

## Mass Spectrometry

# Reproducible trace analysis of PCBs in environmental matrices using triple quadrupole GC-MS/MS

## Authors

Kjell Hope<sup>1</sup>, Giulia Riccardino<sup>2</sup>, Adam Ladak<sup>3</sup>, and Paul Silcock<sup>3</sup>

<sup>1</sup> Pacific Rim Laboratories Inc., Canada

<sup>2</sup> Thermo Fisher Scientific, Milan, IT

<sup>3</sup> Thermo Fisher Scientific, Hemel Hempstead, UK

## Keywords

Polychlorinated biphenyls (PCBs), environment, gas chromatography-mass spectrometry, GC-MS, triple quadrupole, TSQ 9610 mass spectrometer, NeverVent Advanced Ionization ion source (NV-AEI), TRACE 1610 GC, AI/AS 1610

## Goal

The aim of this application note is to demonstrate the performance of the Thermo Scientific™ TSQ™ 9610 triple quadrupole mass spectrometer coupled to the Thermo Scientific™ TRACE™ 1610 GC for the determination of polychlorinated biphenyls (PCBs) in environmental samples.

## Introduction

Polychlorinated biphenyls (PCBs) are a group of industrial organic chemicals consisting of carbon, hydrogen, and chlorine atoms.<sup>1</sup> Due to their non-flammability, chemical stability, high boiling point, and electrical insulating properties, PCBs were used in hundreds of industrial and commercial applications including electrical, hydraulic equipment, plasticizers, plastics, rubber products, and dyes. The production of these compounds has been banned in the United States since 1977<sup>1</sup> because of their persistence in the environment and their tendency to enter the food chain and bioaccumulate in living organism due to their lipophilicity. There are currently 209 known PCBs congeners that can be divided into two groups according to their structural and toxicological characteristics: the non-dioxin like PCBs (non-DL-PCB) representing the majority of the PCB congeners with a lower degree of toxicity and the dioxin-like PCBs (DL-PCBs) representing the 12 most toxic congeners, which have structure and toxicity similar to dioxins. DL-PCBs are classified as persistent organic pollutants (POPs), and

they have been regulated under the Stockholm Convention for POPs since 2001.<sup>2</sup> Following the Clean Water Act (CWA) in 1972, the United States Environmental Protection Agency (U.S. EPA) developed an analytical method, EPA Method 1668 and following revisions,<sup>3</sup> that can be applied for the determination of PCBs in wastewater, surface waters, soil, sediments, biosolids, and tissue matrices using gas chromatography coupled to high-resolution gas chromatography/high-resolution mass spectrometry (HRGC/HRMS).<sup>3</sup> However recent advances in gas chromatography-triple quadrupole mass spectrometry allow for high sensitivity and selectivity, leading to the consideration of GC-MS/MS as a reliable tool for PCBs analysis.

In this study, the TSQ 9610 triple quadrupole GC-MS/MS was used for the determination of PCBs in environmental (water and soil) samples. The Thermo Scientific™ TRACE™ TR-PCB column was tested for chromatographic separation of the critical pairs; whereas selected reaction monitoring (SRM) acquisition mode ensured appropriate selectivity and sensitivity when complex matrix samples were analyzed. Linearity and instrument detection limits (IDLs) were assessed in the experiments for all compound as well as an extended robustness study over n=100 injections of matrix samples to assess the reproducibility of the detection of trace levels of PCBs.

## Experimental

In the experiments described here, a TSQ 9610 triple quadrupole mass spectrometer equipped with a Thermo Scientific™ NeverVent™ Advanced Electron Ionization (AEI) ion source was coupled to a TRACE 1610 gas chromatograph equipped with a Thermo Scientific™ iConnect™ split/splitless (iConnect-SSL) injector and a Thermo Scientific™ AI/AS 1610 autosampler. The TRACE 1610 GC with its instant connect injector and detector modules permits reconfiguration of the instrument to adapt to different workflows in minutes. The NeverVent technology allows for ion source cleaning, filament replacement, and column exchange without breaking instrument vacuum, therefore ensuring minimum downtime to the laboratory workflow. The AI/AS 1610 ensures ease-of-use and cost-effectiveness for high throughput laboratory work.

Chromatographic separation was achieved on a Thermo Scientific™ TRACE™ TR-PCB 8 MS capillary column, 50 m × 0.25 mm × 0.25 μm (P/N 26AJ148P). The column has been developed to ensure outstanding robustness for separation of the critical congeners, coupled with high thermal stability (with operating temperatures up to 360/370 °C) and low bleed for reliable and reproducible performance.

Additional GC-MS/MS and autosampler parameters as well as a complete list of the target compounds are detailed in Table 1 and Appendix 1, respectively.

**Table 1. GC-MS/MS and autosampler experimental conditions for the analysis of PCBs**

AI/AS 1610 autosampler parameters	
Injection type	Standard
Sample mode	Standard
Fill strokes	10
Sample depth	Bottom
Injection mode	Fast
Pre-injection delay time (s)	0
Post-injection delay time (s)	0
Pre-injection wash cycles	0
Post-injection wash cycles	4
Post-injection solvent wash volume (μL)	6.0
Sample wash cycles	1
Sample wash volume (μL)	1.0
Injection volume (μL)	1.0
SSL parameters	
Injection temperature (°C)	280
Liner	Thermo Scientific™ LinerGOLD™ splitless/split liner single taper with wool (P/N 453A1925-UI)
Inlet module and mode	SSL, splitless
Split flow (mL/min)	75
Splitless time (min)	1.2
Septum purge flow (mL/min)	5, constant
Carrier gas, flow (mL/min)	He, 1.2

Table 1 (continued). GC-MS/MS and autosampler experimental conditions for the analysis of PCBs

TRACE 1610 GC parameters	
<b>Oven temperature program</b>	
Temperature (°C)	90
Hold time (min)	1.00
Rate (°C/min)	25
Temperature 2 (°C)	270
Rate 2 (°C/min)	4
Temperature 3 (°C)	330
Hold time (min)	2
GC run time (min)	25.20
<b>Column</b>	
TRACE TR-PCB 8 MS	50 m, 0.25 mm, 0.25 µm (P/N 26AJ148P)

TSQ 9610 mass spectrometer parameters	
Transfer line temperature (°C)	280
Ion source type and temperature (°C)	NeverVent AEI, 300
Ionization type	EI
Emission current (µA)	50
Acquisition mode	timed-SRM
Q1 and Q3 resolution	Normal (0.7 amu)
Tuning parameters	AEI SmartTune
Collision gas and pressure (psi)	Argon at 70
Detector gain	X 7

## Data acquisition, processing, and reporting

Data was acquired, processed, and reported using Thermo Scientific™ Chromeleon™ Chromatography Data System (CDS) software, version 7.3. Integrated instrument control ensures full automation of the analytical workflow combined with an intuitive user interface for data analysis, customizable reporting, and storage in compliance with the U.S. Food and Drug Administration Title 21 Code of Federal Regulations Part 11 (Title 21 CFR Part 11). In particular, PCB quantitative analysis requires the use of isotope dilution (this feature is available in Chromeleon CDS from software version 7.2.9 onwards).

## Standard and sample preparation

### Standard preparation

The EPA Method 1668C standard solution kit (P/N 68C-CVS) at six calibration levels (68C-CS0.2 to 68C-CS5) containing native as well as <sup>13</sup>C mass-labeled PCB congeners and mass-labeled PCB internal standards was purchased from Wellington laboratories, Inc. The lowest calibration level (68C-CS02) was further diluted 1:2 in nonane to expand the calibration curve from 0.1 to 2,000 ng/mL. For the calculation of IDLs, the lowest calibration level was diluted 1:4 in nonane.

### Sample preparation

Water and soil samples were extracted and provided by Pacific Rim Laboratories Inc., Canada. A schematic of the sample preparation workflow is reported in Figure 1. Samples were dried before shipment and reconstituted with 50 µL of nonane, sonicated in the ultra-sonic bath for few minutes, and vortexed before injection into the chromatographic system.

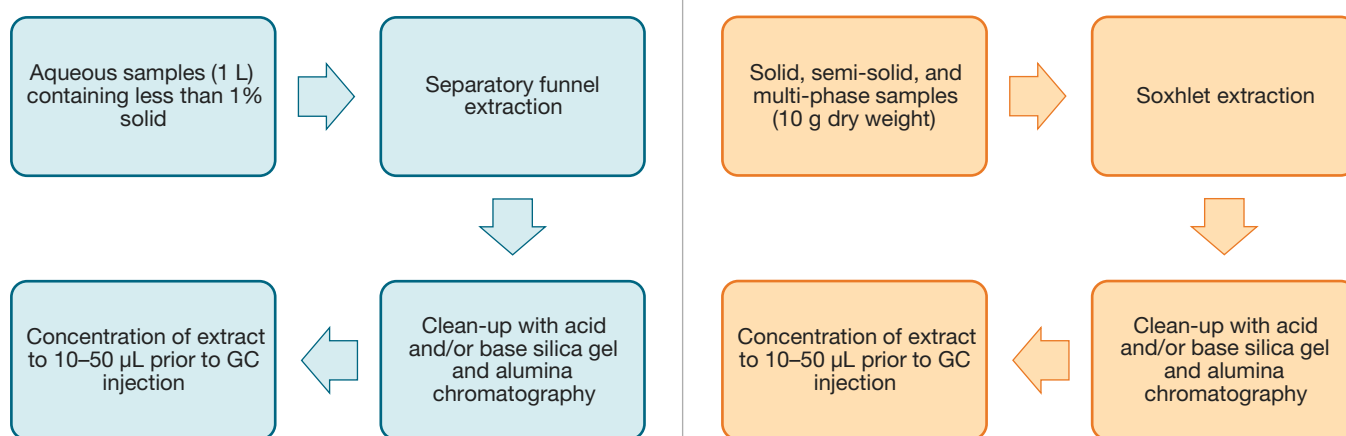


Figure 1. Sample preparation procedure for aqueous, solid, semi-solid and multi-phase samples

## Results and discussion

### Chromatography

The high selectivity of the TRACE TR-PCB 8 MS capillary column ensured the chromatographic resolution of the target analytes in 21 minutes, including the pentachlorobiphenyl critical pair PCB-123/PCB-118 for which the calculated resolution was 3% at the valley height. Moreover, Gaussian peak shape was achieved for the high molecular weight compounds such as PCB-209 (MW = 498.6) with calculated asymmetry factor of 1.2 as shown

in Figure 2. Two specific precursor ions, each with one specific corresponding product ion, were used to set up the timed-selected reaction monitoring (t-SRM) acquisition method. This allowed for high selectivity to discriminate between the target compounds and the complex matrix, thus ensuring a confident and selective identification of analytes. As an example, the total ion chromatograms (TIC) of a real sample acquired in EI, full-scan (FS,  $m/z$  100–600) showing the complexity of the matrices and the selectivity of the SRM acquisition is reported in Figure 3.

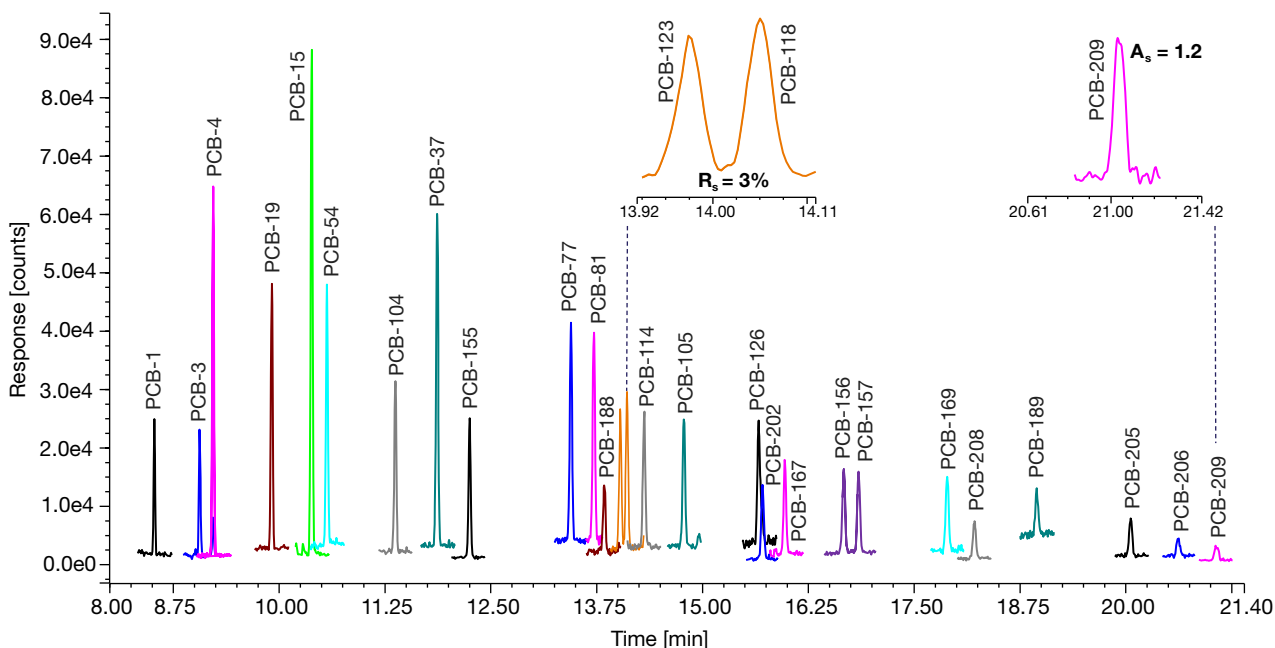


Figure 2. t-SRM acquisition showing baseline chromatographic separation for the investigated compounds in the lowest calibration standard diluted 1:2 (0.1 ng/mL). The insets highlight the resolution of the critical pair and the calculated asymmetry factor for the high boiling point congeners (PCB-209).

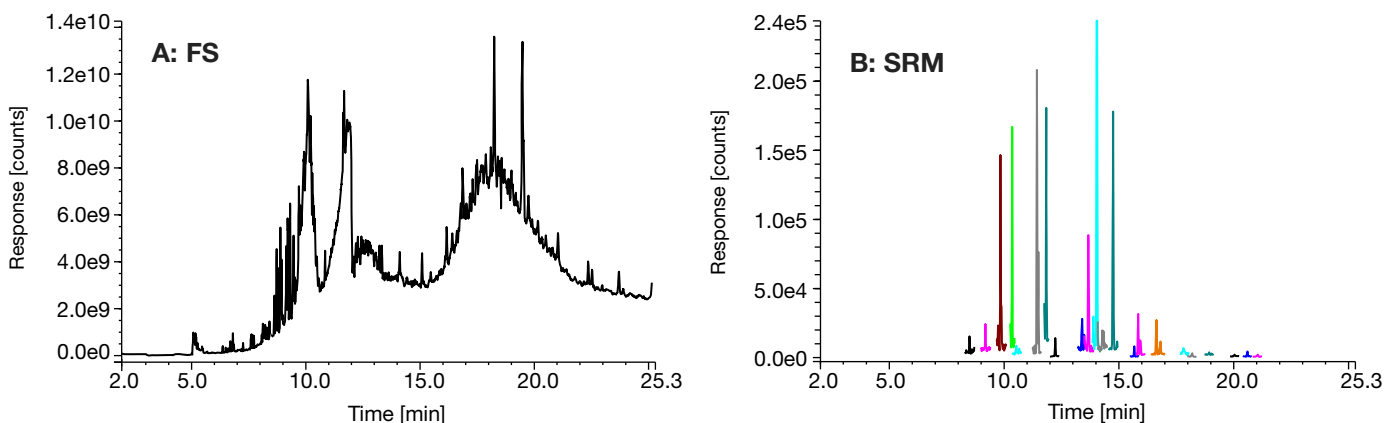


Figure 3. TIC (A) FS:  $m/z$  100–600, and (B) t-SRM acquisitions for environmental sample extract containing PCBs showing the complexity of the matrix (FS acquisition) and the selectivity of the t-SRM acquisition

## Linearity, instrument detection limit (IDL), and limit of quantitation (LOQ)

The TSQ 9610 NeverVent AEI ion source is equipped with the Thermo Scientific™ XLXR™ detector, which is an electron multiplier that offers extended detector lifetime and dynamic range. Calibration curves ranging from 0.10 to 2,000 ng/mL were prepared as detailed in the *Standard preparation* section. Each calibration level was injected in triplicate. Native PCB congeners were quantified using their corresponding isotopes using isotope dilution quantitation, the target analytes showed a linear trend with coefficient of determination ( $R^2$ ) > 0.990 and residual values (measured as %RSD of average response factors, AvCF %RSD) < 20%, thus confirming a wider linear range can be easily achieved as reported in Appendix 2. Full range calibration curves (0.10–2,000 ng/mL) for some selected DL-PCBs (PCB-77, 123, 118) and non-DL-PCBs (PCB-4, 209) as well as zoomed detail (0.1–1.0 ng/mL) are shown as examples in Figure 4.

Very often, data acquired using t-SRM have little noise, therefore the calculation of the IDLs and the LOQs based on the signal-to-noise (S/N) approach may be inadequate. The IDL was therefore determined for the individual congeners by diluting the CS0.2 standard four times, so that a final concentration of 0.05 ng/mL was achieved. This solution was repeatedly injected ( $n=10$ ). IDLs were calculated taking into account the one-tailed Student's *t*-test values for the corresponding  $n-1$  degrees of freedom at 99% confidence, the injected on-column (OC) concentration, and the absolute peak area %RSD (<15%) for each analyte. Calculated IDLs ranged from 3 fg to 19 fg OC, corresponding to 0.15 pg/L to 0.95 pg/L in water and to 0.015 to 0.095 ng/kg in soil samples as reported in Figure 5. The standard concentration used to assess the IDL was chosen as LOQ as (i) the ion ratios were within  $\pm 15\%$  of the expected values calculated as an average across a calibration curve ranging from 0.10 to 2,000 ng/mL, (ii) the absolute peak area repeatability, and (iii) the response factor (RF) RSD were <15%. The calculated ion ratios, as well as RF and peak area %RSD for the investigated compounds are detailed in Appendix 3.

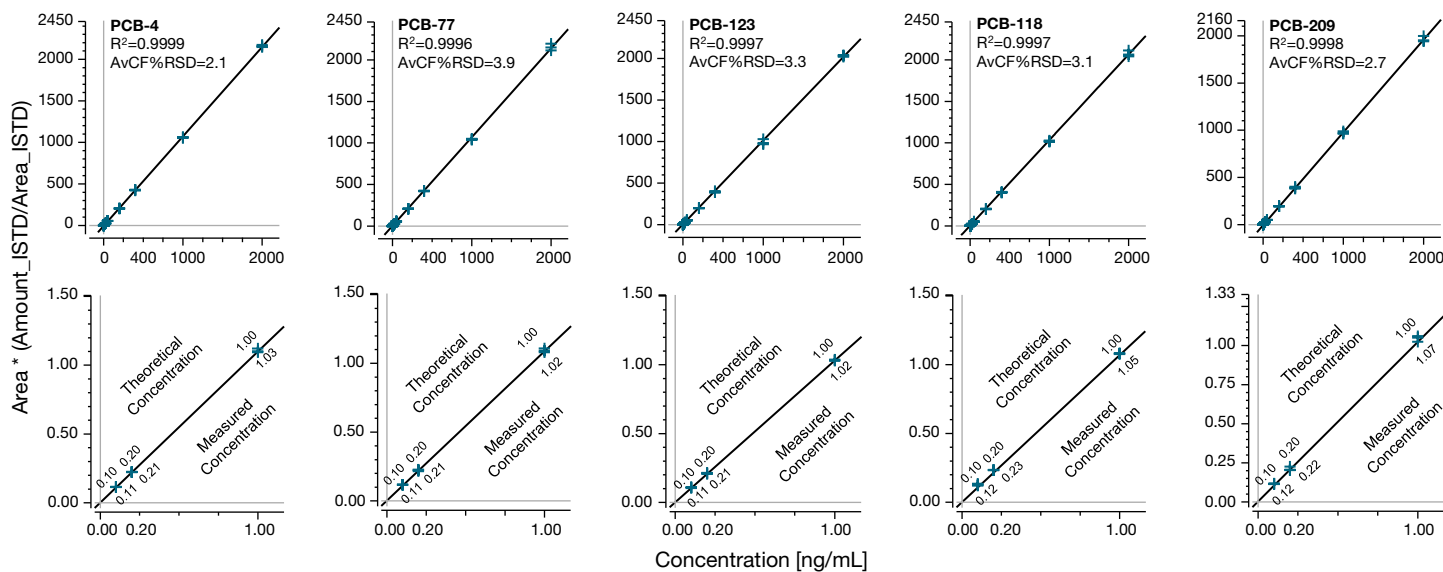


Figure 4. Example of solvent (nonane) calibration curves for some selected DL-PCBs (PCB-77, 123, 118) and non-DL-PCBs (PCB-4, 209) and zoomed detail (0.1–1.0 ng/mL). Each calibration level was injected in triplicate. Coefficient of determination ( $R^2$ ) and AvCF %RSD are annotated.

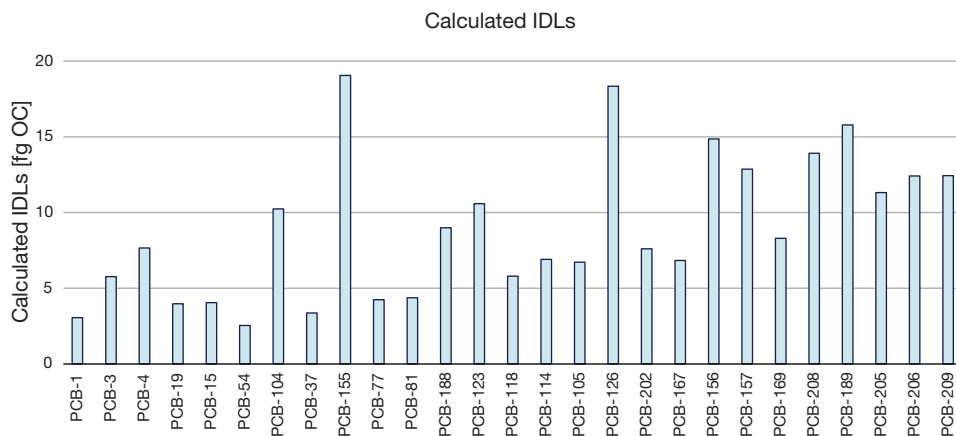


Figure 5. Calculated IDLs for PCB individual congeners. Calculated IDLs ranged from 3 fg to 19 fg OC, corresponding to 0.15 pg/L to 0.95 pg/L in water samples and to 0.015 ng/kg to 0.095 ng/kg in soil samples.

## Robustness

Analytical testing laboratories need to process a high number of samples every day, therefore it is critical that the instrument performs consistently. The Thermo Scientific™ SmartTune™ tool allows the user to check the tune status of the system with a few mouse clicks in an easy and quick fashion. The SmartTune tool uses the MS parameters established during the initial tuning with a clean source and intelligently assesses the performance of the system, only re-tuning when MS performance has been compromised. Instrument robustness for everyday analysis and quantitative performance was evaluated by repeatedly injecting

various environmental extracts (n=100). A quality control standard in nonane (QC) at a concentration of 1.0 ng/mL was injected in duplicate every 10 samples to monitor the system stability. The SmartTune feature was used to check the instrument status at the beginning, middle, and end of the sequence. No inlet or MS re-tuning or maintenance was required during the robustness evaluation. The QC showed stable response across the injections with ion ratios consistently within 15% of the calculated average from the calibration curve, calculated concentration within  $\pm 20\%$  of the spiked level, and QC absolute peak area %RSD <11% as shown in Figure 6.

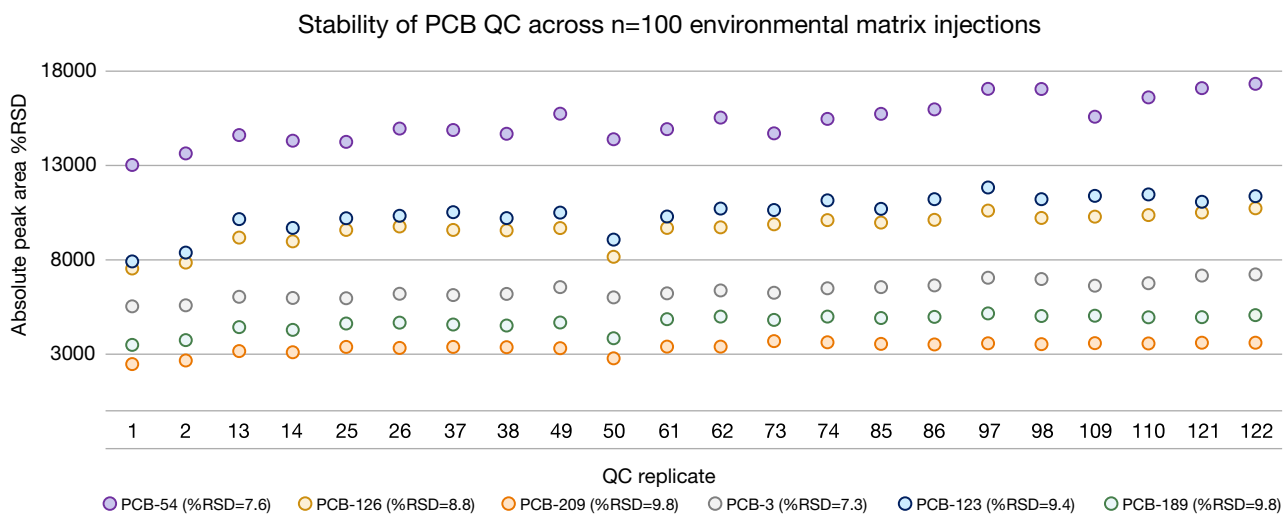


Figure 6. QC absolute peak area and %RSD across a sequence of n=100 injections of various environmental extracts

## Conclusion

The results obtained in these experiments demonstrate that the TSQ 9610 mass spectrometer equipped with the NeverVent AEI ion source in combination with the TRACE 1610 GC and the AI/AS 1610 liquid autosampler represents a reliable tool for analysis of PCBs in environmental samples.

- The high selectivity of the TRACE TR-PCB column ensured chromatographic separation of the target analytes in about 21 minutes. Calculated resolution of the critical pair PCB-123 / PBDE-118 was 3%. Furthermore, the column thin film phase, high thermal stability, and low column bleed ensured elution of the high boiling point PCBs (e.g., PCB-209) with improved peak shapes.
- The XLXR detector allowed for extended linearity over a concentration range of 0.10 to 2,000 ng/mL with coefficient of determination of  $R^2 > 0.990$  and AvCF %RSDs <20. Moreover, the CM advanced reprocessing capability allowed for isotope dilution quantitative analysis.

- The engineered design and the improved sensitivity of the NeverVent AEI ion source allowed for low instrument detection limits ranging from 3 fg to 19 fg OC (corresponding to 0.15 pg/L to 0.95 pg/L in water samples and to 0.015 to 0.095 ng/kg in soil samples) and LOQ set at 0.05 ng/mL, showing ion ratios within 15% of the expected values calculated as an average across a calibration curve, absolute peak area and RF %RSD < 15 even at such low analyte concentrations.
- The enhanced robustness and reliability of the AI/AS 1610 liquid autosampler combined with the inertness of the flow path and the stability of the NeverVent AEI ion source allowed for n=100 matrix injections without requiring any system re-tuning or MS or inlet maintenance.

## References

- United States Environmental Protection Agency, U.S. EPA, Learn about Polychlorinated Biphenyls (PCBS), <https://www.epa.gov/pcbs/learn-about-polychlorinated-biphenyls-pcbs>
- Stockholm Convention. <http://chm.pops.int/Implementation/IndustrialPOPs/PCBs/Overview/tabid/273/Default.aspx>
- United States Environmental Protection Agency, U.S. EPA, Method 1668C Chlorinated Biphenyl Congeners in Water, Soil, Sediment, Biosolids, and Tissue by HRGC/HRMS, April 2010, [https://www.epa.gov/sites/default/files/2015-09/documents/method\\_1668c\\_2010.pdf](https://www.epa.gov/sites/default/files/2015-09/documents/method_1668c_2010.pdf)

Appendix 1. List of target analytes, retention times, precursor and product ions, and collision energy

Compound	Retention time (min)	Window (min)	Precursor ion (Da)	Production (Da)	Collision energy (V)
PCB-1	8.5	0.5	188.04	153.04	22
PCB-1	8.5	0.5	190.04	153.04	22
PCB-1L13C	8.5	0.5	200.08	165.10	22
PCB-1L13C	8.5	0.5	202.08	165.10	22
PCB-3	9.03	0.5	188.04	153.04	22
PCB-3	9.03	0.5	190.04	153.04	22
PCB-3L13C	9.03	0.5	200.08	165.10	22
PCB-3L13C	9.03	0.5	202.08	165.10	22
PCB-4	9.19	0.5	222.00	152.06	22
PCB-4	9.19	0.5	224.00	152.06	22
PCB-4L13C	9.19	0.5	234.04	164.10	22
PCB-4L13C	9.19	0.5	236.04	164.10	22
PCB-19	9.88	0.5	255.96	186.02	22
PCB-19	9.88	0.5	257.96	186.02	22
PCB-19L13C	9.88	0.5	268.00	198.02	22
PCB-19L13C	9.88	0.5	270.00	198.02	22
PCB-15	10.36	0.5	222.00	152.06	22
PCB-15	10.36	0.5	224.00	152.06	22
PCB-15L13C	10.36	0.5	234.04	164.10	22
PCB-15L13C	10.36	0.5	236.04	164.10	22
PCB-54	10.54	0.5	289.92	219.98	22
PCB-54	10.54	0.5	291.92	219.98	22
PCB-54L13C	10.54	0.5	301.96	232.02	22
PCB-54L13C	10.54	0.5	303.96	232.02	22
PCB-104	11.34	0.5	323.90	253.95	22
PCB-104	11.34	0.5	325.90	255.95	22
PCB-104L13C	11.34	0.5	335.92	265.99	22
PCB-104L13C	11.34	0.5	337.92	267.99	22
PCB-37	11.84	0.5	255.96	186.02	22
PCB-37	11.84	0.5	257.96	186.02	22
PCB-37L13C	11.84	0.5	268.00	198.02	22
PCB-37L13C	11.84	0.5	270.00	198.02	22
PCB-155	12.2	0.5	357.80	287.90	24
PCB-155	12.2	0.5	359.80	289.95	24
PCB-155L13C	12.2	0.5	369.90	299.51	24
PCB-155L13C	12.2	0.5	371.90	301.95	24
PCB-101L13C	12.59	0.5	335.92	265.99	22
PCB-101L13C	12.59	0.5	337.92	267.99	22
PCB-111L13C	13.13	0.5	335.92	265.99	22
PCB-111L13C	13.13	0.5	337.92	267.99	22
PCB-77	13.42	0.5	289.92	219.98	22
PCB-77	13.42	0.5	291.92	219.98	22
PCB-77L13C	13.42	0.5	301.96	232.02	22
PCB-77L13C	13.42	0.5	303.96	232.02	22

Appendix 1 (continued). List of target analytes, retention times, precursor and product ions, and collision energy

Compound	Retention time (min)	Window (min)	Precursor ion (Da)	Production (Da)	Collision energy (V)
PCB-81	13.69	0.5	289.92	219.98	22
PCB-81	13.69	0.5	291.92	219.98	22
PCB-81L13C	13.69	0.5	301.96	232.02	22
PCB-81L13C	13.69	0.5	303.96	232.02	22
PCB-188	13.8	0.5	391.80	321.90	25
PCB-188	13.8	0.5	393.80	323.90	25
PCB-188L13C	13.8	0.5	403.80	333.90	25
PCB-188L13C	13.8	0.5	405.80	335.90	25
PCB-123	13.97	0.5	323.90	253.95	22
PCB-123	13.97	0.5	325.90	255.95	22
PCB-123L13C	13.97	0.5	335.92	265.99	22
PCB-123L13C	13.97	0.5	337.92	267.99	22
PCB-118	14.05	0.5	323.90	253.95	22
PCB-118	14.05	0.5	325.90	255.95	22
PCB-118L13C	14.05	0.5	335.92	265.99	22
PCB-118L13C	14.05	0.5	337.92	267.99	22
PCB-114	14.28	0.5	323.90	253.95	22
PCB-114	14.28	0.5	325.90	255.95	22
PCB-114L13C	14.28	0.5	335.92	265.99	22
PCB-114L13C	14.28	0.5	337.92	267.99	22
PCB-105	14.75	0.5	323.90	253.95	22
PCB-105	14.75	0.5	325.90	255.95	22
PCB-105L13C	14.75	0.5	335.92	265.99	22
PCB-105L13C	14.75	0.5	337.92	267.99	22
PCB-126	15.64	0.5	323.90	253.95	22
PCB-126	15.64	0.5	325.90	255.95	22
PCB-126L13C	15.64	0.5	335.92	265.99	22
PCB-126L13C	15.64	0.5	337.92	267.99	22
PCB-202	15.68	0.5	427.80	357.80	25
PCB-202	15.68	0.5	429.80	357.80	25
PCB-202L13C	15.68	0.5	439.80	369.90	25
PCB-202L13C	15.68	0.5	441.80	369.90	25
PCB-167	16	0.5	357.80	287.90	24
PCB-167	16	0.5	359.80	289.95	24
PCB-167L13C	16	0.5	369.90	299.51	24
PCB-167L13C	16	0.5	371.90	301.95	24
PCB-156	16.6	0.5	357.80	287.90	24
PCB-156	16.6	0.5	359.80	289.95	24
PCB-156L13C	16.6	0.5	369.90	299.51	24
PCB-156L13C	16.6	0.5	371.90	301.95	24
PCB-157	16.82	0.5	357.80	287.90	24
PCB-157	16.82	0.5	359.80	289.95	24
PCB-157L13C	16.82	0.5	369.90	299.51	24
PCB-157L13C	16.82	0.5	371.90	301.95	24

Appendix 1 (continued). List of target analytes, retention times, precursor and product ions, and collision energy

Compound	Retention time (min)	Window (min)	Precursor ion (Da)	Production (Da)	Collision energy (V)
PCB-169	17.86	0.5	357.80	287.90	24
PCB-169	17.86	0.5	359.80	289.95	24
PCB-169L13C	17.86	0.5	369.90	299.51	24
PCB-169L13C	17.86	0.5	371.90	301.95	24
PCB-208	18.18	0.5	461.70	391.80	25
PCB-208	18.18	0.5	463.70	393.80	25
PCB-208L13C	18.18	0.5	473.80	403.80	25
PCB-208L13C	18.18	0.5	475.80	405.80	25
PCB-189	18.92	0.5	391.80	321.90	25
PCB-189	18.92	0.5	393.80	323.90	25
PCB-189L13C	18.92	0.5	403.80	333.90	25
PCB-189L13C	18.92	0.5	405.80	335.90	25
PCB-205	20.04	0.5	427.80	357.80	25
PCB-205	20.04	0.5	429.80	357.80	25
PCB-205L13C	20.04	0.5	439.80	369.90	25
PCB-205L13C	20.04	0.5	441.80	369.90	25
PCB-206	20.6	0.5	461.70	391.80	25
PCB-206	20.6	0.5	463.70	393.80	25
PCB-206L13C	20.6	0.5	473.80	403.80	25
PCB-206L13C	20.6	0.5	475.80	405.80	25
PCB-209	21.03	0.5	495.70	425.80	25
PCB-209	21.03	0.5	497.70	427.80	25
PCB-209L13C	21.03	0.5	507.70	437.80	25
PCB-209L13C	21.03	0.5	509.70	439.80	25

Appendix 2. List of target analytes, calculated coefficient of determination ( $R^2$ ), and residual values (measured as %RSD of average response factors, AvCF %RSD)

Compound	Retention time (min)	Coefficient of determination ( $R^2$ )	AvCF %RSD	Compound	Retention time (min)	Coefficient of determination ( $R^2$ )	AvCF %RSD
PCB-1	8.49	0.100	1.5	PCB-114	14.27	0.100	3.6
PCB-3	9.03	0.100	1.2	PCB-105	14.74	0.100	3.2
PCB-4	9.19	0.100	2.1	PCB-126	15.62	0.100	1.9
PCB-19	9.88	0.100	1.6	PCB-202	15.67	0.100	2.7
PCB-15	10.35	0.100	1.2	PCB-167	15.93	0.997	10.0
PCB-54	10.53	0.100	2.1	PCB-156	16.62	0.995	13.8
PCB-104	11.34	0.100	2.1	PCB-157	16.80	0.994	14.3
PCB-37	11.83	0.100	1.9	PCB-169	17.84	0.994	14.4
PCB-155	12.21	0.992	17.3	PCB-208	18.16	0.100	1.8
PCB-77	13.40	0.100	3.9	PCB-189	18.90	0.100	2.6
PCB-81	13.68	0.999	5.0	PCB-205	20.00	0.100	3.6
PCB-188	13.80	0.100	2.9	PCB-206	20.57	0.100	1.9
PCB-123	13.96	0.100	3.3	PCB-209	21.02	0.100	2.7
PCB-118	14.04	0.100	3.1				

Appendix 3. Calculated IDLs (fg OC), as well as ion ratios (IR, expected and measured), peak area %RSD, and RRF at the chosen LOQ (0.05 ng/mL) for the investigated compounds

Compound	Absolute peak area %RSD	RF %RSD	Expected IR	Average measured IR (n=10)	Calculated IDL (fg OC)
PCB-1	2.2	2.4	33	33	3
PCB-3	4.1	4.3	33	35	6
PCB-4	5.4	5.2	64	65	8
PCB-19	2.8	2.9	62	67	4
PCB-15	2.9	2.3	64	67	4
PCB-54	1.8	2.8	64	65	3
PCB-104	7.3	6.3	95	99	10
PCB-37	2.4	2.4	61	63	3
PCB-155	13.5	6.5	124	123	19
PCB-77	3.0	1.9	63	66	4
PCB-81	3.1	2.9	63	65	4
PCB-188	6.4	6.2	157	148	9
PCB-123	7.5	7.5	102	94	11
PCB-118	4.1	3.5	101	96	6
PCB-114	4.9	4.1	96	97	7
PCB-105	4.8	5.7	95	93	7
PCB-126	13.0	11.6	90	83	18
PCB-202	5.4	6.6	64	66	8
PCB-167	4.8	5.3	123	119	7
PCB-156	10.5	8.2	123	130	15
PCB-157	9.1	5.4	122	128	13
PCB-169	5.9	10.4	129	132	8
PCB-208	9.9	6.6	98	98	14
PCB-189	11.2	10.9	154	151	16
PCB-205	8.0	6.4	64	64	11
PCB-206	8.8	6.2	97	98	12
PCB-209	8.8	6.6	110	111	12