O2	M+Hac-H	321.09142	0.037	-557.4	1794.0	110522	no	no
C8H13Cl5	8	5	C8H13Cl6	M+Cl	320.91244	100.000	C11H21Cl3	C13H24Cl3O2	M+Hac-H	321.08936	0.010	-551.0	1814.9	110522	no	no
C8H13Cl5	8	5	C8H13Cl6	M+Cl	320.91244	100.000	C11H21Cl3	C13H24Cl3O2	M+Hac-H	321.09569	0.004	-570.7	1752.2	110522	no	no
C8H13Cl5	8	5	C8H13Cl6	M+Cl	320.91244	100.000	C16H33Cl1	C18H36Cl1O2	M+Hac-H	321.23798	31.996	-1013.4	986.8	110522	no	no
C8H13Cl5	8	5	C8H13Cl6	M+Cl	320.91244	100.000	C16H33Cl1	C18H36Cl1O2	M+Hac-H	321.24764	1.790	-1043.4	958.4	110522	no	no
C8H13Cl5	8	5	C8H13Cl6	M+Cl	320.91244	100.000	C16H33Cl1	C18H36Cl1O2	M+Hac-H	321.24518	0.411	-1035.8	965.5	110522	no	no
C8H13Cl5	8	5	C8H13Cl6	M+Cl	320.91244	100.000	C16H33Cl1	C18H36Cl1O2	M+Hac-H	321.25056	0.081	-1052.5	950.1	110522	no	no
C8H13Cl5	8	5	C8H13Cl6	M+Cl	320.91244	100.000	C16H33Cl1	C18H36Cl1O2	M+Hac-H	321.24850	0.015	-1046.1	955.9	110522	no	no
C8H13Cl5	8	5	C8H13Cl6	M+Cl	320.91244	100.000	C8H13Cl5	C8H13Cl6	M+Cl	320.92210	0.171	-30.1	33222.5	110522	no	no
C8H13Cl5	8	5	C8H13Cl6	M+Cl	320.91244	100.000	C8H13Cl5	C8H13Cl6	M+Cl	320.92502	0.007	-39.2	25507.3	110522	no	no

m/z 300-1500
C_8 t0 C_{36} and Cl_4 to Cl_{n+2}

Orbitrap
resolution 140000 @ 200

Abundance
1 %

interfering pairs:
181347

interfering pairs (>1% abundance):
45641

potential interferences LR (>1% abundance, R =<10000):
12803

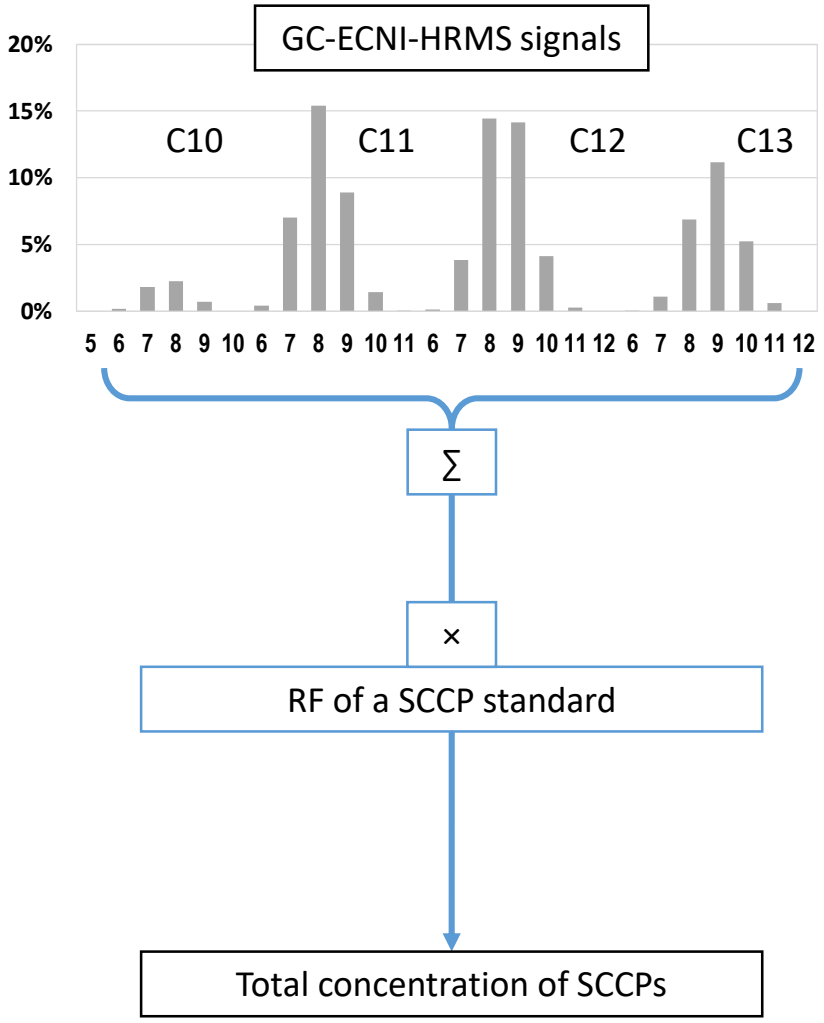
Potential interferences Orbitrap Q-Exactive (>1% abundance):
2892

Quantification: signal response factor

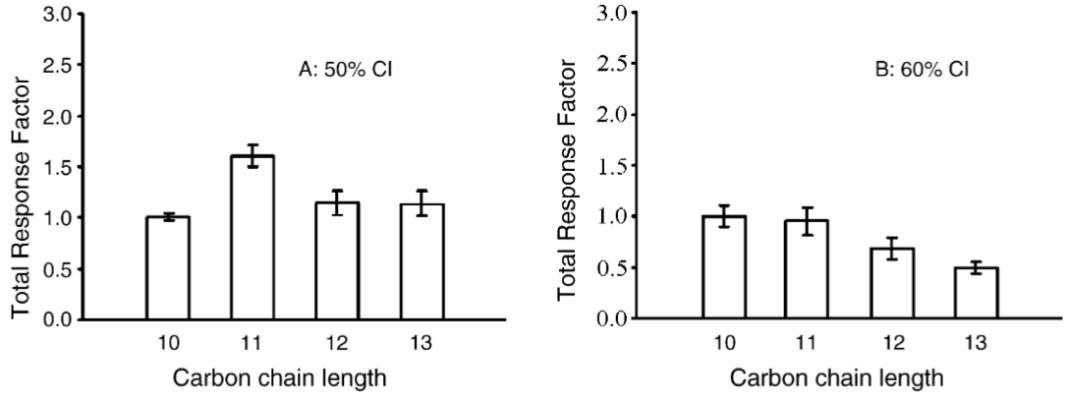
Concentration = Instrumental signal × Response Factor (RF)

Quantifying total SCCPs

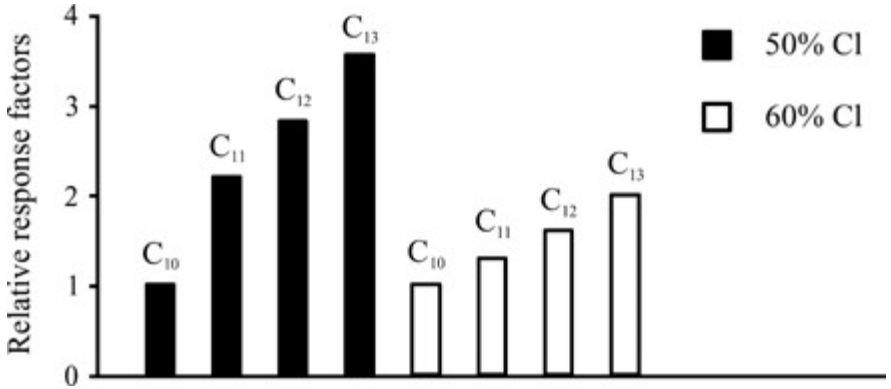
$$\text{Concentration (SCCPs)} = \frac{\sum[\text{instrumental signal } (C_xCl_z \text{ of SCCPs})]}{\text{RF (the most similar SCCP std)}}$$



Anal. Chem., **1997**, 69 (14), 2762-2771



GC-ECNI-MS

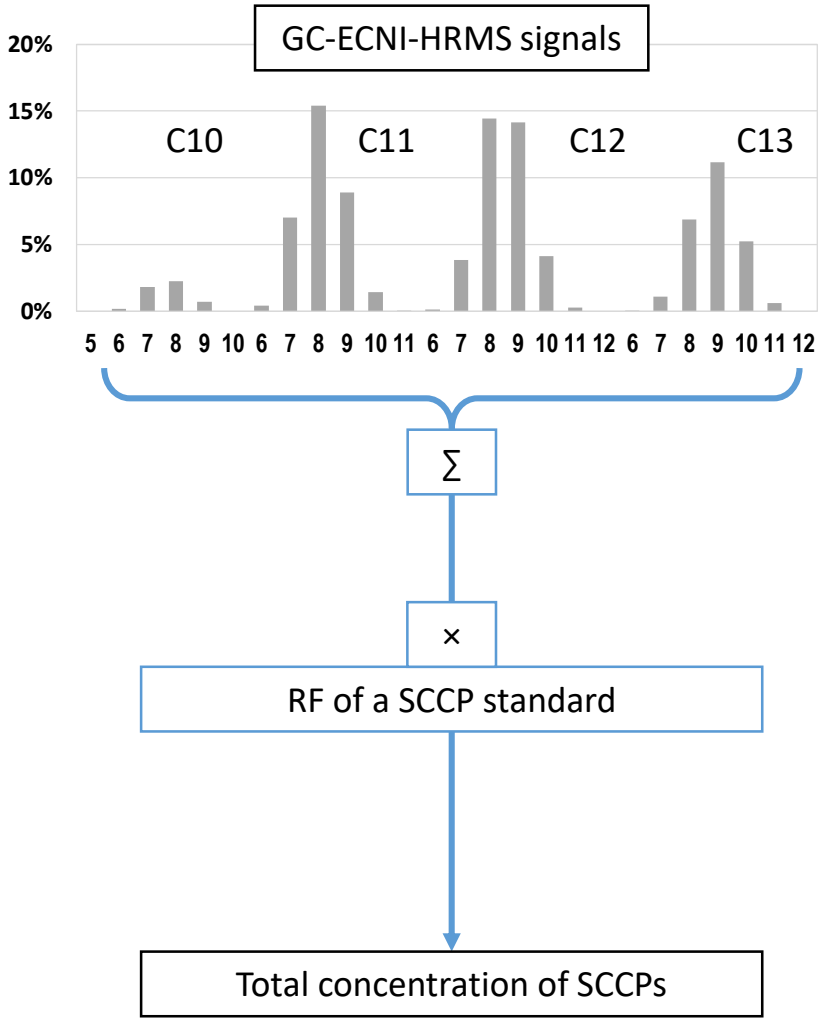


LC-APCI-MS

J. Chromatogr. A. 2005,108, 225–231
Rapid Commun. Mass Spectrom. 2004, 18, 2235–2240

Quantifying total SCCPs

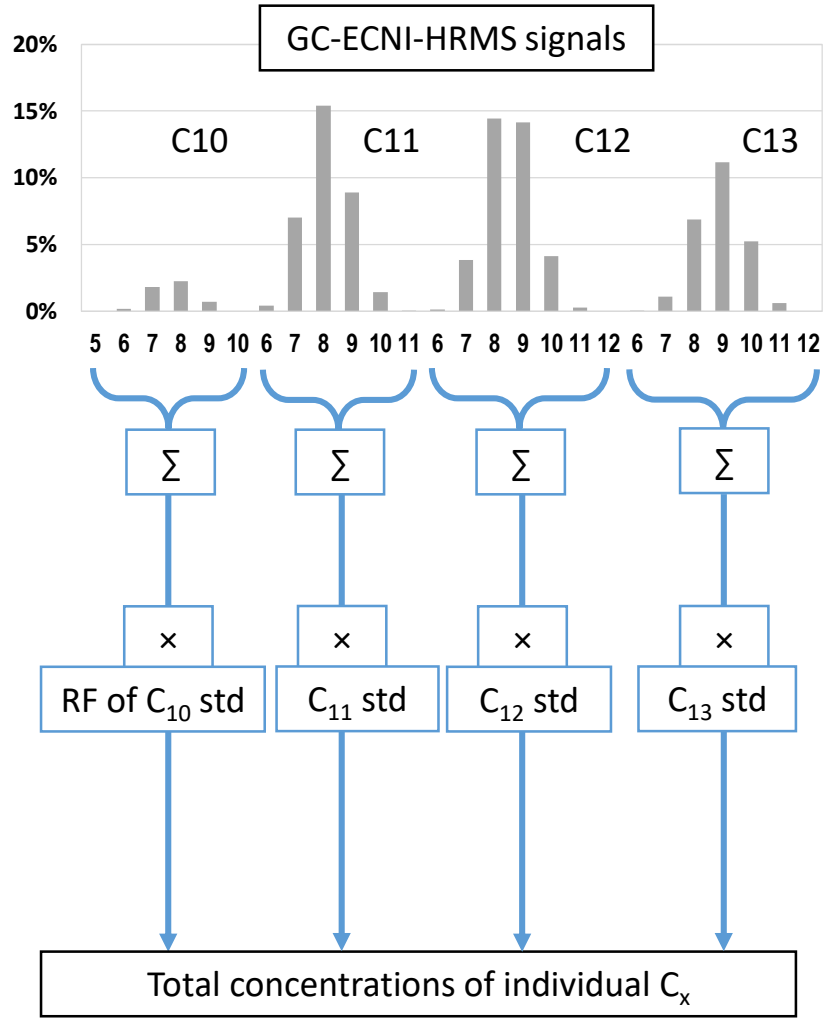
$$\text{Concentration (SCCPs)} = \frac{\sum[\text{instrumental signal } (C_xCl_z \text{ of SCCPs})]}{\text{RF (the most similar SCCP std)}}$$



Anal. Chem., **1997**, 69 (14), 2762-2771

Quantifying total C_x

$$\text{Concentration } (C_x) = \frac{\sum[\text{instrumental signal } (C_xCl_z \text{ of } C_x)]}{\text{RF (the most similar } C_x \text{ std)}}$$



Environ. Pollut., **2013**, 175, 16-21

homologue-dependent ionization efficiency

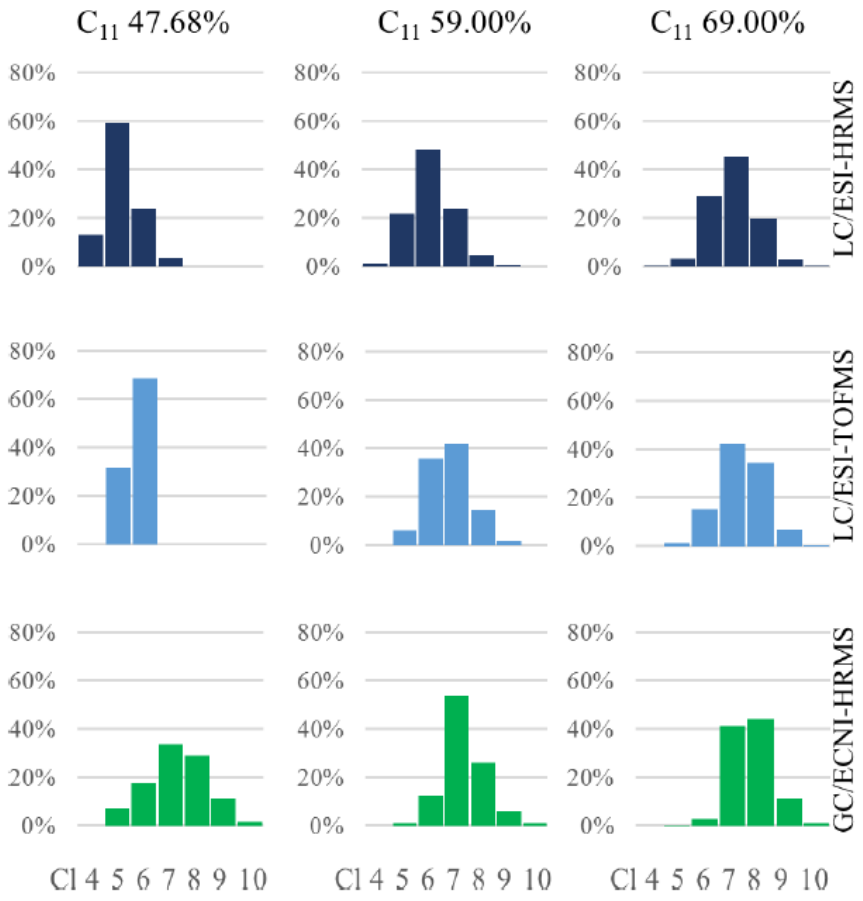
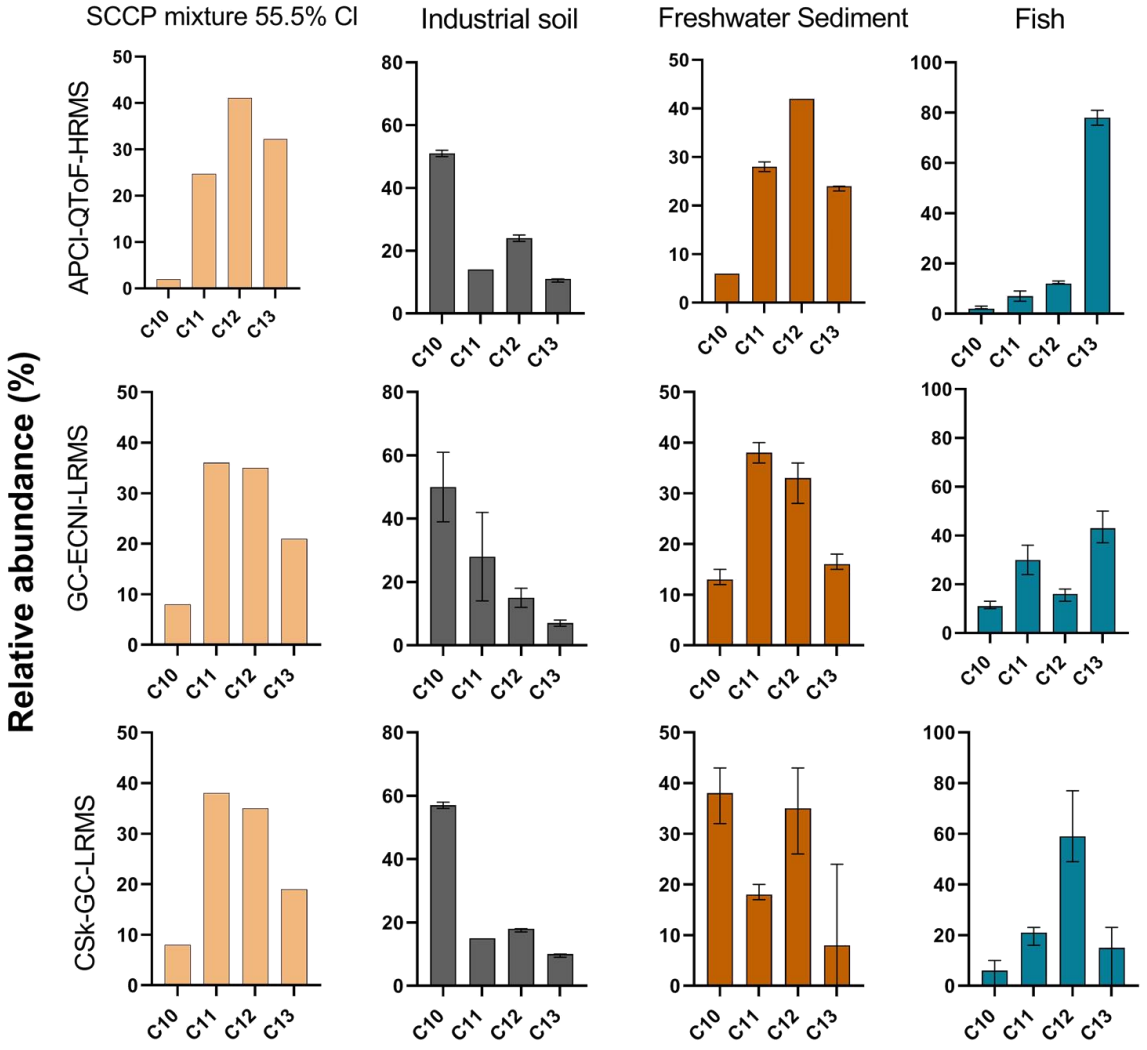


Figure 2. Comparison of Hohenheim single-chain CP-standard instrumental responses between the three instrument set-ups.

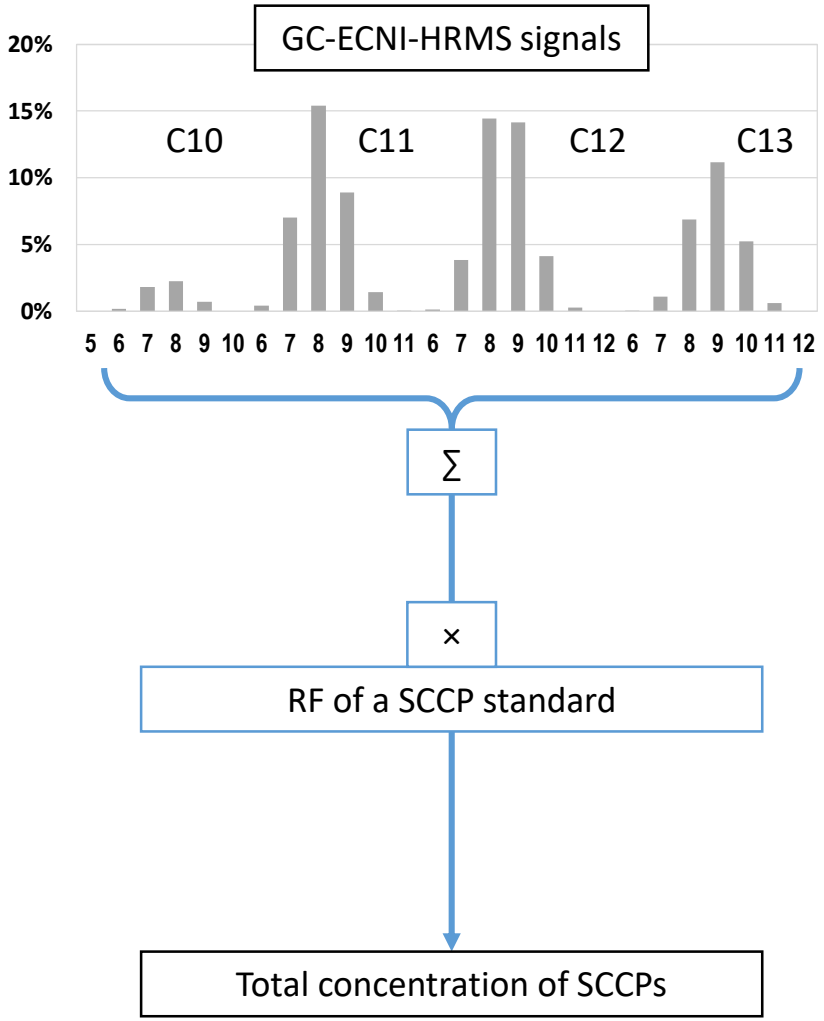
Mézière et al. / *J. Am. Soc. Mass Spectrom.* 2020



van Mourik et al. / *J. Chromatogr. A* 2020

Quantifying total SCCPs

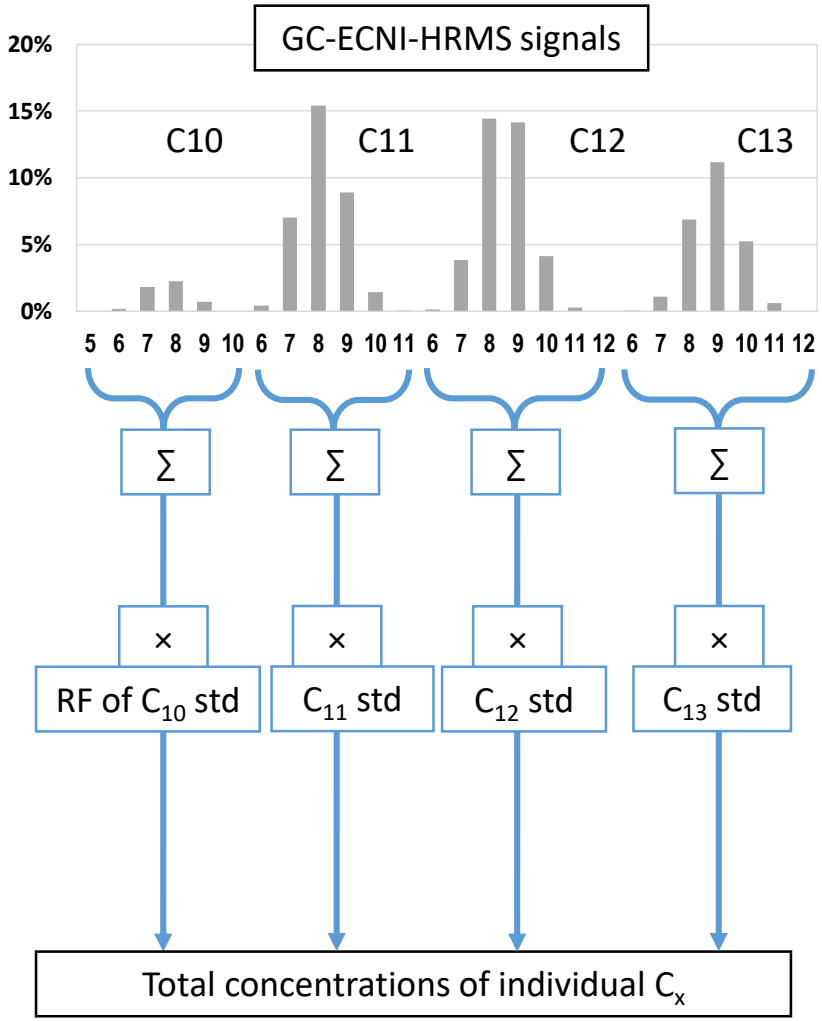
$$\text{Concentration (SCCPs)} = \frac{\sum[\text{instrumental signal } (C_xCl_z \text{ of SCCPs})]}{\text{RF (the most similar SCCP std)}}$$



Anal. Chem., **1997**, 69 (14), 2762-2771

Quantifying total C_x

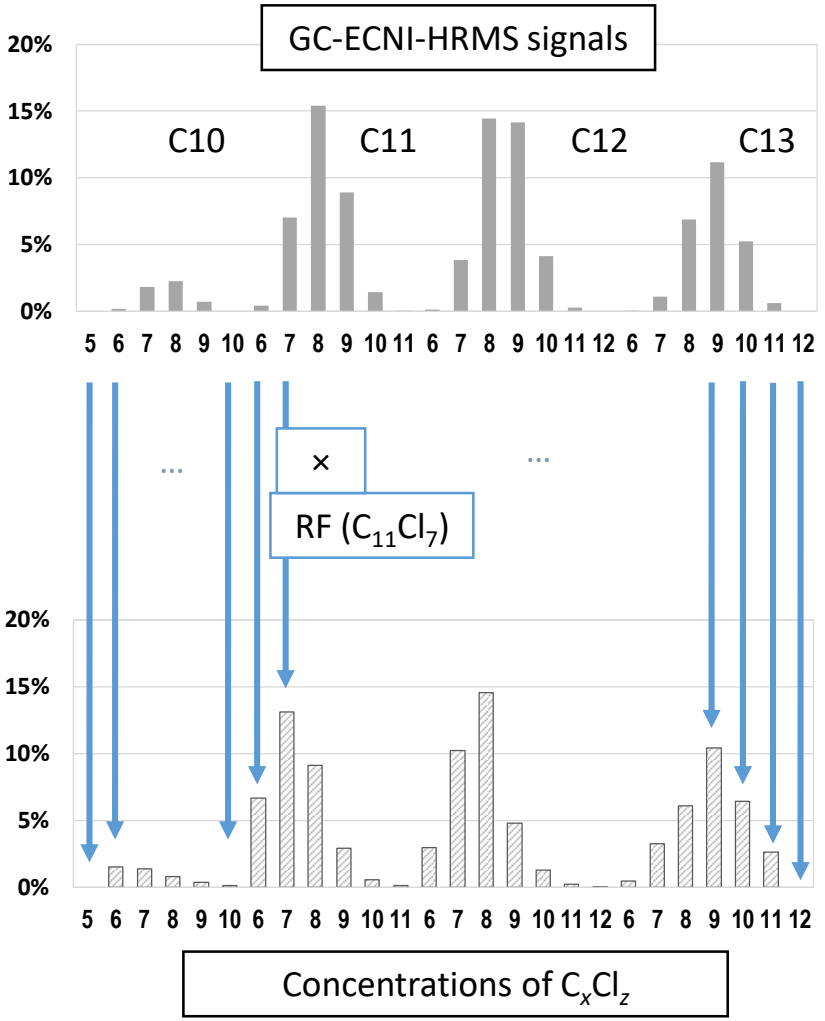
$$\text{Concentration } (C_x) = \frac{\sum[\text{instrumental signal } (C_xCl_z \text{ of } C_x)]}{\text{RF (the most similar } C_x \text{ std)}}$$



Environ. Pollut., **2013**, 175, 16-21

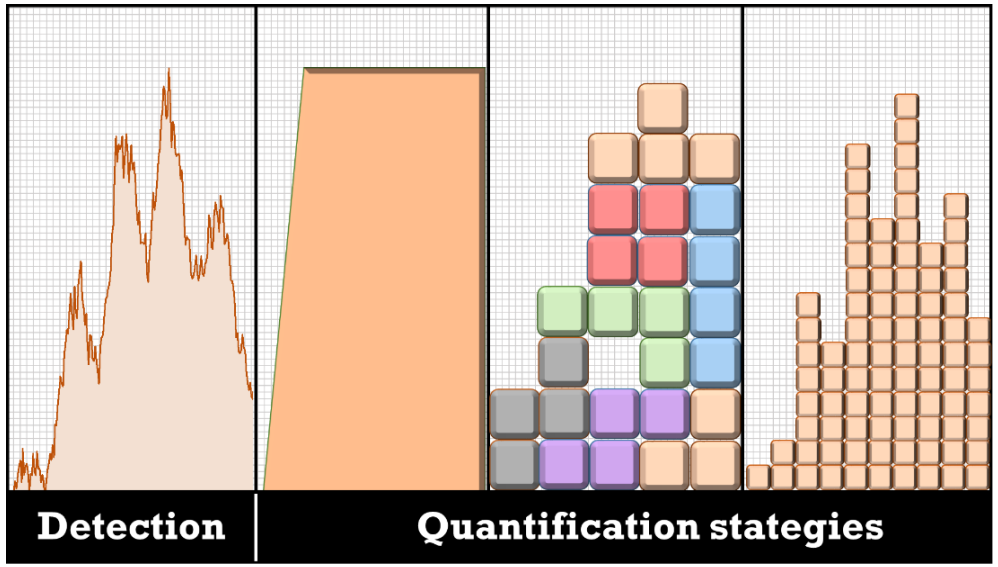
Quantifying homologue C_xCl_z

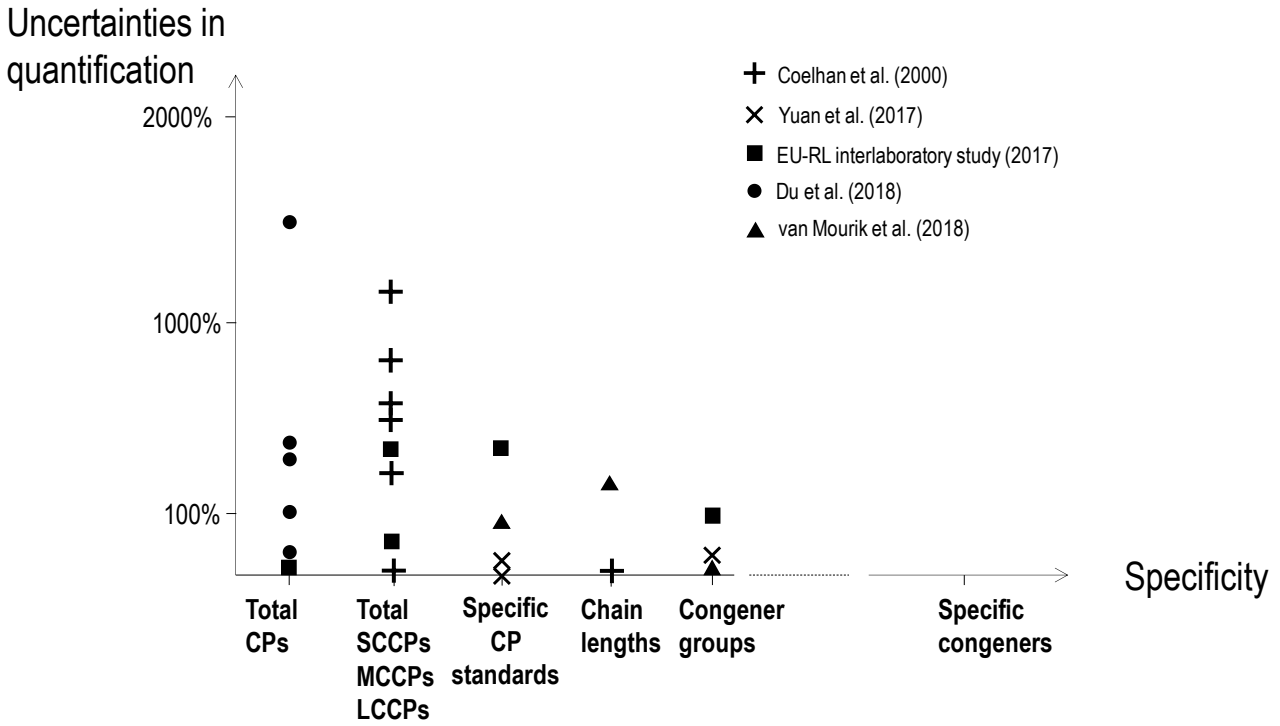
$$\text{Concentration } (C_xCl_z) = \frac{\text{instrumental signal } (C_xCl_z)}{\text{RF } (C_xCl_z)}$$



Environ. Sci. Technol. **2017**, 51, 10633−10641

Quantification uncertainties





Total concentration of SCCPs

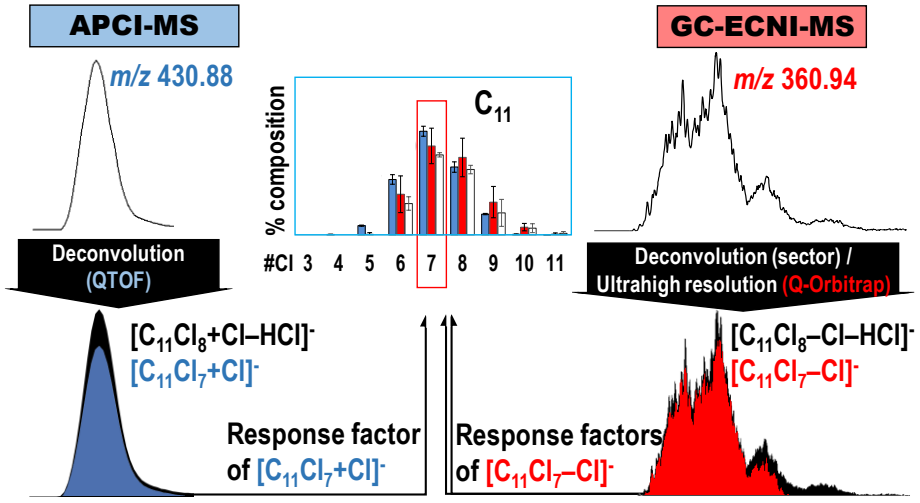
Total concentrations of individual C_x

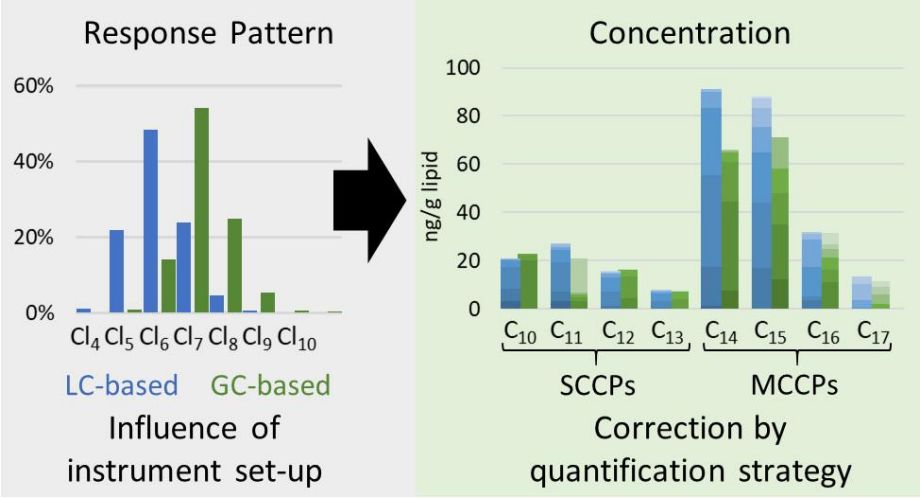
Concentrations of C_xCl_z

Stockholm University

Future directions

Quantificaion at the C_xCl_z level





GC-Orbitrap-MS

Table 1
Homologue percentage compositions (%) in SCCP mixtures with nominal 51.5%, 55.5%, and 63% Cl content and in SCCP-CS, as calculated using data acquired by GC–EI/ECNI-Orbitrap-HRMS analysis.

Homologue	SCCP mixture with 51.5% Cl content	SCCP mixture with 55.5% Cl content	SCCP mixture with 63% Cl content	SCCP-CS (1:1 mixture of the SCCP mixtures with 55.5% and 63% Cl content)
$C_{10}Cl_3$	0	0	0	0
$C_{10}Cl_4$	2.11	1.81	0.06	0.93
$C_{10}Cl_5$	2.57	3.66	0.82	2.24
$C_{10}Cl_6$	0.67	1.93	3.08	2.51
$C_{10}Cl_7$	0.09	0.49	2.93	1.71
$C_{10}Cl_8$	0	0.07	1.05	0.56
$C_{10}Cl_9$	0	0	0.17	0.09
$C_{10}Cl_{10}$	0	0	0	0
$C_{11}Cl_3$	0	0.00	0	0

LC-ESI-MSMS

Environ. Sci. Technol. 51 (2017) 10633-10641

J. Am. Soc. Mass Spectrom. (2020)

Chemosphere 244 (2020) 125531

Synthesis of new reference chemicals

New standards of polychlorinated alkanes (SCCPs)

Liu H, Gozhina O, Gorovoy A, Johansen JE

Chiron AS, Stiklestadveien 1, Trondheim, Norway, Jon.Johansen@chiron.no

Environmental Science & Technology Letters

Review

Cite This: Environ. Sci. Technol. Lett. 2018, 5, 708−717

pubs.acs.org/journal/estlcu

Analysis of Medium-Chain and Long-Chain Chlorinated Paraffins: The Urgent Need for More Specific Analytical Standards

Lena Schinkel,*[,†,‡] Christian Bogdal,[§,#] Elia Canonica,[†,∥] Ronan Cariou,[⊥] Davide Bleiner,[†] Kristopher McNeill,[‡] and Norbert V. Heeb*[,†]

[†]Laboratory for Advanced Analytical Technologies, Swiss Federal Laboratories for Materials Science and Technology (Empa), Überlandstrasse 129, 8600 Dübendorf, Switzerland

[‡]Institute of Biogeochemistry and Pollutant Dynamic, Swiss Federal Institute of Technology (ETH Zurich), Universitätsstrasse 16, 8092 Zurich, Switzerland

[§]Institute for Chemical and Bioengineering, Swiss Federal Institute of Technology (ETH Zurich), Vladimir-Prelog-Weg 1, 8093 Zürich, Switzerland

[∥]Institute of Chemistry and Biotechnology, Zurich University of Applied Sciences (ZHAW), Grüentalstrasse 14, 8820 Wädenswil, Switzerland

[⊥]Laboratoire d'Étude des Résidus et Contaminants dans les Aliments (LABERCA), Oniris, INRA, Université Bretagne Loire, 44307 Nantes, France

Chemosphere 228 (2019) 762–768

Contents lists available at ScienceDirect

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journal homepage: www.elsevier.com/locate/chemosphere

Characterization of single chain length chlorinated paraffin mixtures with nuclear magnetic resonance spectroscopy (NMR)

Jannik Sprengel, Nina Wiedmaier-Czerny, Walter Vetter*

University of Hohenheim, Institute of Food Chemistry, Garbenstr. 28, D-70599, Stuttgart, Germany

Chemosphere 255 (2020) 126959

Contents lists available at ScienceDirect

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journal homepage: www.elsevier.com/locate/chemosphere

Short Communication

Characterization of synthetic single-chain CP standard materials – Removal of interfering side products

Norbert V. Heeb [a, *], Silvan Iten [a, b], Lena Schinkel [a, 1], Marco Knobloch [a, c], Jannik Sprengel [d], Peter Lienemann [b], Davide Bleiner [a, c], Walter Vetter [d]

[a] *Empa, Swiss Federal Laboratories for Materials Science and Technology,Laboratory for Advanced Analytical Technologies, Überlandstrasse 129, CH-8600 Dübendorf, Switzerland*

[b] *ZHAW, Zurich University of Applied Sciences, Institute of Chemistry and Biological Chemistry, Reidbach, CH-8820, Wädenswil, Switzerland*

[c] *University of Zürich, Department of Chemistry, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland*

[d] *University of Hohenheim, Institute of Food Chemistry, Garbenstrasse 28, D-70599 Stuttgart, Germany*

Interlaboratory studies and certified reference materials

Stockholm University

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journal homepage: www.elsevier.com/locate/chemosphere

Interlaboratory studies on chlorinated paraffins: Evaluation of different methods for food matrices

K. Krätschmer*, A. Schächtele

European Union Reference Laboratory (EURL) for Halogenated Persistent Organic Pollutants (POPs) in Feed and Food, 79114, Freiburg, Germany

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Food Control

journal homepage: www.elsevier.com/locate/foodcont

Optimization and validation of an analytical method for the quantification of short- and medium-chained chlorinated paraffins in food by gas chromatography-mass spectrometry

Thomas J. McGrath[a,*], Giulia Poma[a], Jasper Bombeke[a], Franck Limonier[b], Els Van Hoeck[b], Laure Joly[b], Adrian Covaci[a,**]

[a] *Toxicological Centre, University of Antwerp, Universiteitsplein 1, 2610, Wilrijk, Belgium*
[b] *Sciensano, Chemical and Physical Health Risks Department, Rue Juliette Wytsman 14, B-1050, Ixelles, Belgium*

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Journal of Chromatography A

journal homepage: www.elsevier.com/locate/chroma

The underlying challenges that arise when analysing short-chain chlorinated paraffins in environmental matrices

L.M. van Mourik[a,b,*], R. Lava[c,1], J. O'Brien[a], P.E.G. Leonards[b], J. de Boer[b], M. Ricci[c]

[a] *Queensland Alliance for Environmental Health Science (QAEHS), The University of Queensland, 20 Cornwall Street, Woolloongabba, 4102, Qld, Australia*
[b] *Department of Environment and Health (E&H), Vrije Universiteit, De Boelelaan 1085, 1081 HV, Amsterdam, the Netherlands*
[c] *European Commission, Joint Research Centre, Retieseweg 111, 2440 Geel, Belgium*

Journal of the American Society for Mass Spectrometry

pubs.acs.org/jasms Research Article

Addressing Main Challenges Regarding Short- and Medium-Chain Chlorinated Paraffin Analysis Using GC/ECNI-MS and LC/ESI-MS Methods

Marie Mézière,[⊥] Kerstin Krätschmer,[⊥] Ingus Pērkons, Dzintars Zacs, Philippe Marchand, Gaud Dervilly, Bruno Le Bizec, Alexander Schächtele, Ronan Cariou,* and Walter Vetter

Cite This: https://dx.doi.org/10.1021/jasms.0c00155 Read Online

Thank you for your attention

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