Waters™

Note d'application

# Routine Quantitation of Polychlorinated Biphenyls (PCBs) in Sediments Using Electron Ionization GC-MS/MS

Kari L. Organtini, Stephanie Crombie, Serge Moore, Kenneth J. Rosnack

Waters Corporation, Environment and Climate Change Canada

This is an Application Brief and does not contain a detailed Experimental section.

## Abstract

This application brief demonstrates to evaluate the Xevo TQ-GC as a fit for purpose electron ionization (EI) GC-MS/MS for the routine analysis of polychlorinated biphenyls (PCBs) extracted from sediment samples.

### Benefits

Xevo TQ-GC is a fit for purpose GC-MS/MS solution for routine analysis of PCBs in sediment samples.


## Introduction

Polychlorinated biphenyls (PCBs) are a class of man-made chemicals that, although were banned in the late 1970's, are still persistent in the environment. Exposure to PCBs is well known to cause a variety of adverse health effects. There are 209 congeners varied by the number and substitution pattern of chlorines on the biphenyl backbone. Toxicity varies by congener and the World Health Organization hosts additional information about toxicity on their website. Therefore, environmental monitoring of these compounds is still necessary.

Various sediment sample extracts previously prepared on site at Environment and Climate Change Canada Quebec Laboratory for Environmental Testing (QLET) were used for this evaluation. A suite of 41 PCBs ($Cl_3$ through $Cl_{10}$) were chosen based on toxicity, abundance in Aroclor mixes, and persistence in the environment. This list of PCBs was evaluated on the Xevo TQ-GC for routine performance criteria such as sensitivity, accuracy, and robustness based on analysis of the extracted sediment samples.

## Results and Discussion

For analysis, a calibration range of 0.1–20 µg/kg was utilized and the Xevo TQ-GC demonstrated excellent linearity for all compounds with $R^2$ values ≥0.997. Sensitivity was evaluated by determining limit of detection (LOD) values using solvent standards for each PCB based on 5 replicate injections. Table 1 highlights the overall results of the LODs for each congener group. On average, the LODs were well below 0.100 µg/kg, demonstrating sensitivity into the parts per trillion (ppt) range.

| Congener class | Average LOD (µg/kg) | LOD range (µg/kg) |
|---|---|---|
| $Cl_3$ | 0.010 | 0.003–0.016 |
| $Cl_4$ | 0.015 | 0.005–0.027 |
| $Cl_5$ | 0.032 | 0.013–0.090 |
| $Cl_6$ | 0.068 | 0.022–0.114 |
| $Cl_7$ | 0.045 | 0.017–0.058 |
| $Cl_8$ | 0.051 | 0.028–0.074 |
| $Cl_9$ | 0.059 | 0.056–0.062 |
| $Cl_{10}$ | 0.045 | 0.045 |

*Table 1. Average LOD and LOD range for each PCB congener class included in method. LOD calculated from 5 replicate injections of solvent standard.*

Quantitation of PCBs can be performed multiple ways depending on reporting requirements. Quantitative values can be determined for individual PCBs, by congener group, or by Aroclor mix. The totals functionality in TargetLynx allows for the latter two quantitative schemes as well as options for custom reports. Figure 1 demonstrates the pentachlorinated PCB MRM channel, with only the targeted penta PCBs summed on the top trace, and the entire congener group summed on the bottom trace. Four sediment samples were evaluated, and total PCB congener sums are shown for each sample in Figure 2. The total PCB concentration ranged widely between samples, ranging from 16–2000 µg/kg.

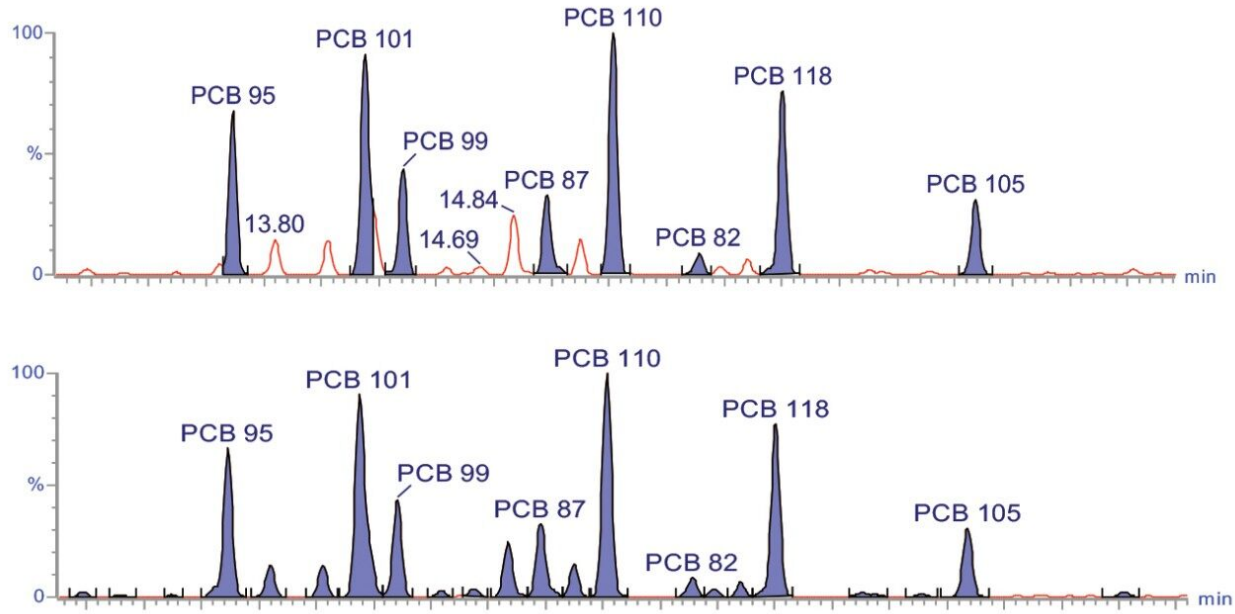


*Figure 1. MRM channel for pentachlorinated PCBs demonstrating individual compound quantitation (top) and congener group quantitation (bottom). Full method details for PCB analysis on TQ-GC can be accessed in Quanpedia (www.marketplace.waters.com).*

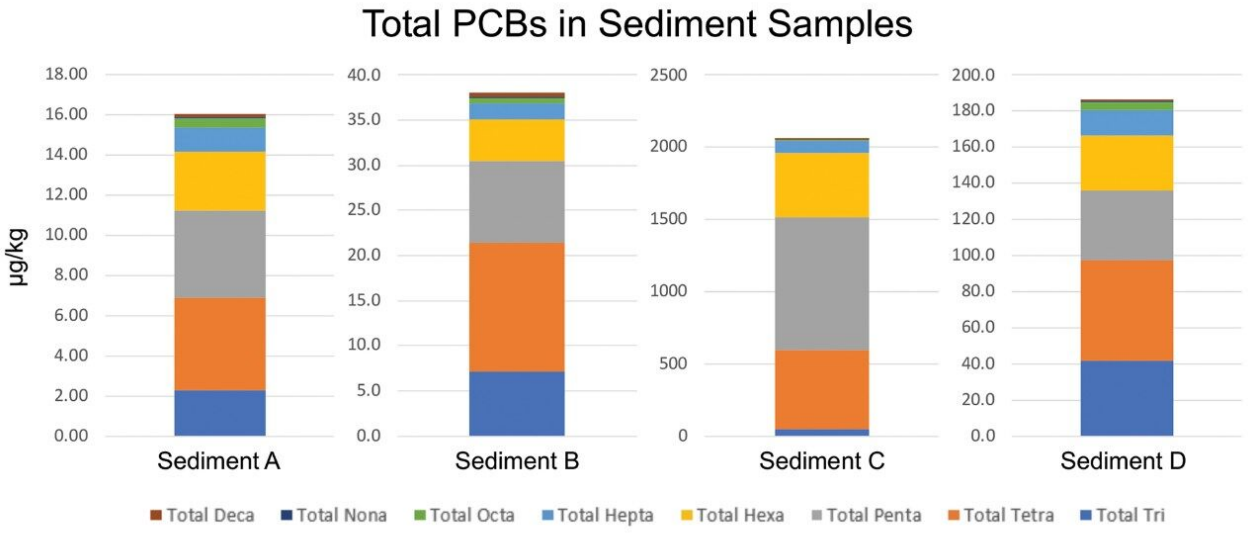


*Figure 2. Quantitation of PCBs by congener group for each sediment sample evaluated.*

Finally, robustness of the quantitative method was evaluated using 50 replicate injections of one of the sediment samples. Percent RSD was monitored for the reported calculated concentration of all detected PCBs in the sample. Figure 3 demonstrates the Trendplot of PCB 17 ($Cl_3$) and PCB 209 ($C_{l10}$) over the 50 injections with % RSD values of 1.1 and 7.4, respectively. All detected PCBs demonstrated % RSDs <10%, with a majority <5%. This establishes that the analysis of PCBs on the Xevo TQ-GC is robust and suitable for routine use.

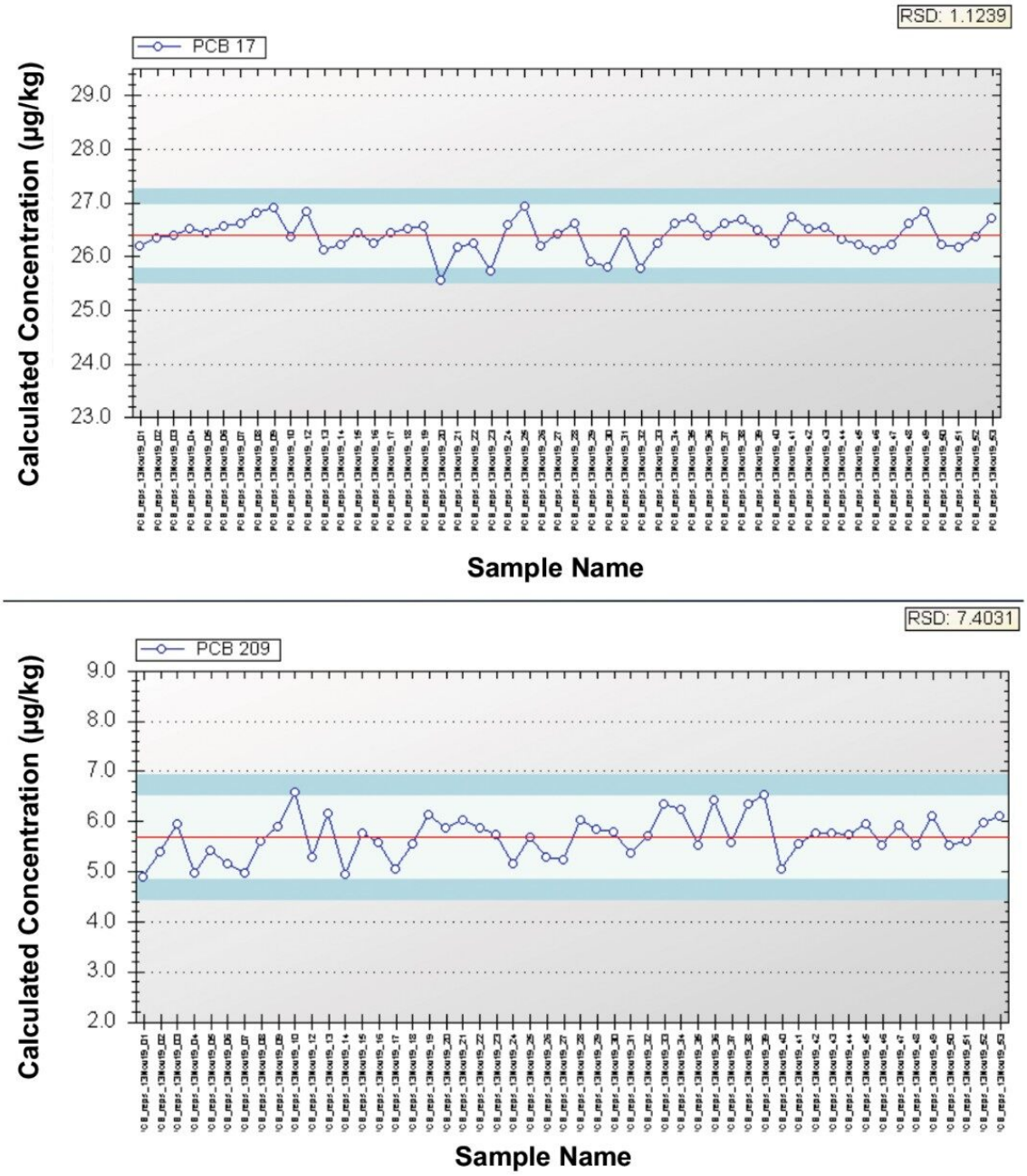


*Figure 3. Calculated concentration plotted over 50 injections of a sediment sample for PCB 17 (top) and PCB 209 (bottom). Red line indicates mean, light blue highlights 2 standard deviations from mean, dark blue highlights 3 standard deviations from mean.*

## Conclusion

The Xevo TQ-GC is demonstrated to be suitable for the routine, accurate, and robust analysis and quantitation of PCBs in sediment samples. Average limits of detection for each congener group ranged from 0.010 to 0.068 µg/kg, indicating the Xevo TQ-GC can detect trace levels of PCBs in sediment samples, allowing the instrument to meet and exceed global regulatory requirements. Analytical laboratories could extend this application for PCB analysis to other types of environmental and food matrices and analyses with proper sample preparation consideration.

## Featured Products

Xevo TQ-GC Mass Spectrometry System <https://www.waters.com/134977323>

TargetLynx <https://www.waters.com/513791>

720006885, July 2020