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Comprehensive determination of 209 PCBs using two-dimensional gas chromatography triple quadrupole mass spectrometry

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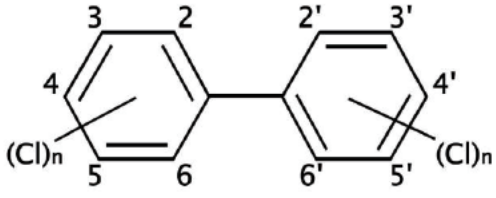
Overview

- 198 of the 209 PCB congeners separated by GC×GC-MS/MS
- Dioxin-like PCB congeners fully separated without interferences
- Triple quadrupole mass spectrometry as an alternative detector for GC×GC

Introduction

Polychlorinated biphenyls (PCBs) are classified as Persistent Organic Pollutants (POPs) by Stockholm Convention. PCBs received attention because of their persistence, bioaccumulation, potential for long-range environmental transport and toxicity.
Depending on the level of chlorination, 209 PCB congeners are grouped into 10 homologue groups containing 1-46 compounds. The World Health Organization (WHO) has assigned dioxin toxic equivalency factors (TEF) of 12 coplanar PCBs, also known as dioxin like PCBs, which present high concentrations.



PCBs ($C_{12}H_{10-x}Cl_x$)

Figure 1 Structure and formula of PCBs

Table 1 Homologue groups of PCBs

Homologue group	Formula	Congener #
Mono-CBs	$C_{12}H_9Cl$	3
Di-CBs	$C_{12}H_8Cl_2$	12
Tri-CBs	$C_{12}H_7Cl_3$	24
Tetra-CBs	$C_{12}H_6Cl_4$	42
Penta-CBs	$C_{12}H_5Cl_5$	46
Hexa-CBs	$C_{12}H_4Cl_6$	42
Hepta-CBs	$C_{12}H_3Cl_7$	24
Octa-CBs	$C_{12}H_2Cl_8$	12
Nona-CBs	$C_{12}HCl_9$	3
Deca-CBs	$C_{12}Cl_{10}$	1

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The separation of 209 PCBs remains a challenge. No single column can separate all 209 congeners. GC×GC coupled with TOFMS and mECD detectors has been applied on PCB analysis.

Table 2 Conclusion on PCB congener separation on GC×GC

1st column	2nd column	Detector	Separated congener #	Deconvoluted congener #	Reference
HT-8	BPX-50	TOFMS	188	4	Focant et al. (2004)
DB-XLB	BPX-70	mECD	194	0	Harju et al. (2003)
Rtx-PCB	DB-17	TOFMS	196	0	Osemwiege and Sovocool (2009)
SPB-Octyl	SLB-IL59	TOFMS	196	0	Zapadlo et al. (2011)

Methods

Two-dimensional gas chromatography coupled with triple quadrupole mass spectrometry (GC×GC-MS/MS) was applied in the separation and quantification of 209 PCB congeners.

Table 3 Instrument for PCB analysis

Instrument	Shimadzu comprehensive two-dimensional gas chromatography triple quadrupole mass spectrometry (GC×GC-MS/MS)
1st column	SPB-Octyl (30m, 0.25mm i.d., 0.25mm df)
2nd column	BPX-50 (1m, 0.1mm i.d., 0.1mm df)
Ion source	Electron Ionization (EI)
Acquisition mode	Multiple Reaction Monitoring (MRM)

Figure 2 Shimadzu GC×GC-MS/MS

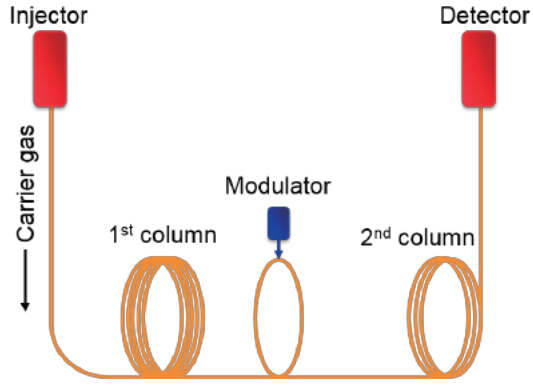

Figure 3 GC×GC schematic

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Results

Method development for 209 PCB congeners

198 of 209 PCB congeners are separated using MRM acquisition mode on GC×GC-MS/MS, together with 4 doublets and 1 triplet.

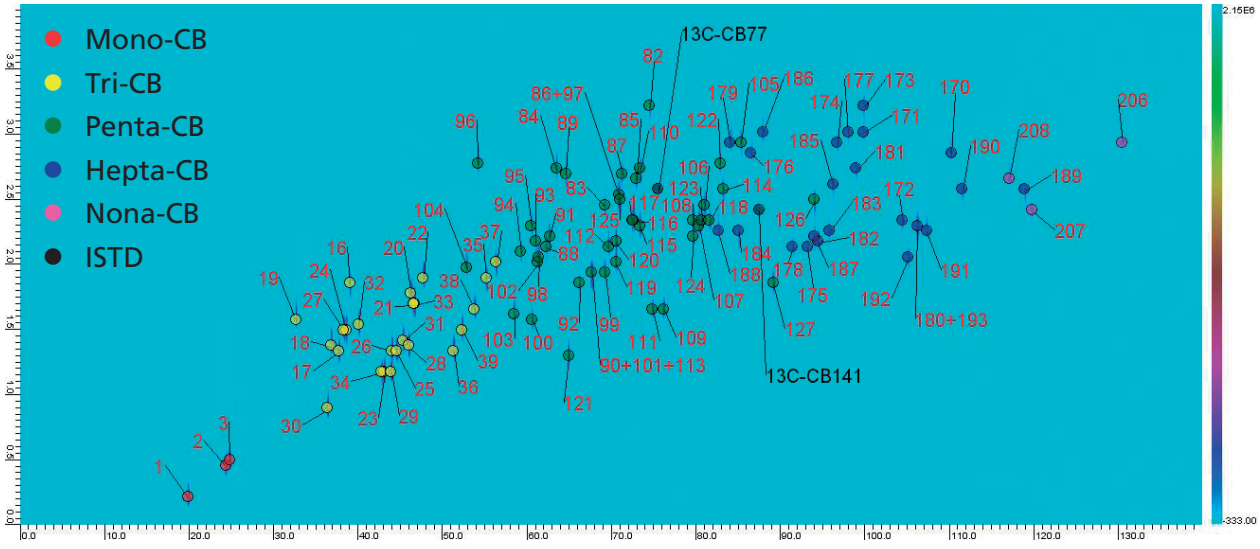

Figure 4 2D chromatogram of **odd number chlorine** substituted PCBs

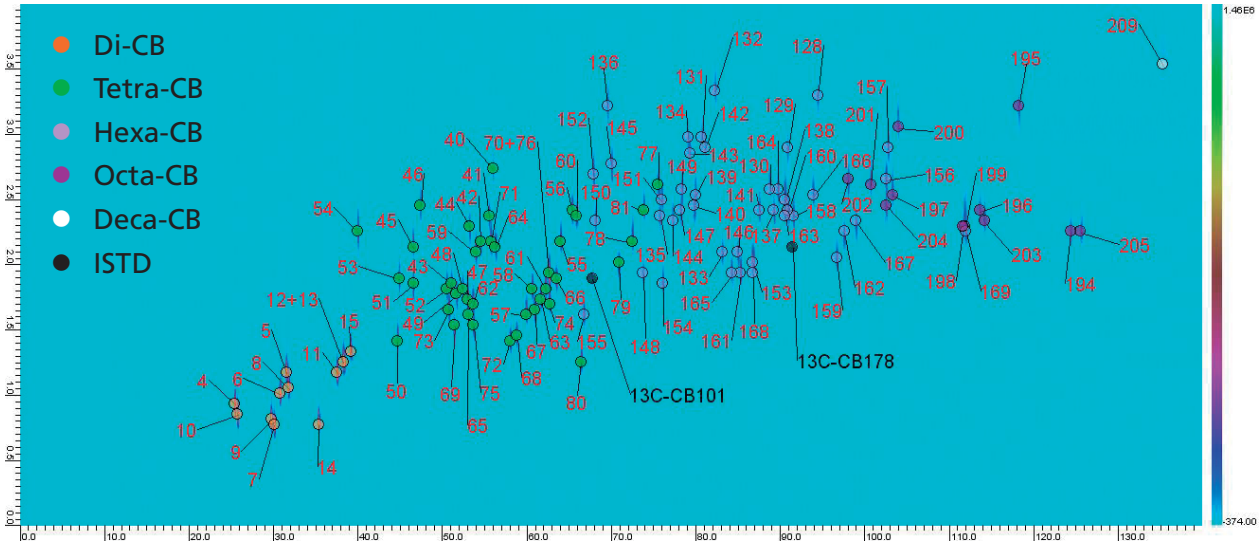

Figure 5 2D chromatogram of **even number chlorine** substituted PCBs

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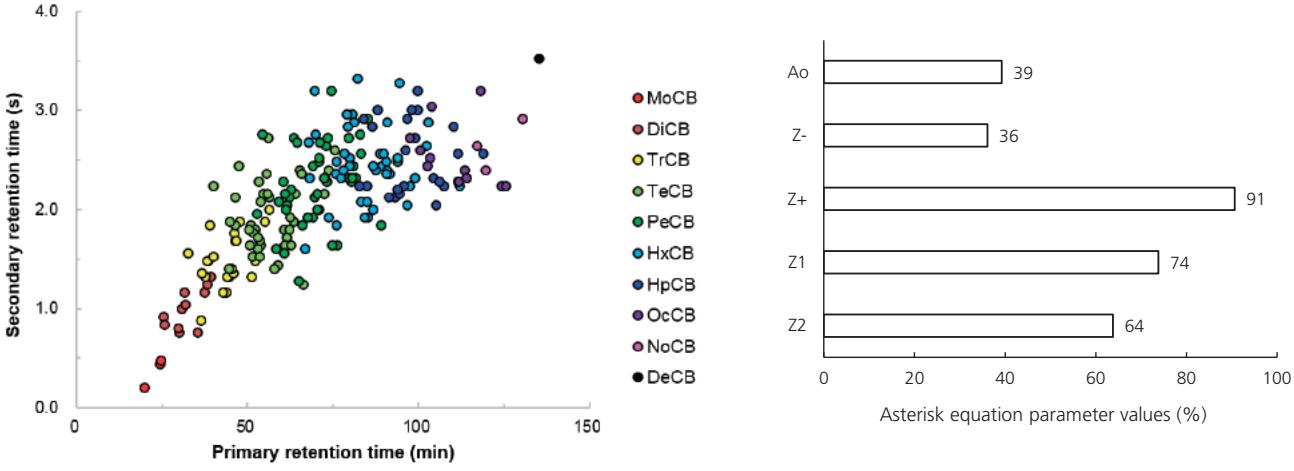

Figure 6 GC×GC separation of 209 PCBs and degree of orthogonality by asterisk equations

Separation of 12 dioxin-like PCBs

12 dioxin-like PCB congeners are separated without interferences from any other PCBs.

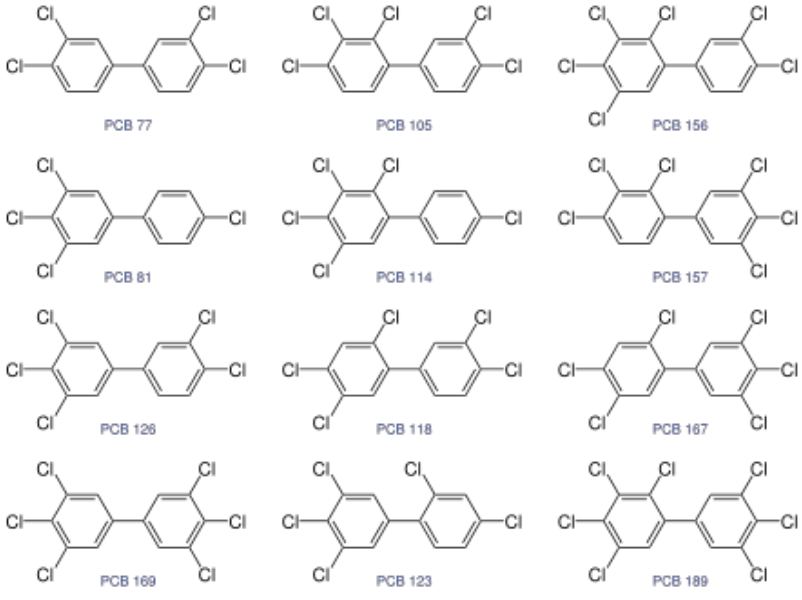

Figure 7 Structure of dioxin-like PCBs

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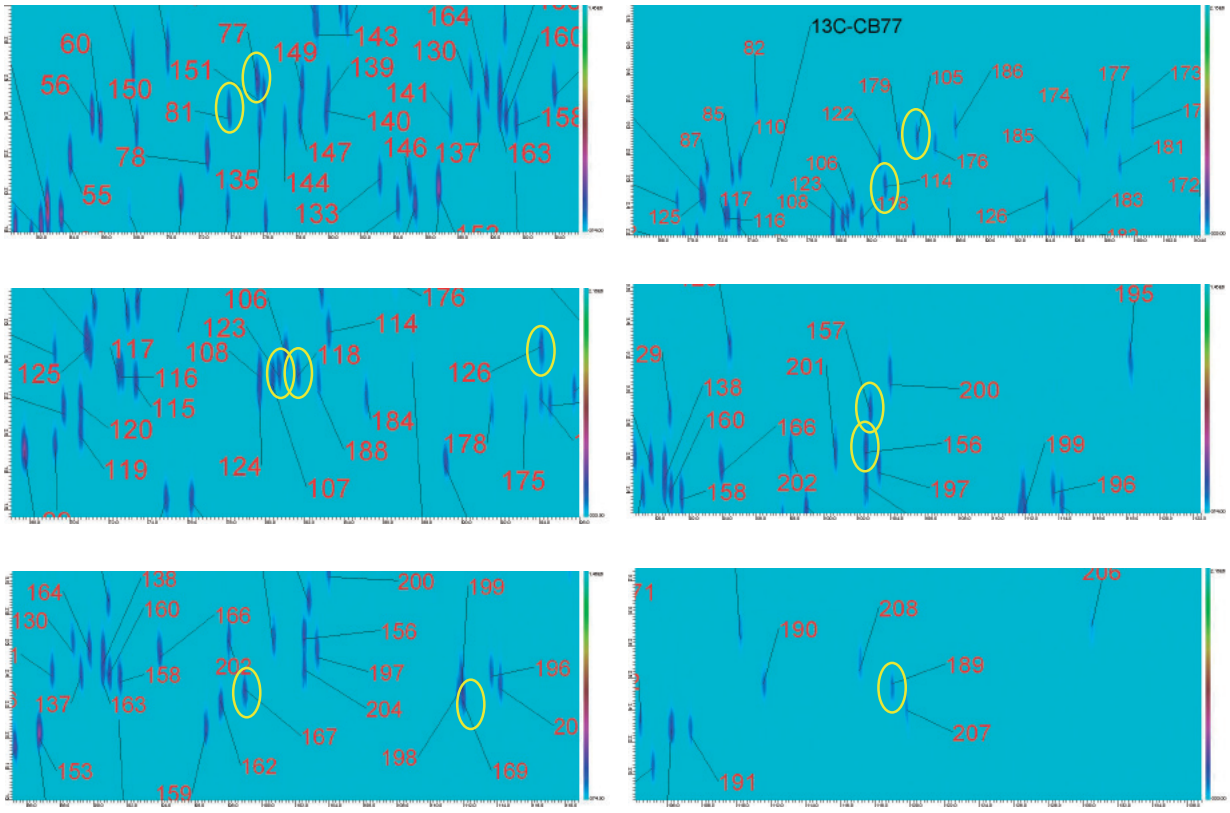

Figure 8 2D chromatogram of dioxin-like PCBs

Conclusions

- Shimadzu GC×GC-MS/MS is able to separate 198 of 209 PCB congeners, together with 4 doublets and 1 triplet.
- The lower cost and easier operational triple quadrupole mass spectrometer is an alternative detector for GC×GC.

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