Increasing Sample Throughput in Ultra-trade Environmental Analysis with the TSQ-9610 GC-MS/MS

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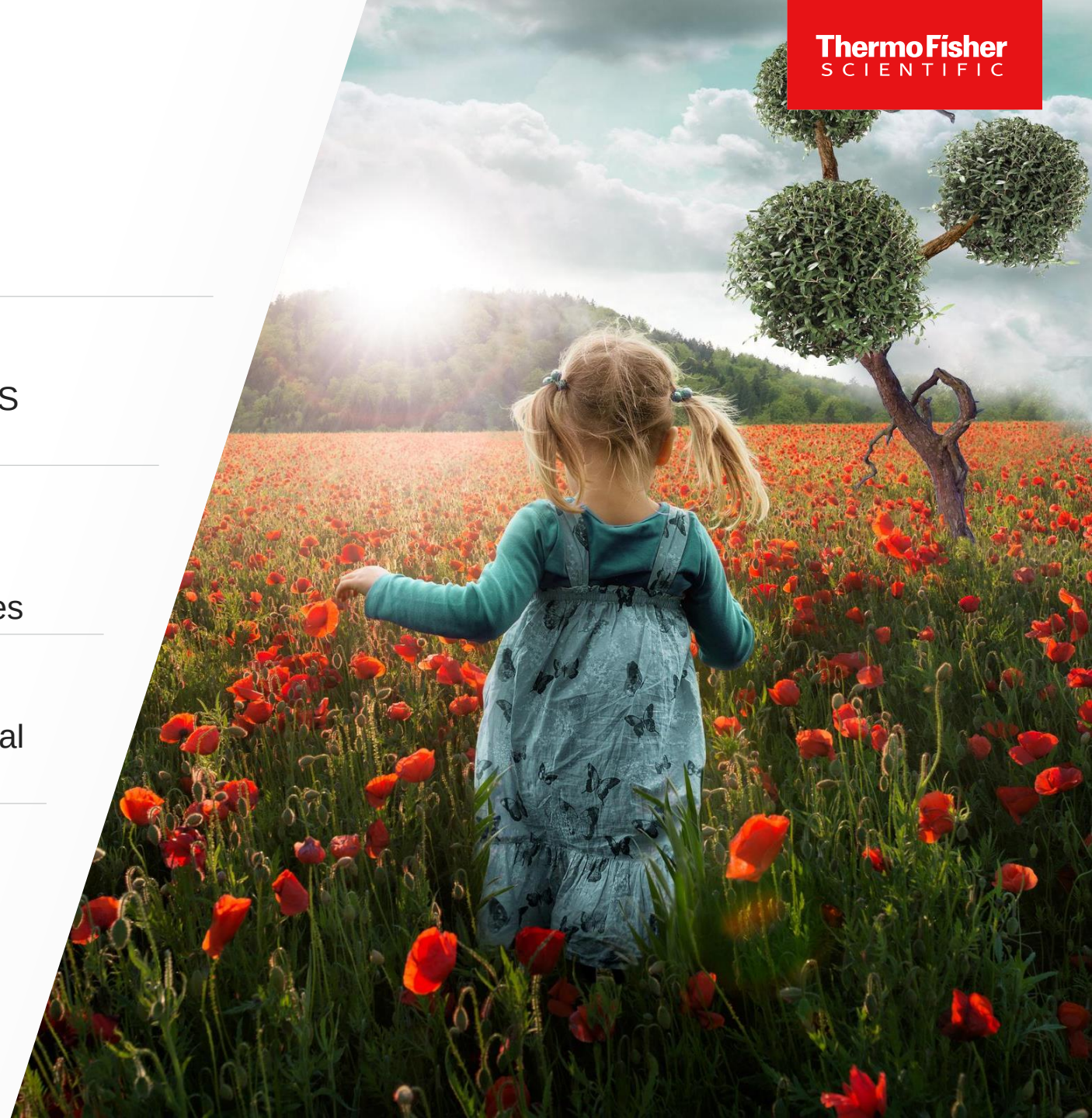
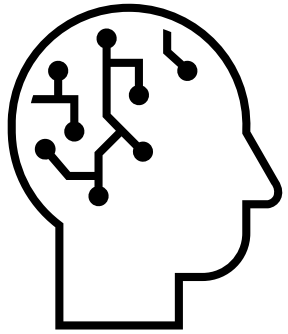
Agenda

1. Introduction
2. Challenges associated with ultra-trace GC-MS/MS analysis in environmental samples
3. TSQ-9610 features to address analysis challenges
4. Applicability of TSQ-9610 to various environmental samples: PBDEs, “BOP”, Chlorophenolics
5. Conclusions



Analytical Challenges in the Environmental Laboratory



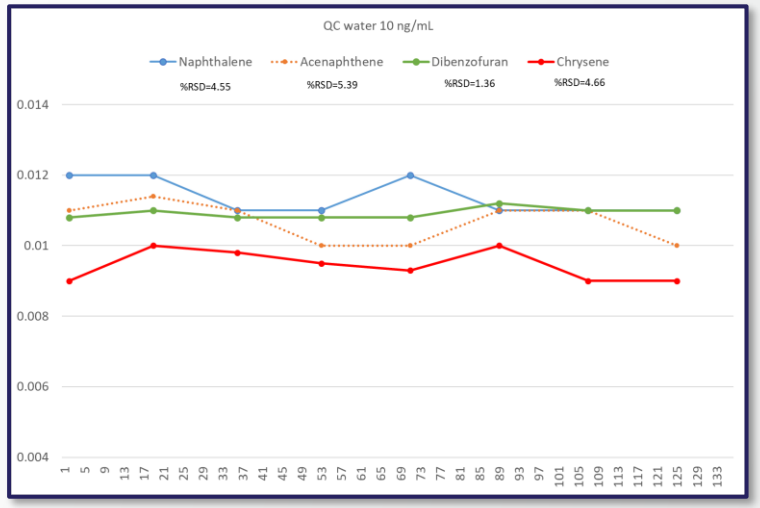
- Maximizing sample throughput, minimizing instrument downtime
- Sensitivity, linearity, and applicability to multiple methods, analytical targets, and matrices
- Ensuring repeatability and instrument robustness for compliance
- Ease-of-use for both hardware and software

Increasing instrument uptime

NeverVent™ Technology

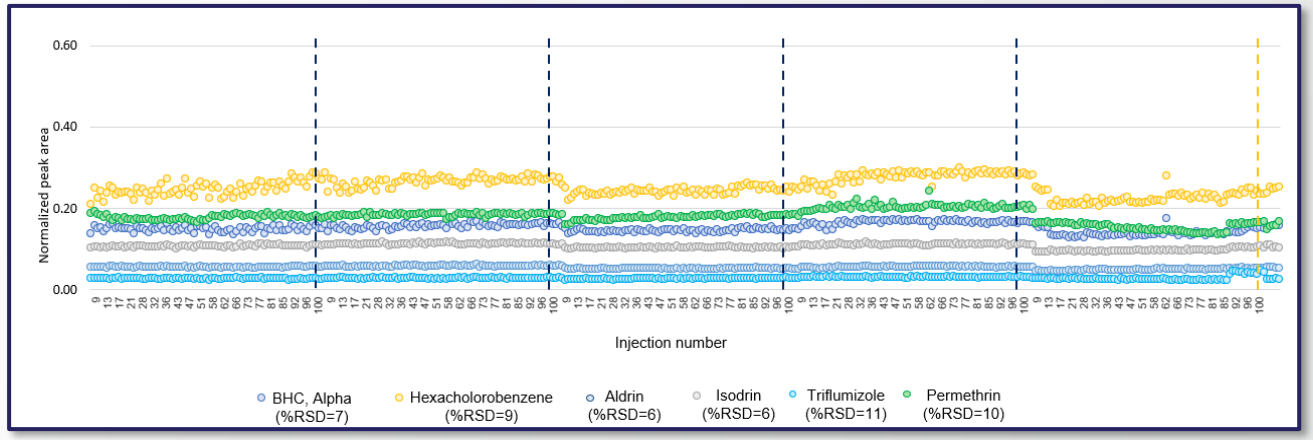
- Thermo Scientific™ NeverVent™ technology allows analytical laboratories to perform maintenance without interrupting their workflow
- Remove and maintain ionization source without venting the mass analyzer
- Return to routine analysis in minutes

		Maintenance activity		
		Column change (hrs:mins)	Exchange ion source (hrs:mins)	Replace filaments (hrs:mins) (only available on NV-AEI)
Standard GC-MS	Requires vacuum system venting and pump down operations	4:35	4:00	4:00
NeverVent GC-MS	Venting and pump down not required	00:35	00:05	00:05
NeverVent time savings		87%	98%	98%



↑ Analysis of PAH in water at 0.01 ppm over 130 injections on ISQ-7610

↓ 500 injections of baby food matrix, monitoring pesticides at 10 ug/kg.

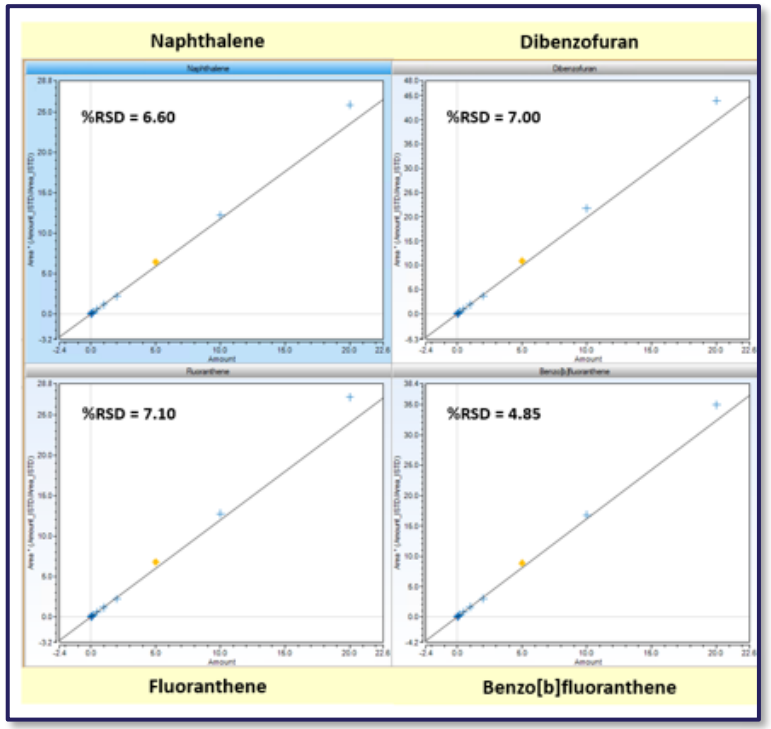


Maximizing sample throughput

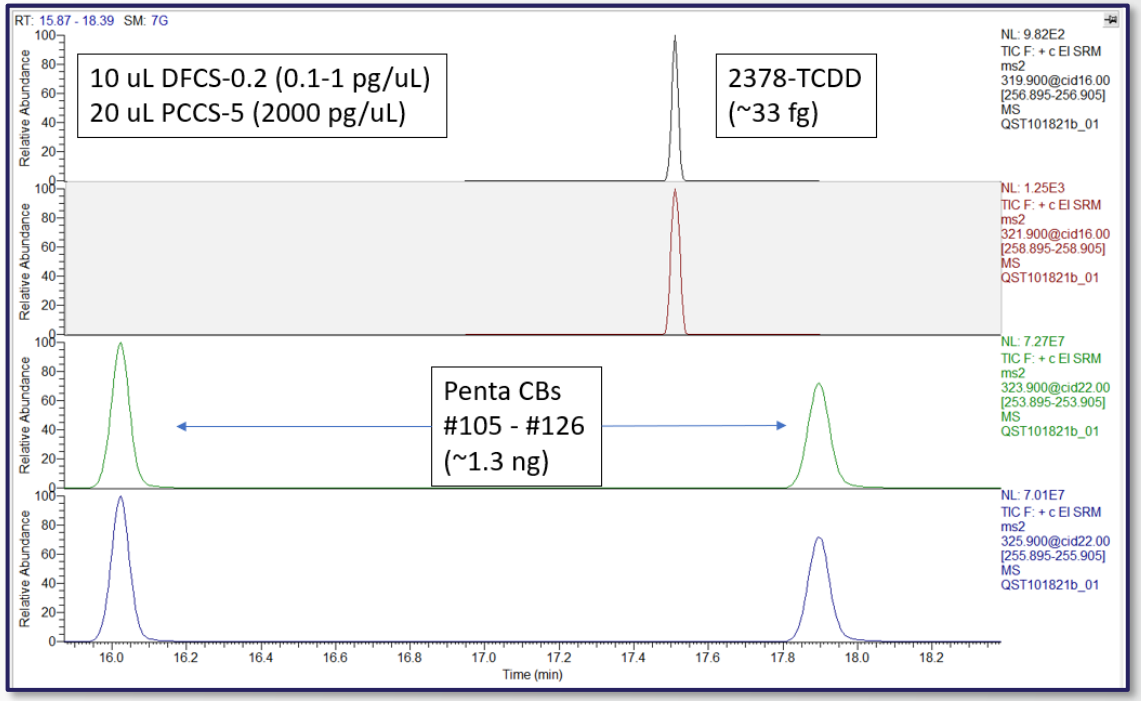
Extended dynamic range and lifetime detector

- The XLXR detector provides extended dynamic range and lifetime allowing method consolidation and increased instrument uptime

- 7x increased detector lifespan



Linearity of PAH spans over 4 orders of magnitudes, from 2.5 to 20000 ng/mL

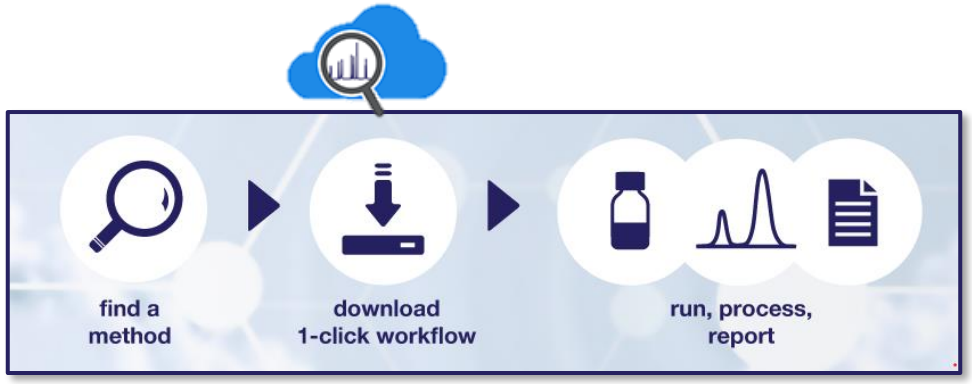


Analysis of trace concentrations of dioxins and high concentration PCBs in a single method using the TSQ 9610 AEI

Ensuring ease-of-use

Ready to use methods, optimization tools and instrument health

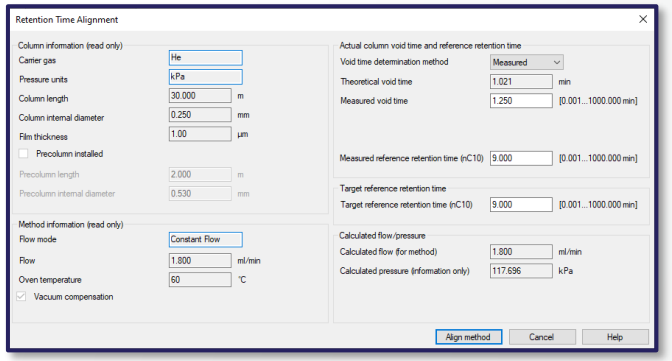
- Apps Lab provides methods that are ready to implement. Intelligent software tools allow methods to be optimized with ease. Instrument health enables real-time maintenance decisions to be made.

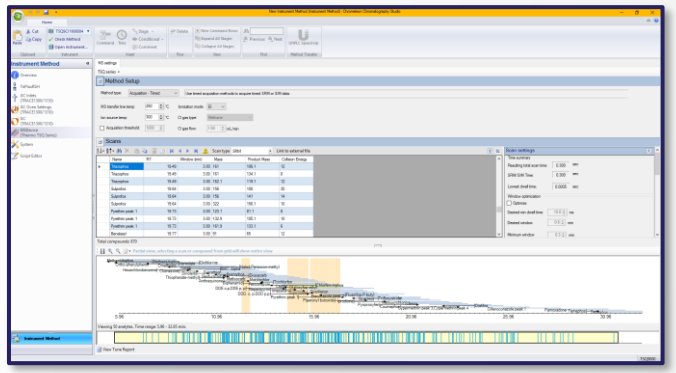


Instrument health records:

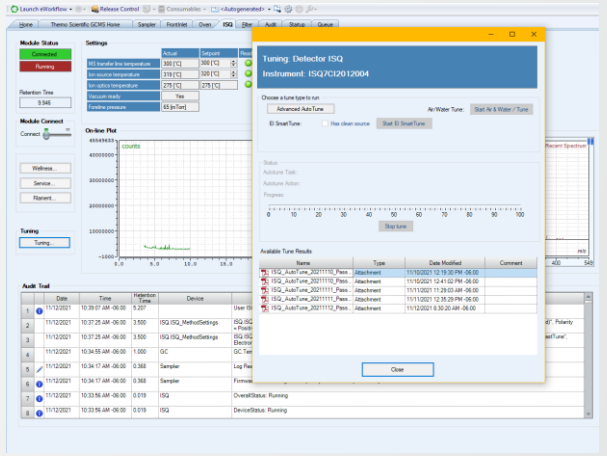
- Injections on current consumables
- Column health
- Filament lifetime
- Tuning status
- Detector lifetime

Gives user intelligent data to make maintenance decisions





Intelligent software tools including retention time alignment and Time SRM for optimizing methods



In-sequence tuning for compliance

TSQ 9610 GC-MS/MS summary

NeverVent technology

- Available with ExtractaBrite and AEI
- Increases instrument uptime

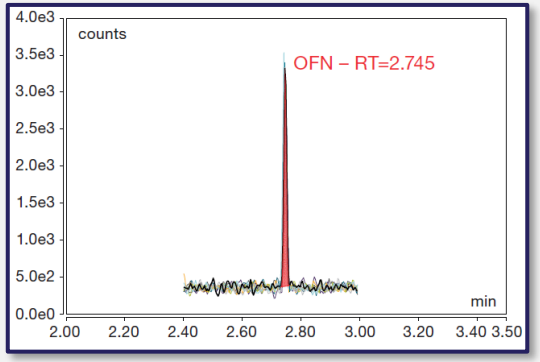
Off -axis ion guide pre-filter

- Eliminates the neutral noise

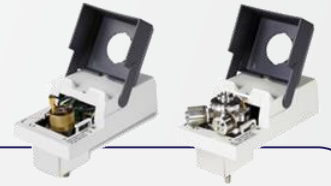
Evo collision cell

- Allows analysis of more compounds
- Shortens runtimes without loss of signal

Class-leading sensitivity



8 x 1 fg on-column OFN injections with %RSD of 4.1%. IDL is 0.12 fg



TRACE 1600 GC series

- Unique modular injector and detector design
- Easy-to-use touchscreen with real-time instrument monitoring and video guides

Software productivity tools

- Compliant-ready software
- Instrument health

XLXR detector as standard

- Extended dynamic range (2X more than previous model)
- Extended lifetime (7X more than previous model)

Application to Environmental Market

- Demonstrate utility of features for specific environmental analysis
- Collaborative effort between Pacific Rim Laboratories and Thermo Fisher Scientific
- Seek to expand utility of the TSQ-9610, consolidate methods, reduce analytical time to increase throughput

PACIFIC RIM LABORATORIES INC

Pacific Rim Laboratories

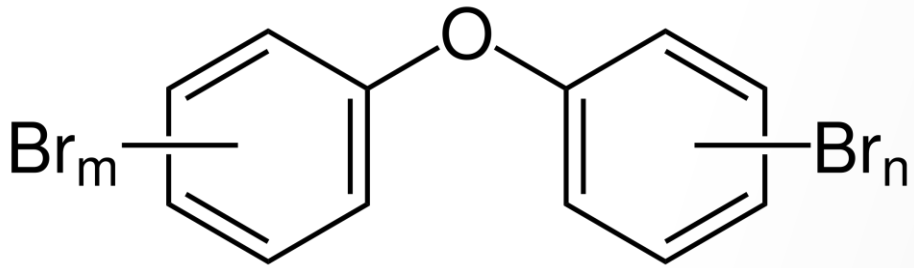
- Based in Surrey, British Columbia, Canada
- 16 employees
- ISO 17025 CALA accredited
- Work with governments, regulatory agencies and corporations the require environmental tests down to ppq levels
- Global client base
- www.pacificrimlabs.com

CALA
Canadian Association for Laboratory Accreditation Inc.

PACIFIC RIM LABORATORIES INC

PBDEs

- Polybrominated diphenyl ethers
- Widely used as flame retardants in everything from electronics, foams, building materials, etc.
- Another POP under growing scrutiny – shown to reduce fertility in humans



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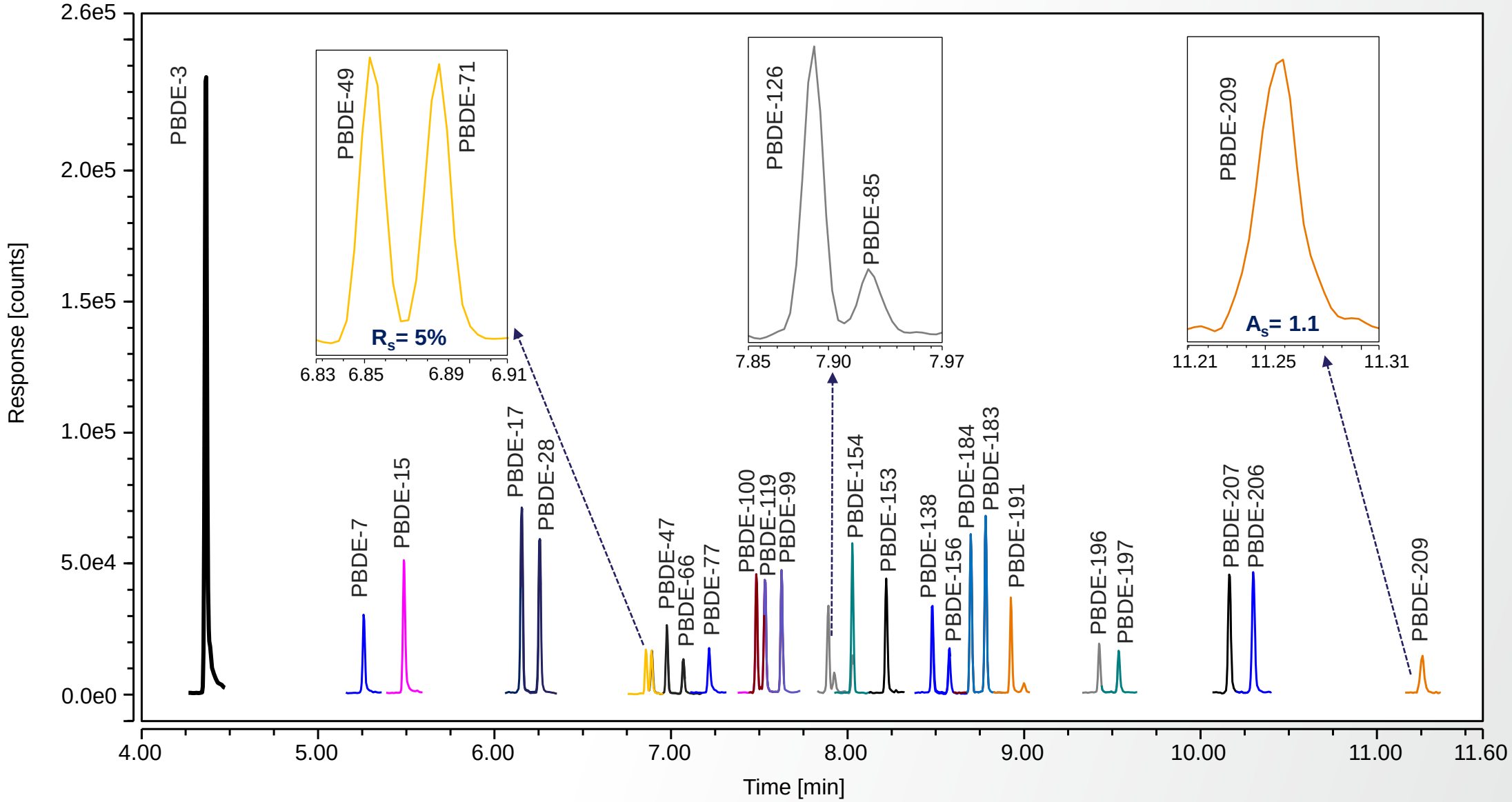
PBDEs @ 1.0-5.0 ng/mL CS1 STD



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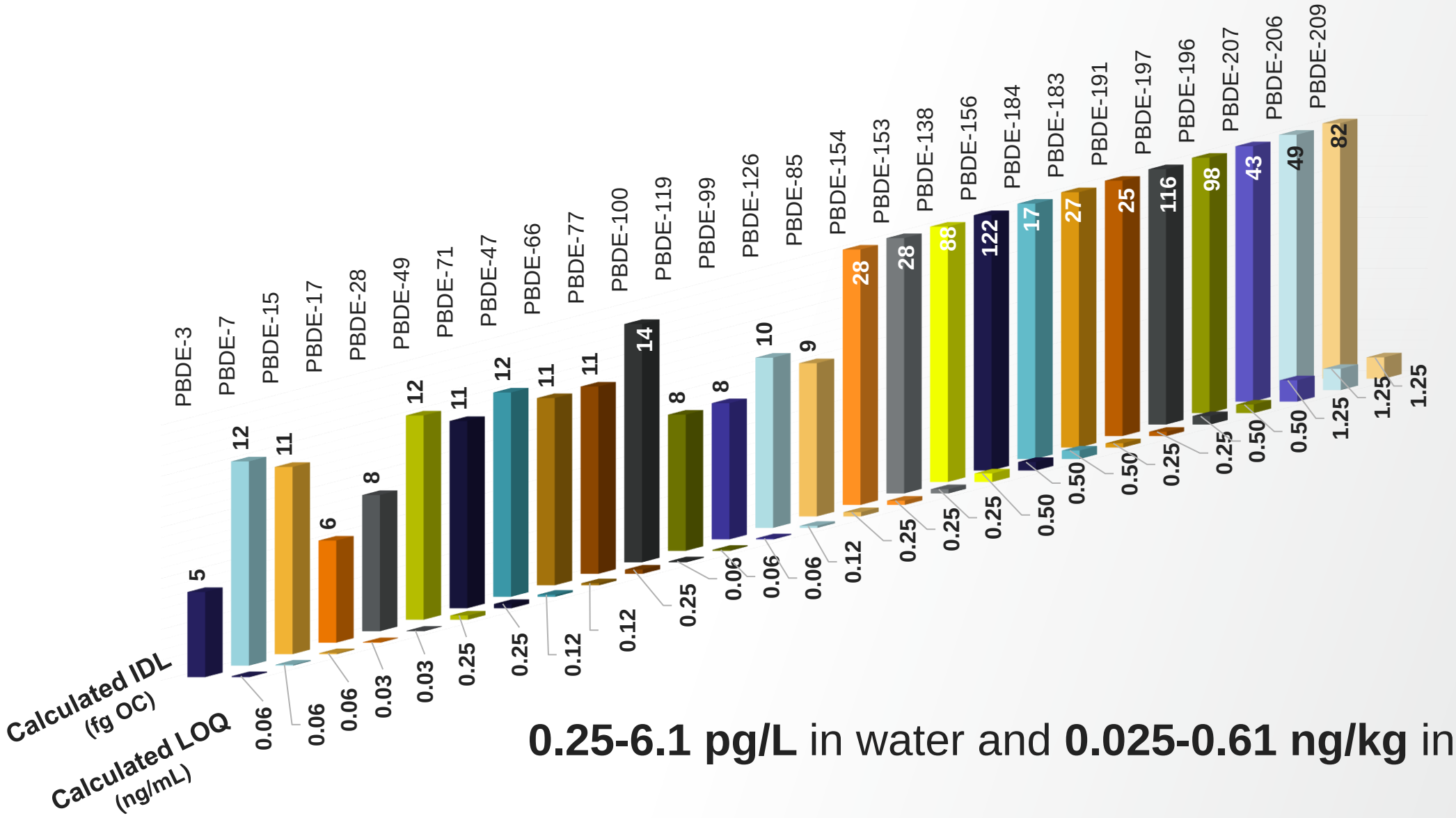
Calculated IDL and LOQ



0.25-6.1 pg/L in water and **0.025-0.61 ng/kg** in soil

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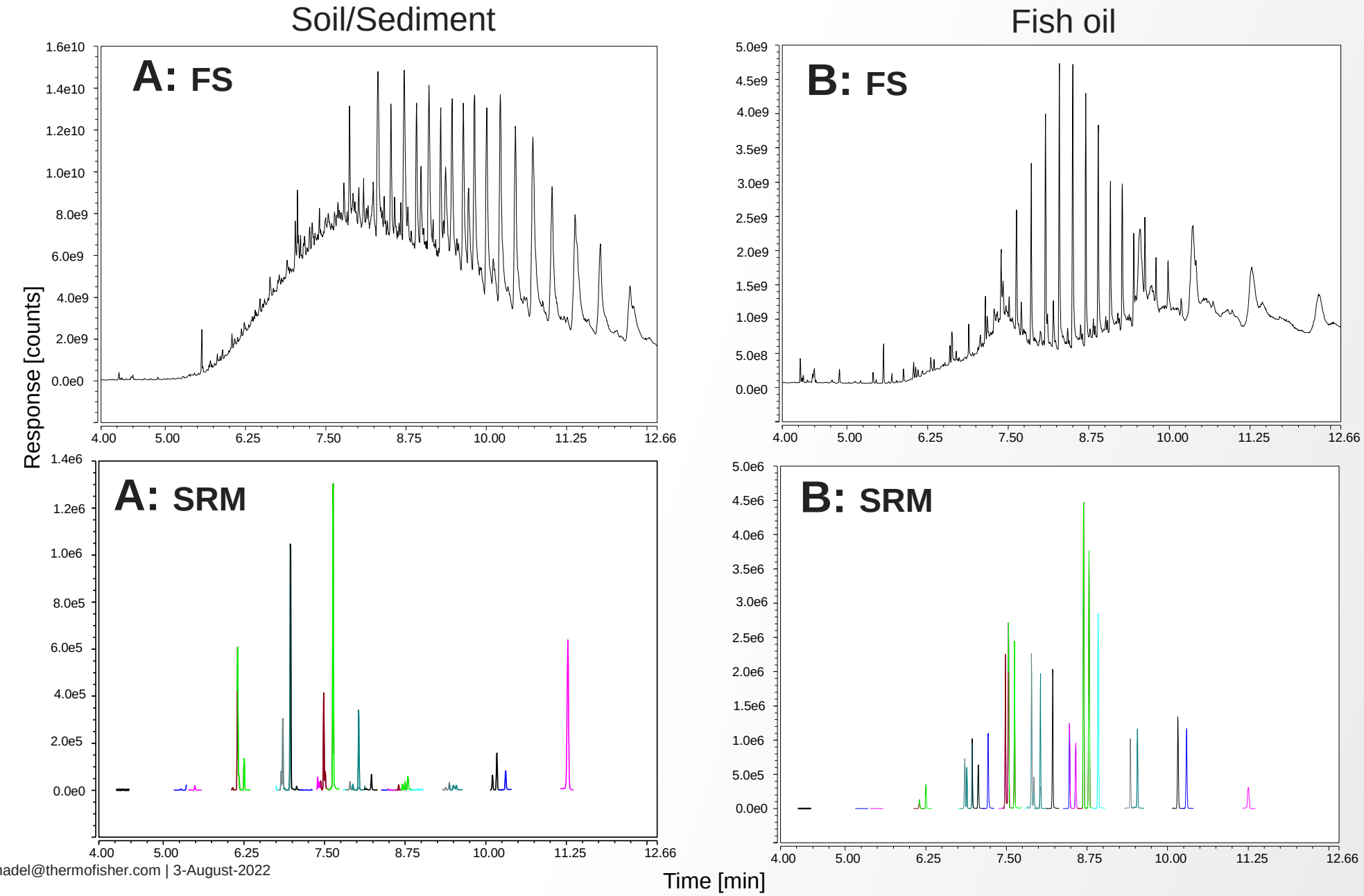
SRM for Matrix Interference Reduction



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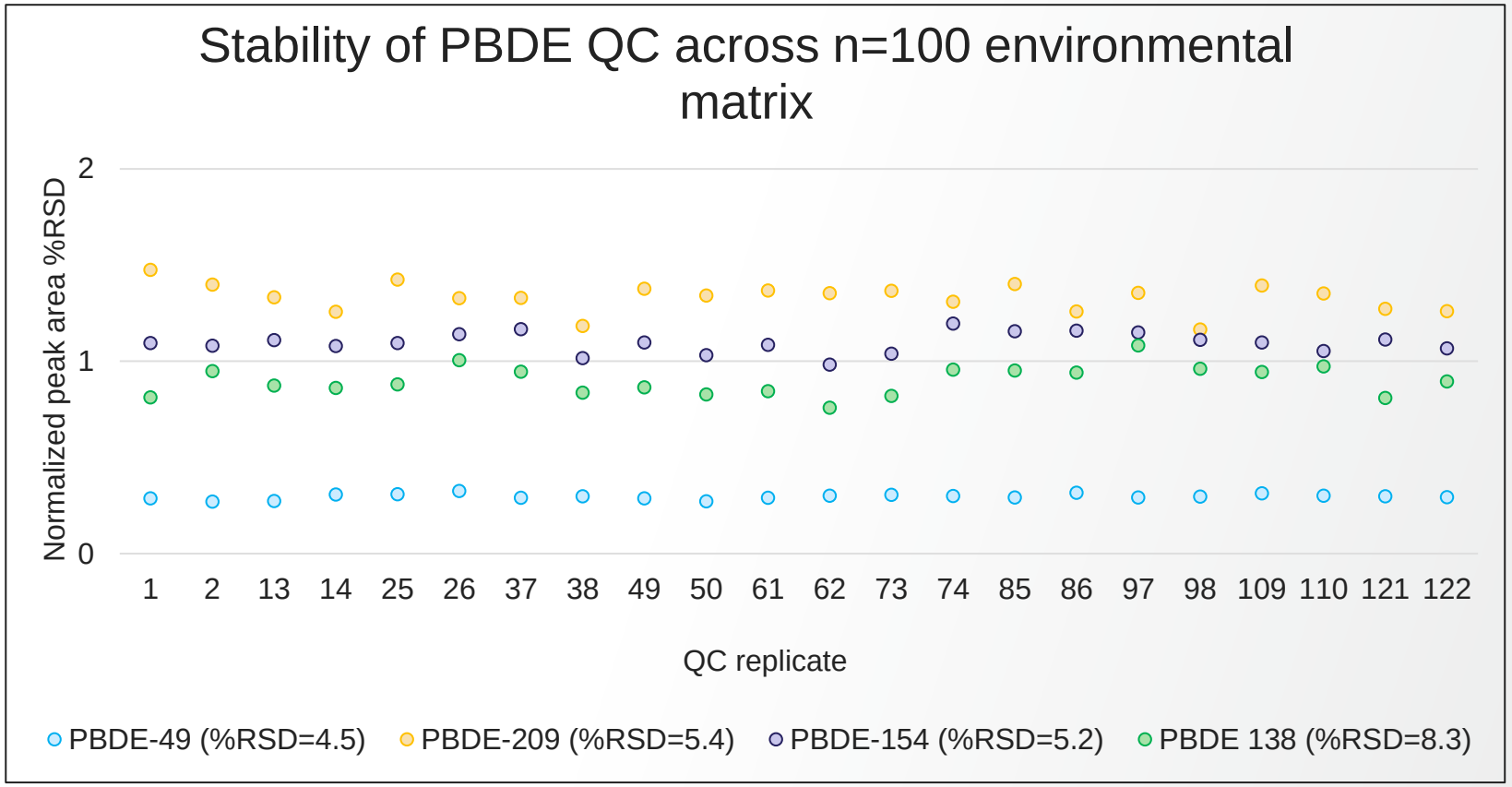
PBDE Stability

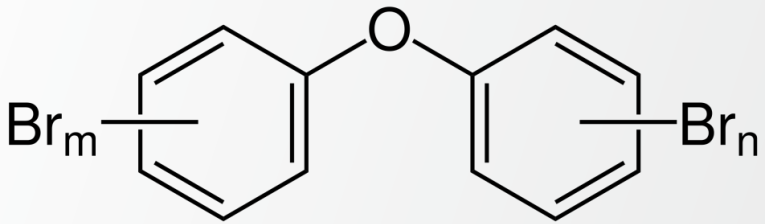


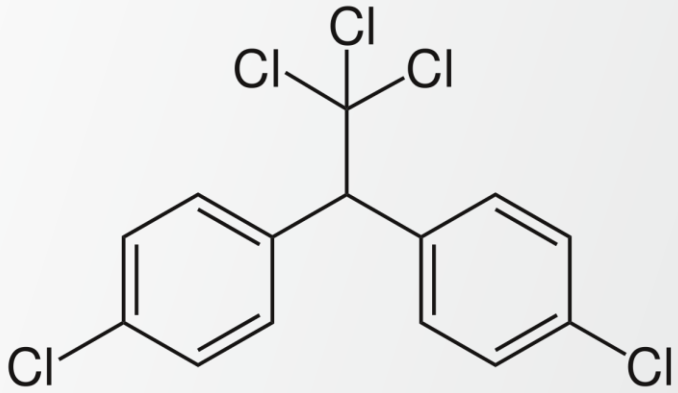
QC standard at 5.0 – 25.0 ng/mL every 10 samples to monitor stability

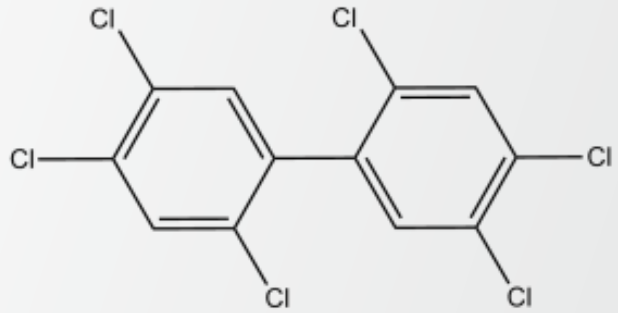
Consolidated “BOP” Method

- **BOP**
- **B**DE – Brominated diphenyl ethers
- **O**CP – Organochlorine Pesticides
- m**P**CB – Polychlorinated Biphenyls

- Series of contaminants commonly found in the same samples. Would be ideal to consolidate methods to increase throughput…





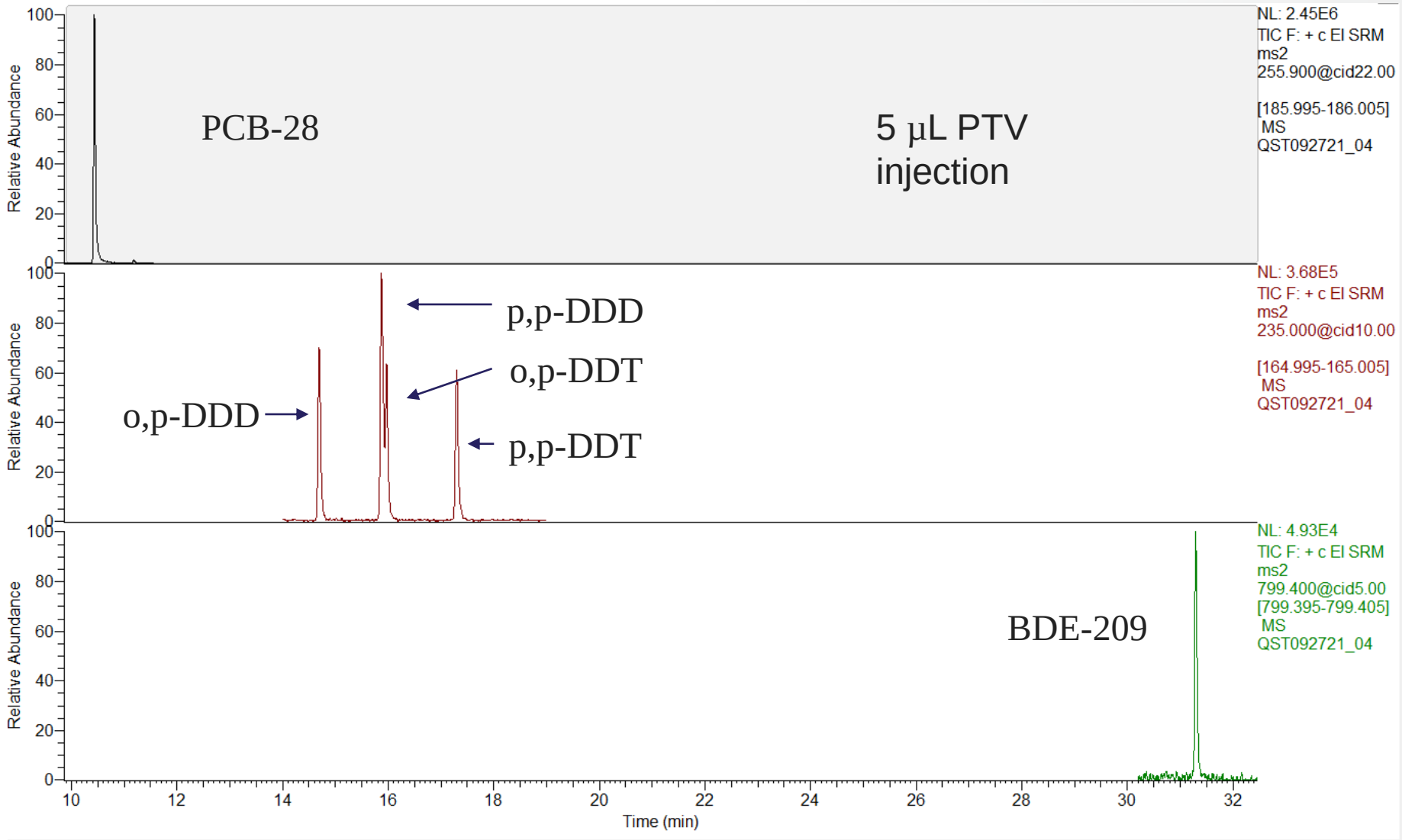


Consolidated “BOP” Method

P

O

B



BOP Fish oil MDL & LOQ

Analyte	MDL	LOQ
	ng/g	ng/g
PCB 28	0.18	0.6
PCB 52	0.26	0.88
PCB 101	0.23	0.78
PCB 138	0.26	0.85
PCB 153	0.27	0.89
PCB 180	0.18	0.6

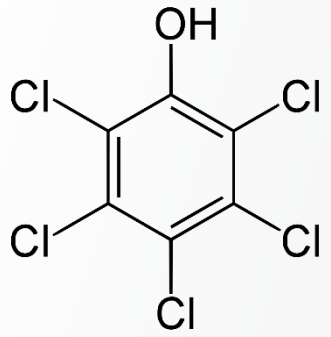
Analyte	MDL	LOQ
	ng/g	ng/g
Lindane (γ-HCH)	0.22	0.75
HCB	0.36	1.19
o,p'-DDE	0.27	0.92
p,p'-DDE	0.08	0.27
o,p'-DDD	0.19	0.62
p,p'-DDD	0.16	0.55
o,p'-DDT	0.16	0.53
p,p'-DDT	0.17	0.58
Aldrin	0.63	2.11
Dieldrin	0.86	2.88
Endrin	0.48	1.6

Analyte	MDL	LOQ
	ng/g	ng/g
BDE-17	0.08	0.26
BDE-28	0.1	0.33
BDE-49	0.15	0.5
BDE-47	0.19	0.62
BDE-66	0.19	0.63
BDE-77	0.14	0.48
BDE-100	0.17	0.57
BDE-99	0.27	0.92
BDE-85	0.27	0.91
BDE-154	0.08	0.28
BDE-153	0.13	0.44
BDE-138	0.16	0.52
BDE-183	0.2	0.66
BDE-209	0.75	2.52

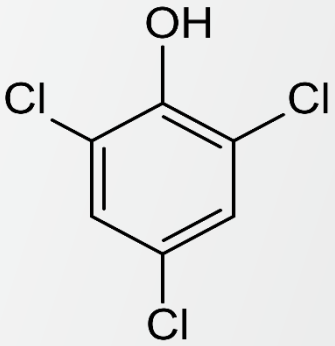
- LOQs are slightly higher in the combined method than those being run individually, but still within usable specification.

Chlorophenolic compounds

- Used in industrial manufacturing
- Ubiquitous in environment from pesticides, industrial waste, breakdown of other chlorinated compounds, and chlorination of phenols in water
- EPA 1653 used to regulate these, but little understanding of toxicity
- Extracted based on EPA 1653 – actually acetylated derivatives

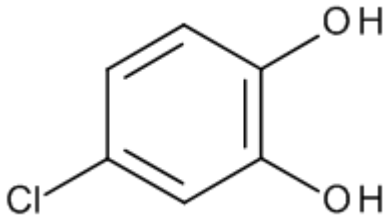


pentachlorophenol

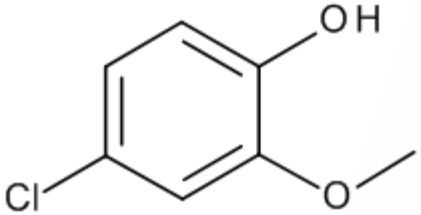


2,4,6-trichlorophenol

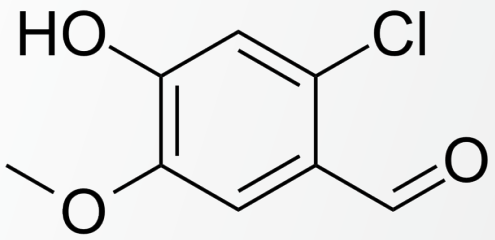
2 µg/L



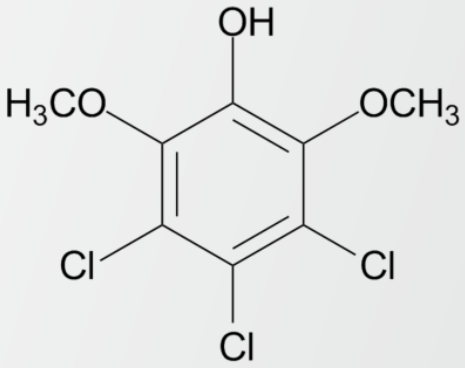
4-chlorocatechol



4-chloroguiacol



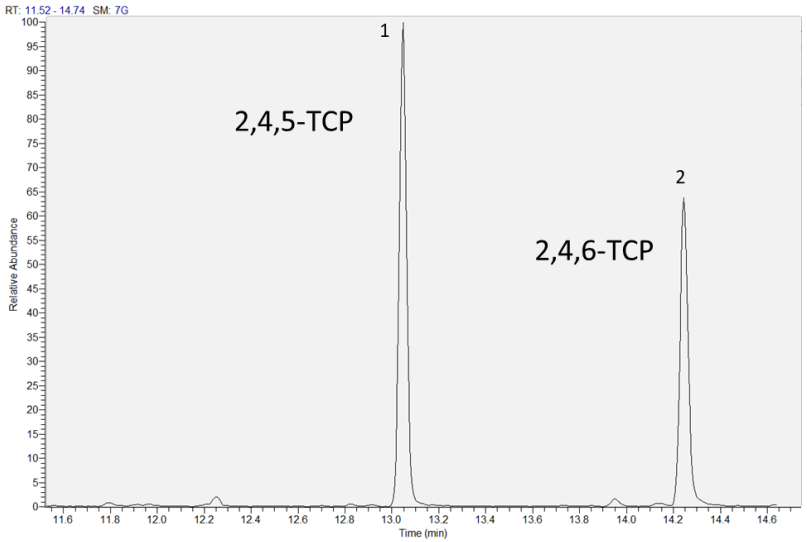
6-chlorovanillin

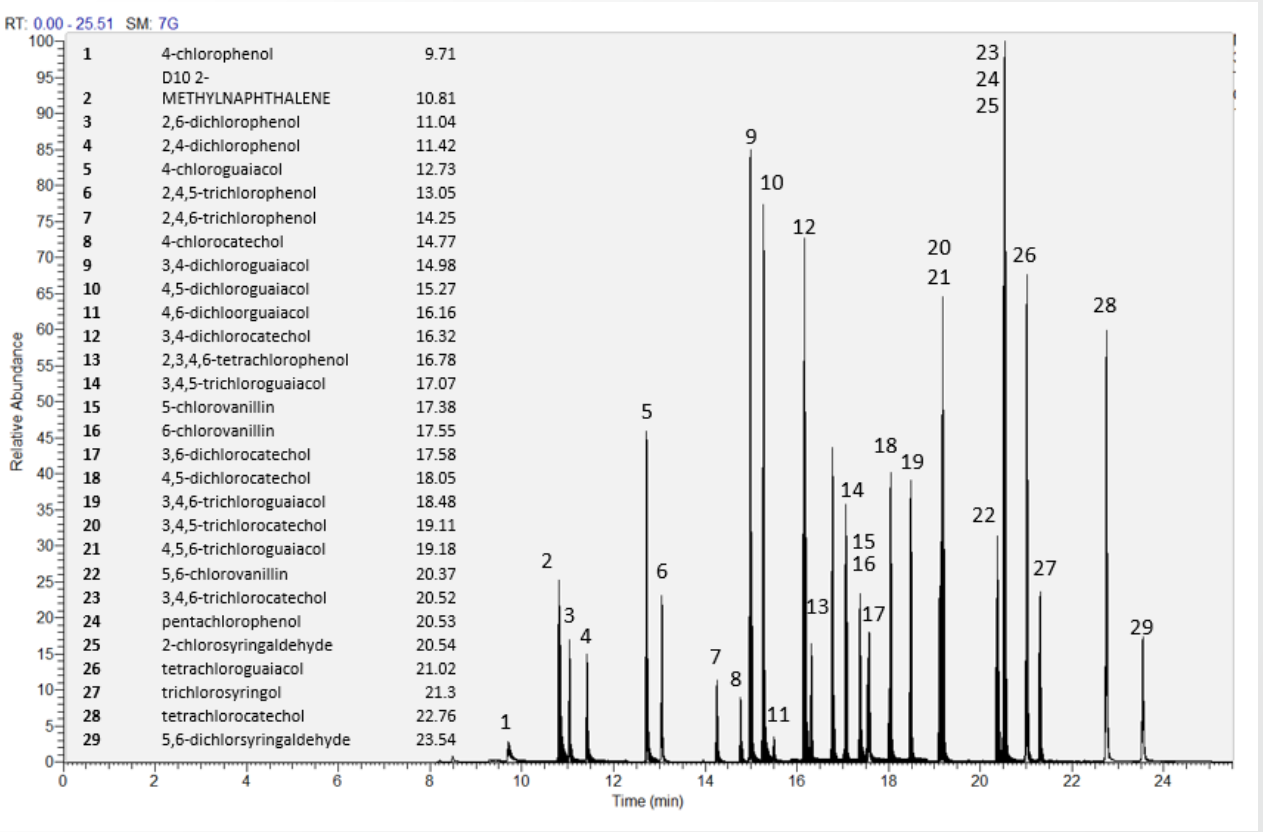


trichlorosyringol

Chlorophenolic compounds

- Chlorophenolics at 100-200 ng/mL
- 2,4,6 TCP is compound #7, well separated
- 2,4,6 and 2,4,5 TCP at 5 ng/L shown below





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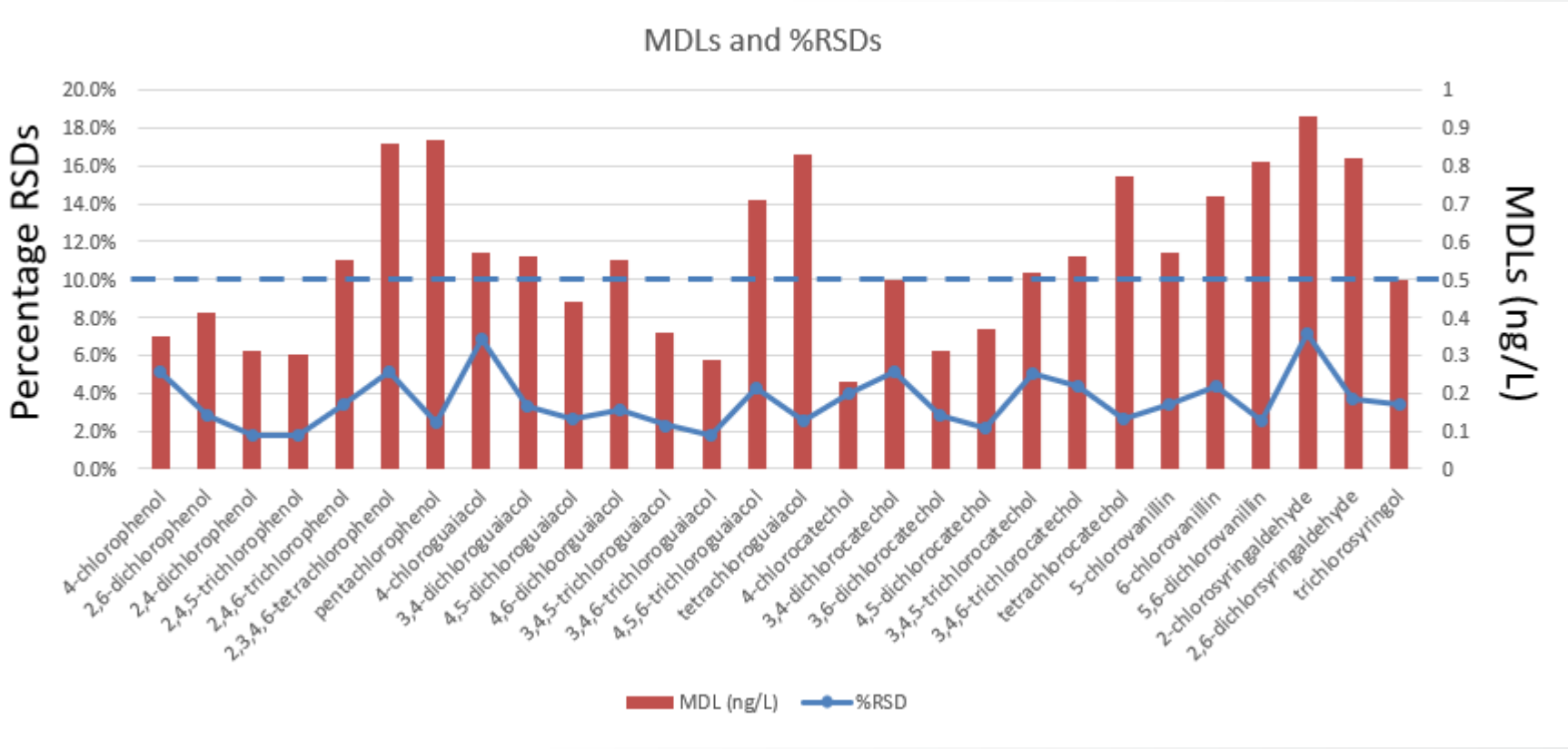
Chlorophenolic compounds



- 9 injections of spiked sample at 2.5-10 ng/L, 3x the std. deviation of results
- MDL for all compounds < 1 ng/L, regulatory guideline of 2 µg/L

Conclusions

The new TSQ-9610 GC-MS/MS offers a range of features aimed at addressing common laboratory challenges

- NeverVent technology with unique EI source
- XLXR Detector for extended life and dynamic range
- Software functionality for tuning and ease-of-use

The TSQ-9610 is well-suited to analysis of various environmental sample matrices and analytical targets, including:

- PBDEs
- A consolidated “BOP” method – easy transfer from HR-GCMS
- Chlorophenolics
- Others not presented here (PCBs, etc.)

Productivity is enhanced through method consolidation facilitated through ionization source efficiency and detector sensitivity, allowing analysis of compounds across a large range of concentrations in a single run.

- This allows for increased throughput

Acknowledgments

Analytical work was completed in collaboration between Pacific Rim Laboratories (Surrey, BC) and Thermo Fisher Scientific

Thank you