

# Determining PCB Aroclors in Matrix by GC MSMS Tandem Mass Spectrometry

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January 2013  
Poster #



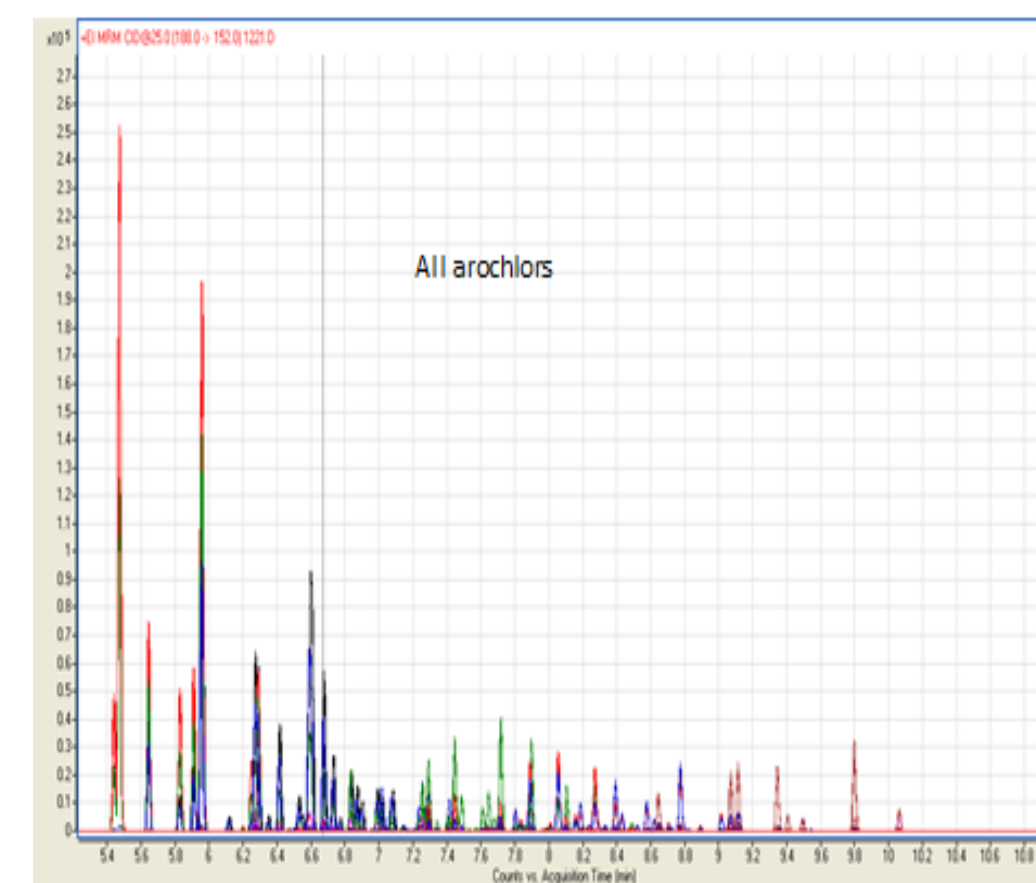
## Introduction

Poly chlorinated biphenyls or PCB Aroclors are ubiquitous synthetic entities not known to naturally occur in the environment. These compounds were synthesized primarily for use as coolants and insulating fluids in electrical equipment. Initially PCB Aroclors were valued for their chemical stability however, the fact that they are so stable resulted in environmental persistence and ultimately, a ban on PCB production

Aroclors are PCB mixtures that were produced from approximately 1930 to 1979. Aroclor is one of the most commonly known trade names for PCB mixtures. There are many types of Aroclors and each has a distinguishing suffix number that indicates the degree of chlorination. The numbering standard for the different Aroclors is as follows:

The first two digits generally refer to the number of carbon atoms in the phenyl rings (for PCBs this is 12), the second two numbers indicate the percentage of chlorine by mass in the mixture. For example, the name Aroclor 1254 means that the mixture contains approximately 54% chlorine by weight.

Herein is a presentation of Data collected on Agilent's GC-tandem mass spectrometer GCMS/MS 7000B which offers both superior sensitivity and selectivity for the analysis of PCB Aroclors in matrices. The purpose of the analysis is to quantitatively identify the amount of PCB Aroclors present in the matrix



## Instrument Parameters

Deca	497.7	Wide	427.7	Wide	20	25
Nona	461.7	Wide	391.8	Wide	20	25
Octa	427.8	Wide	357.8	Wide	20	25
Hepta	393.8	Wide	323.9	Wide	20	25
Hexa	359.8	Wide	289.9	Wide	20	25
Penta	325.9	Wide	255.9	Wide	20	25
Tetra	291.9	Wide	222	Wide	20	25
Tri	258	Wide	186	Wide	20	25
Di	222	Wide	152	Wide	20	25
Mono	188	Wide	152	Wide	20	25
Acenaphthene D10	164	Wide	160	Wide	20	50
Acenaphthene D10	164	Wide	82	Wide	20	50

GC-MS/MS Conditions  
MMI Inlet (He)  
Injection Volume: 1 µL  
Mode: splitless injection  
Injector split/splitless: 250 °C

Column #1  
HP5MSUI (30 m x 250 µm x 0.25 µm)  
Constant Flow: 0.72 mL/min

Oven Program:  
70 °C for 1.5 min  
16 °C/min to 200 °C for 1.5 min

MS Transfer Line: 280 °C

EI Mode, Source: 280 °C

Run Time: 10.125 min

## Results and Discussion

### Analytical Method

A Multi point calibration curve was used for unknown's analysis and quantification. The PCB Aroclor calibration concentrations are as follows:  
5ng/ml, 10ng/ml, 20ng/ml, 40ng/ml, 50ng/ml

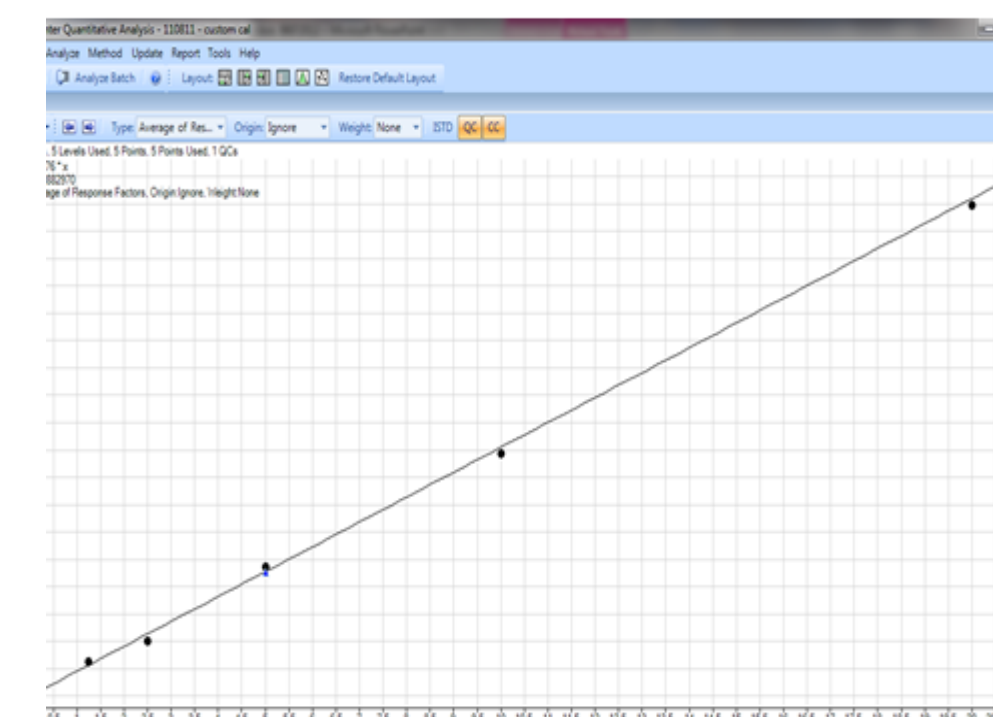
A single time segment was used to monitor the Mono through Nona transitions.

For Mass Quantification the Relative Response Factor (RRF) method was used to determine the amount of each Aroclor present in the sample. Mass quantification was on the sum of all relevant transitions for the particular Aroclor

Quantification is based on the following:  
(Formula based on injection and quantification of a known mass of Internal Standard (IS) and a calibration standard containing individual Aroclors of interest, an RRF was calculated for each Aroclor.

All individual Aroclors were then combined into a single calibration curve Table which is used in the analysis of unknowns) the assumption used is that the RRF stays the same between the calibration standard and sample. Example RRF calculations are as follows:

From the calibration standard data:  
RRF Aroclor 1260 = (mass 1260 in calibration standard/area 1260 in calibration standard) / (mass IS in calibration standard/area IS in calibration standard)  
From the sample, data rearranging the RRF equation to solve for Aroclor mass and plugging in the RRF calculated above: Mass Aroclor 1260 = (RRF Aroclor 1260)x(area Aroclor1260 in sample)x(mass IS in sample/area IS in sample)



9 unique Aroclor standards were used for acquiring the calibration curves. When analyzing unknown samples there is often co-eluting Aroclors. In these instances a subset of the Aroclors total areas is used to isolate and identify the Aroclor from other Aroclors.

In these instances it is necessary to use both the Quantitative and Qualitative program in Mass Hunter to make the appropriate determination as to what co-elution's exist and the effect that it has on the concentration of a particular Aroclor.

Based on previous work by Dr. Frame<sup>(1)</sup> the following table shows the predicted ratios of 5 individual Aroclors.

Table 3. Typical PCB Homologue Composition % wt. of Pure PCB Aroclors PCB Homologue	Aroclor 1016 (%)	Aroclor 1242 (%)	Aroclor 1248 (%)	Aroclor 1254 (%)	Aroclor 1260 (%)
Mono-CB	0.7	0.8	0	0	0
Di-CB	17.6	15.0	0.4	0.2	0.1
Tri-CB	54.7	44.9	22.0	1.3	0.2
Tetra-CB	26.6	32.8	56.6	16.4	0.8
Penta-CB	0.8	0.4	15.6	53.0	8.6
Hexa-CB	0	0.3	2.0	26.8	43.4
Hepta-CB	0	0	0.6	2.7	38.9
Octa-CB	0	0	0	0	8.3
Nona-CB	0	0	0	0	0.7
Deca-CB	0	0	0	0	0
Percentage	12.88	51.76	8.78	15.73	10.61

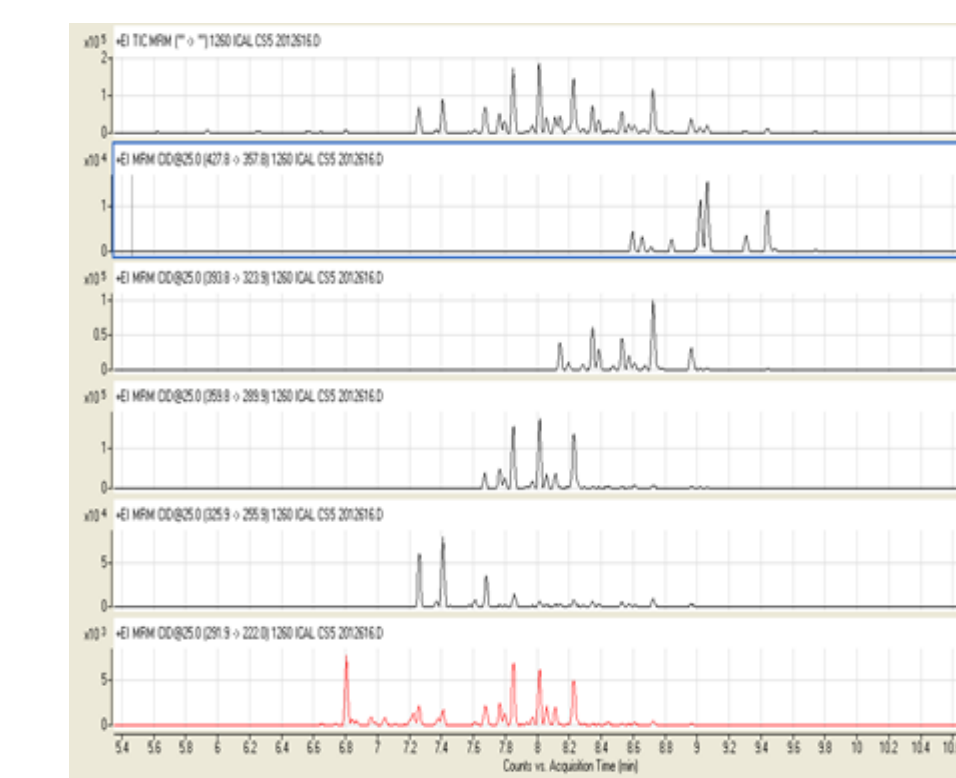
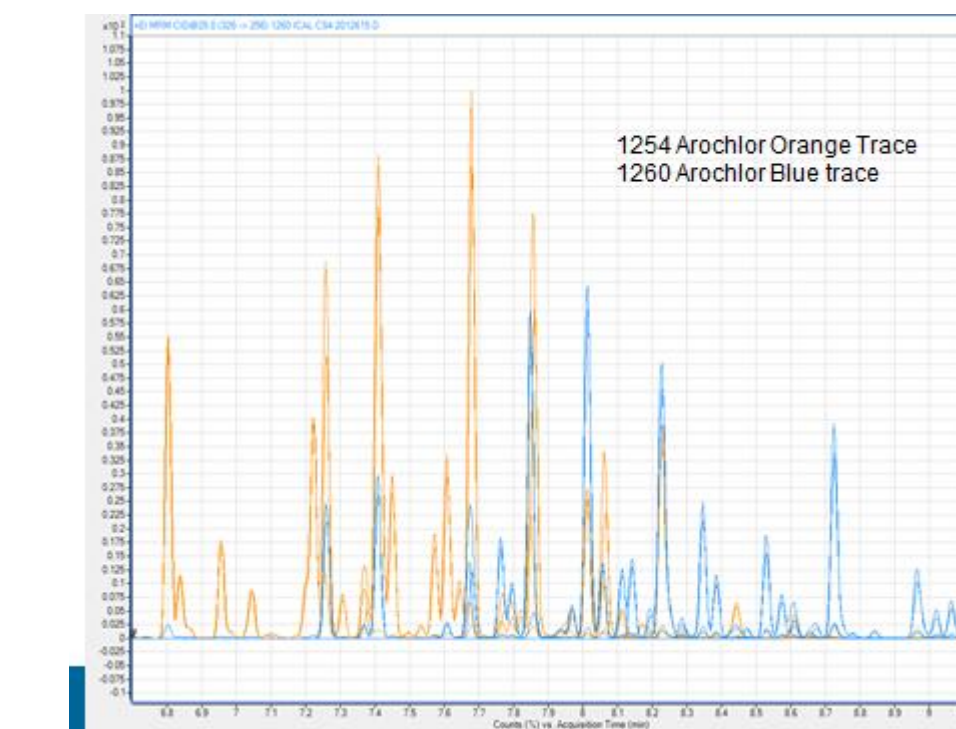
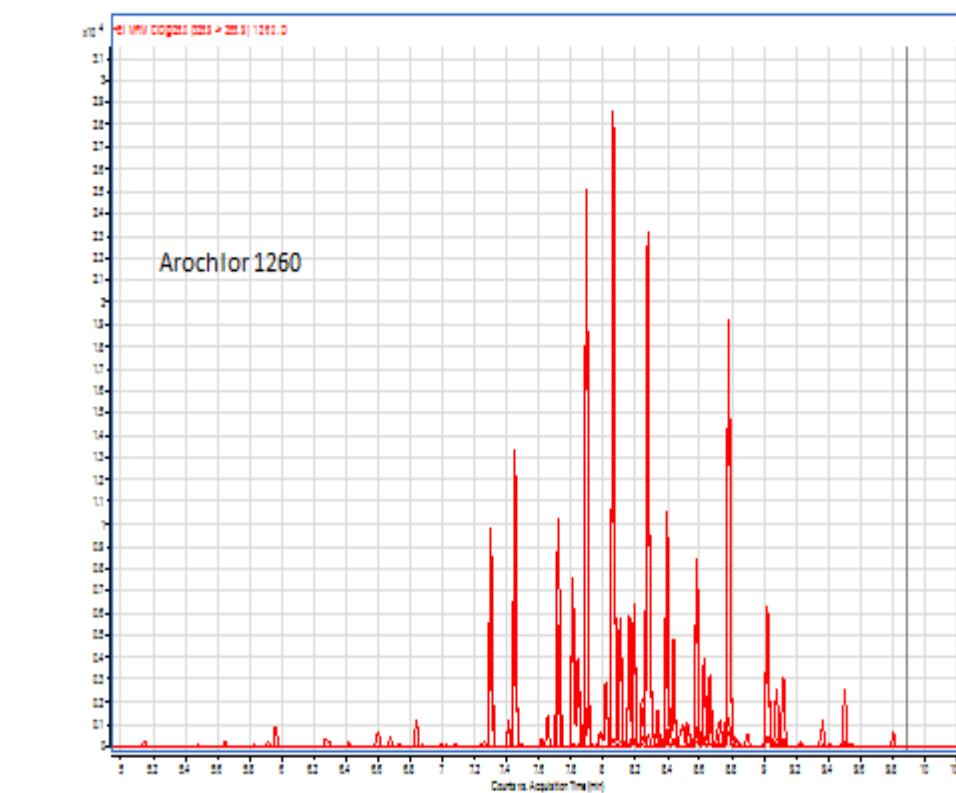
## Results and Discussion

PCB Aroclors are persistent environmental pollutants. In the United States and other countries around the world, PCBs were widely used as dielectric fluids in transformers and capacitors and also used as coolants. In 1979, PCB production was banned in the late twentieth century.

The work presented herein demonstrates the applicability of GC tandem mass spectrometry to monitor exposure to PCB Aroclors in matrix. The same methodology is also applied to matrices such as gas-phase air, particulate phase air, sediment and sediment pore water. Human health studies concluded that PCB Aroclors are probable carcinogens and exposure can also result in deleterious effects on the immune, reproductive and endocrine systems.

Traditionally the analysis for PCB Aroclors is done by GC Electron Capture Detector (ECD) methodology. Historically a traditional single stage GCMS system has lacked the ability to achieve the detection limits of an ECD due to matrix interferences.

In this study we employed the use of a GC-tandem mass spectrometry (GC-MS/MS) The GC-MS/MS not only achieved but surpassed the required detection limits of the traditional GC ECD detector. In addition to achieving the detection limits the system also offers confirmation of the compound by using the individual Congener groups to positively identify the compounds by utilizing both the GC retention times and the MRM transition for the Aroclor. Comparing the data with that obtained via GC-ECD suggests that GC-MS/MS is an appropriate tool and offers a confirmatory technique. Labs may now expand GC-MS/MS for the analysis of PCB Aroclors in matrix.



## Bibliography

1. Frame et al. (1996) has reported on the detailed analyses of the PCB congener distributions present in Aroclors 1016, 1242, 1248, and 1254. Because of variation to the chlorination process during chemical synthesis, no two batches of the same Aroclor had identical PCB congener distributions. In fact, substantial differences in congener profiles between batches of the same Aroclor could lead to significant differences in biological effects (Kodavanti et al., 2001).