

## ASMS 2019 TP303

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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.

		Table 1 Homologue groups of PCBs		
		Homologue group	Formula	Congener #
32 2'_	3'	Mono-CBs	C <sub>12</sub> H <sub>9</sub> Cl	3
	_\_	Di-CBs	$C_{12}H_8CI_2$	12
4⟨/_ \>──<\	$\langle \rangle^4$	Tri-CBs	$C_{12}H_7CI_3$	24
	N X CD-	Tetra-CBs	$C_{12}H_6CI_4$	42
5 6 6	5'	Penta-CBs	$C_{12}H_5CI_5$	46
		Hexa-CBs	$C_{12}H_4CI_6$	42
PCBs (C <sub>12</sub> H <sub>10-x</sub> Cl <sub>x</sub> )		Hepta-CBs	$C_{12}H_3CI_7$	24
		Octa-CBs	$C_{12}H_2CI_8$	12
Figure 1 Structure and formula of PCBs		Nona-CBs	C <sub>12</sub> HCl <sub>9</sub>	3
		Deca-CBs	C <sub>12</sub> Cl <sub>10</sub>	1

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.

1 <sup>st</sup> column	2 <sup>nd</sup> 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)

Table 2 Conclusion on PCB congener separation on GC×GC

# 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)
1 <sup>st</sup> column	SPB-Octyl (30m, 0.25mm i.d., 0.25mm df)
2 <sup>nd</sup> column	BPX-50 (1m, 0.1mm i.d., 0.1mm df)
lon source	Electron Ionization (EI)
Acquisition mode	Multiple Reaction Monitoring (MRM)



Figure 2 Shimadzu GC×GC-MS/MS



Figure 3 GC×GC schematic

# 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



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





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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