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A streamlined laboratory workflow for the analysis of common contaminants according to the U.S. EPA 8270E and 8081B methods using GC-MS/MS

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Goal: The goal of this application note is to demonstrate a modernized workflow for the analysis of semivolatile compounds (SVOCs) and pesticide residues according to EPA 8270E[1] and EPA 8081B[2] methods using a single instrument platform based on gas chromatography coupled to triple quadrupole mass spectrometry (GC-MS/MS). This method could also be expanded to include similar environmental methods, providing users with a simplified analysis workflow that can be applied across a variety of application areas to simplify adoption in high-throughput environmental laboratories.

INTRODUCTION

Analytical testing laboratories dealing with environmental analysis must monitor diverse compound classes (SVOCs, pesticides, PCBs, etc.) in multiple matrices (drinking water, surface water, wastewater, soils, sludges) often requiring different instrument configurations and settings. This poses some challenges in terms of reduced productivity and sample throughput as well as increased time and costs for multiple platform maintenance, dedicated consumable usage, as well as staff training. Moreover, staff turnover or reduced laboratory personnel requires analysts to run multiple instrumentation and methods, adding unneeded complexity to their daily work.

Many U.S. EPA methods for environmental analysis recommend the use of gas chromatography coupled to analog detectors such as electron capture detection (ECD),[1] nitrogen phosphorous detection (NPD),[2] and photometric detection (FPD)[3] because they provide a very specific detection for certain functional classes (e.g., organochlorine or organophosphorus pesticides). Despite their high specificity, extensive sample preparation and adequate chromatographic separation are required to differentiate between the target compounds and other co-eluting compounds or matrix interferences. This can result in sample reanalysis using alternative columns and conditions to confirm results. These reruns are often run by mass spectrometry to provide better identification and confirmations. A more effective approach is the use of triple quadrupole mass spectrometry (MS/MS). The selected rection monitoring (SRM) acquisition mode provides greater selectivity compared to single ion monitoring, allowing for simplified sample preparation protocols. Hundreds of analytes can be monitored within a single chromatographic run as typical ion transitions are monitored for each compound. This allows for confident identification of analytes at sub-ppb level sensitivities even without full chromatographic resolution between compounds. Furthermore, timed-SRM mode (t-SRM) allows the operator to process a specific method's list of target analytes, set an acquisition window around each elution time, and subsequently optimize the mass spectrometers dwell time, leading not only to simpler data with smaller file sizes, but also better sensitivity. The adoption of such a platform that can be used for multiple analytical methods would improve laboratories' sample throughput and productivity while reducing the cost of spare parts inventory and instrument management, streamlining operations.

In this study, the same Thermo Scientific™ TSQ™ 9610 GC-MS/MS system configuration was used for analysis of SVOCs and organochlorine pesticides according to the EPA 8270E and EPA 8081B methods. Overall method performance, including linearity, sensitivity, and precision, were evaluated thoroughly for use in a working water testing laboratory.

Key hardware and software for method modernization As part of workflow modernization and cost reduction, many laboratories investigate automation of the sample preparation procedures to promote a safer work environment (reducing the analyst's exposure to toxic chemicals) and save analyst's valuable time, improve data quality, and reduce possible errors, cross- contamination, and waste. The Thermo Scientific™ TriPlus™ RSH Smart autosampler[4] combines highly versatile sample injection capability (liquid, headspace, and solid-phase microextraction (SPME)) with automated sample preparation procedures, eliminating typical GC-MS workflow bottlenecks. Daily operations such as dilutions, standard curve generation, and derivatization up to more complex, multi-step sample preparation protocols can be fully automated leading to substantial cost savings, while gaining efficiency and productivity from system's unattended operations.

Containing costs does not mean that laboratories must give up flexibility and advances in technology. The Thermo Scientific™ TRACE™ 1610 series GC,[5] the only GC with a user-installable modular concept, is designed to enhance the workflow experience through the use of interchangeable injector and detector modules that allow the analyst to easily modify the instrument configuration in minutes without special tools or training and simplify troubleshooting operations without the need for service calls. The GC's advanced multi-functional touch screen with instrument health monitoring of common

maintenance items such as inlet liner or septum changes (among many others) can help avoid unplanned downtime through user- settable alerts on consumables usage and maintenance. The TSQ 9610 GC-MS/MS[6] system using NeverVent™ technology allows for column replacement and ion source cleaning without venting the mass spectrometer, increasing uptime. The ultra-sensitive, ultra-robust Thermo Scientific™ Advanced Electron Ionization™ (AEI) ion source combined with the Thermo Scientific™ XLXR™ electron multiplier detector provide class leading sensitivity and extended dynamic range enables method consolidation for analysis of low- and high-concentrated compounds in a single GC run.

Software is key for a streamlined workflow. The Thermo Scientific™ Chromeleon™ Chromatography Data System (CDS)[7] provides flexibility and scalability to control chromatography (GC, LC, and IC) instruments, as well as single and triple quadrupole mass spectrometers, and even HRAM mass spectrometry instruments like the Thermo Scientific™ Orbitrap Exploris™ GC mass spectrometer with one single software, all while meeting data integrity regulatory requirements of the U.S. Food and Drug Administration Title 21 Code of Federal Regulations Part 11 (21 CFR Part 11). Users can easily switch between instruments, platforms, and methods, managing all the analytical processes and data, from a variety of locations. From instrument control to raw data storage, processing, and generation of the results and approvals, Chromeleon CDS can seamlessly connect multiple sites and worldwide locations to a central data center with the same performance as a fully local operation

EXPERIMENTAL

In all the experiments described here, a TSQ 9610 triple quadrupole mass spectrometer equipped with NeverVent 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 liquid autosampler. The same instrument configuration, chromatographic column, and consumables were used for assessing instrument compliance to EPA 8270E and EPA 8081B methods (Figure 1). A TriPlus RSH SMART autosampler was placed on the bench and used as an off-line sample preparation station for calibration curve dilution and internal standard addition. The use of an automated approach improved analyst's safety by reducing exposure to toxic chemicals such as dichloromethane (DCM).

Chromatographic separation was achieved on a Thermo Scientific™ TraceGOLD™ TG-5SilMS capillary column 30 m × 0.25 mm × 0.25 µm (with integrated 5 m SafeGuard column, P/N 26096-1425). The "-Sil" indicates silylarene groups are incorporated in the polymer backbone, ensuring improved thermal stability and reduced susceptibility to oxidation, resulting in low column bleed and outstanding inertness.

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.

Data acquisition, processing and reporting

Data was acquired, processed, and reported using the Chromeleon CDS, version 7.3.2. Integrated instrument control ensures full automation of the analytical workflow combined with an intuitive user interface for data analysis, processing, customizable reporting, and storage in compliance with 21 CFR Part 11. This integrated instrument control enables users to perform in-sequence tuning, and when combined with the scheduling capability of Chromeleon CDS, instruments can be checked automatically at a desired time, so that additional operator time can be saved and used for more productive purposes.

In addition, the Chromeleon Environmental Analysis Extension Pack for U.S. EPA-based environmental applications provides a comprehensive set of instrument methods, processing methods, and reports, designed for quick sequence set-up and reporting to allow rapid implementation of new instruments with ease.

Figure 1. Unified environmental method schematic for analysis of multiple compound classes using a single analytical platform.

Table 1. GC-MS/MS and autosampler parameters applied for SVOCs and multi-residue analysis of pesticides according to EPA 8270E and EPA 8081B methods as well as parameters used for DFTPP, tailing and degradation performance verification as per EPA 8270E method

AI/AS 1610 autosampler parameters	
Injection type	Standard
Sample mode	Standard
Fill strokes	6
Air volume (µL)	1
Sample depth	Bottom
Injection mode	Fast
Pre-injection wash cycles	0
Pre-injection solvent wash volume (µL)	0
Post-injection wash cycles	6
Post-injection solvent wash volume (DCM, µL)	5
Sample wash cycles	3
Sample wash volume (µL)	1.5
Injection volume (µL)	1
Syringe	10 µL Fixed needle, gas tight syringe 26 Gauge, 50 mm, Cone tip, (P/N 365D2977)

iConnect-SSL parameters		
	EPA 8081	EPA 8270 and DFTPP
Injection temperature (°C)	225	
Liner	For splitless injection: Thermo Scientific™ LinerGOLD™ Splitless liner, Single taper with quartz wool (P/N 453A1925-UI)	
Oven equilibration time (min)	0.2	
Inlet module and mode	SSL, split with surge	SSL, splitless with surge
Surge pressure (psi)	35	35
Surge duration (min)	0.8	0.8
Splitless time (min)	--	0.8
Split flow (mL/min)	--	60
Split ratio	5:1	--
Septum purge flow (mL/min)	Constant 5.0	

(continues on next page)

iConnect-SSL parameters		
	EPA 8081	**EPA 8270 and DFTPP**
Gas saver flow (mL/min)	5	5
Gas saver time (min)	5	5
Carrier gas, flow (mL/min)	Ramped, 1.2 mL/min hold 20 min 1.0 mL/min to 2.0 mL/min hold 9.20 min	Constant,1.2

TRACE 1610 GC parameters		
	EPA 8081 / 8270	**DFTPP**
Oven temperature program		
Oven equilibration time (min)	0.2	0.2
Temperature (°C)	40	90
Hold time (min)	2	1
Rate (ºC/min)	50	30
Temperature 2 (°C)	125	310
Rate (ºC/min)	12	--
Temperature 3 (°C)	150	--
Rate (ºC/min)	20	--
Temperature 4 (°C)	200	--
Rate (ºC/min)	5	--
Temperature 5 (°C)	280	--
Rate (ºC/min)	30	--
Temperature 6 (°C)	330	--
Hold time (min)	4.05	5
GC run time (min)	30	15
Column		
Trace GOLD TG-5SilMS with integrated 5 m SafeGuard	30 m, 0.25 mm, 0.25 µm (P/N 26096-1425)	

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TSQ 9610 mass spectrometer parameters		
	EPA 8081 / 8270	**DFTPP**
Transfer line temperature (°C)	300	300
Ion source type and temperature (°C)	NeverVent AEI, 300	NeverVent AEI, 300
Ionization type	EI	EI
Aquisition mode	Timed SRM	Full Scan, 35–500
Filament delay (min)	--	3.5
Dwell or scan time (s)	--	0.0988
Tuning parameters	AEI Smart Tune	AEI Smart Tune
Collision gas and pressure (psi)	Argon at 70	Argon at 70
Minimum deisred peak width (s)	3	--
Desired scans per peak	20	--
Set resolution for each unique transition	Enabled (see table in **Appendix 1** for individual resolution)	--
Use last tune detector gain	X7	--
Use specified emission current (μA)	25	25

RESULTS AND DISCUSSION

EPA Method 8270E

U.S. EPA Method 8270E is used to determine the concentration of semivolatile organic compounds, such as polycyclic aromatic hydrocarbons (PAHs), in many types of solid waste matrices, soils, air, and water samples by using gas chromatography coupled to mass spectrometry (GC-MS). One of the challenges of this method is that multiple analytes spanning wide concentration ranges must be analyzed in one single run, often leading to non-ideal calibration curves. The Thermo Scientific XLXR detector provides an extended dynamic range that allows laboratories to easily overcome this issue and provides wider calibration ranges, with better linearity, leading to more accurate and repeatable results. Moreover, since many diverse pesticides are listed in the EPA 8270E method, high selectivity is mandatory for a confident identification of compounds. The timed-selected reaction monitoring (t-SRM) acquisition mode allows for simultaneous acquisition of multiple characteristic ion transitions for each target analyte, maintaining high sensitivity combined with high selectivity to discriminate between the target compounds and matrix, thus ensuring a reliable and confident identification of analytes.

Instrument performance verification: DFTPP tune, tailing, and degradation

The EPA 8270E method provides a list of performance criteria that need to be assessed to check instrument suitability for sample analysis. A decafluorotriphenylphosphine (DFTPP) tune check standard is used to assess the instrument response in terms of spectral quality. Other test probes such as benzidine and pentachlorophenol are used to assess instrument inertness, specifically in the sample flow path, and yet more compounds like endrin and DDT breakdown products are used to assess sample degradation within the injector. Although not requested when analysis is performed using product ions for quantitation, a quality control sample containing all test analytes was injected at least once daily to ensure that the system fulfilled all method requirements in terms of ion abundance, tailing, and degradation. The TSQ 9610 GC-MS/MS met all ion ratio performance criteria without requiring any adjustments of the default instrument tuning. Moreover, the high inertness of the GC flow path allowed the peak tailing and degradation evaluation criteria to be easily met. The Chromeleon CDS reporting capability allows for customized tune and breakdown reports, and the Chromeleon 7.3.2 Report Designer 2.0 features allow for quick and easy visual review of the performance tests by using conditional formatting with a Pass/Fail indicator as shown in Figure 2.

Chromatography

Structural isomers are compounds having the same molecular formula but different physical arrangement of the atoms in space; therefore, they often elute very closely to each other in pairs. The EPA 8270E method requires calculations of chromatographic resolution for these "critical pairs" to ensure that the fundamental chromatographic separation is adequate for analysis so that, for example, analytical columns can be exchanged before degradation may affect data quality. Typically, if the peaks are separated by at least 50% resolution, they can be considered chromatographically separated. An example of typical chromatograms for a reference standard mix prepared in DCM at a concentration of 500 µg/L (ppb) is shown in Figure 3. The insets show some examples of critical pair resolution achieved for closely eluting isomers. Resolution was calculated as per the EPA method using the formula in Equation 1 and was ≥ 50%, thus meeting the method suitability requirements.

Equation 1: *Resolution = 1−[valley height]/[average peak height]*

Linearity and detection limits

Linearity and detection limits were assessed by preparing multiple calibration curves diluted in solvent (DCM) ranging from 0.5 µg/L to 250 µg/L. Linearity was determined using an internal standard method by calculating the relative standard deviation (RSD) of the response factor (RF) for each analyte and comparing the result to the limit specified in the EPA methods. All target analytes showed a linear trend with RF %RSD in agreement to the <20% limit specified in the method, thus confirming that a very wide linear range can be easily achieved with the XLXR detector. Full range calibration curves (0.5–250 µg/L) for some selected analytes and the quantifier and qualifier ions at 0. 5 µg/L are reported as an example in Figure 4.

Method detection limits (MDLs) are firmly established with many regulatory bodies and can be defined in multiple ways. According to the most recent U.S. Code of Federal Regulations,[8] MDL is defined as: "the minimum concentration of a substance that can be measured and reported with 99% confidence that the analyte concentration is greater than zero and is determined from analysis of a sample in a given matrix containing the analyte." This methodology can be seamlessly transferred when calculating instrument detection limits (IDLs). Unlike MDL, IDL uses solvent based standards containing the test chemical at concentrations that give a consistent response over several repeat injections.

Thermo Scientific GCMS Report

MS Tune Check, Tailing, and Breakdown - US EPA 8270E

Sample	Tune Check	**Instrument**	TSQ8120103	**Sequence**	20240403 - Calibration 31620
Acquired	04/03/2024 10:25 AM	**Method**	DFTPP	**Analyst**	
Reported	08/01/2024 11:47 AM	**Processing**	EPA 8270E - DFTPP & Tailing V30		

Test Summary

DFTPP:	Pass	Tailing:	Pass	Breakdown:	Pass

Chromatogram

DFTPP

Mass	Criteria	Raw Value	Value	Operator	Value 1	Value 2	Result
68	< 2% of m/z 69	21,657	0.77%	<	2.00%		Pass
69	Present	2,806,230	Present	>	0		Pass
70	< 2% m/z 69	8,208	0.29%	<	2.00%		Pass
197	< 2% of m/z 198	113,379	0.41%	<	2.00%		Pass
198	Base peak or present	27,449,497	Base Peak				Pass
199	5-9% of m/z 198	1,827,621	6.66%	between	5.00%	9.00%	Pass
365	>1% of base peak	485,268	1.77%	>	1.00%		Pass
441	< 150% of m/z 443	4,498,581	20.37%	<	150.00%		Pass
442	Base peak or present	22,086,747	Present				Pass
443	15-24% of m/z 442	3,867,497	17.51%	between	15.00%	24.00%	Pass

Overall Result
Pass

Tailing Check

Peakname	Ret.Time	Area	Tailing Factor	Limit	Result
	min	counts*min			
TIC	TIC	TIC	TIC		TIC
Pentachlorophenol	6.204	31,314,338	1.063	2.000	Pass
Benzidine	7.469	62,293,986	1.241	2.000	Pass

Overall Result
Pass

Breakdown Check

Peakname	Ret.Time	Peak Area	Peak Type	% Breakdown	% Breakdown Limit	Result
	min					
TIC	TIC	TIC				
4,4'-DDE	7.629	40,340	Breakdown	3.33%	20.00%	Pass
4,4'-DDD	7.936	2,042,864	Breakdown			
4,4'-DDT	8.158	60,463,837	Native			

Overall Result
Pass

Peakname	Ret.Time	Peak Area	Peak Type	% Breakdown	% Breakdown Limit	Result
	min					
TIC	TIC	TIC				
Endrin	7.879	43,648,846	Native	4.97%	20.00%	Pass
Endrin aldehyde	8.024	593,071	Breakdown			
Endrin ketone	8.506	1,691,677	Breakdown			

Figure 2. Chromeleon CDS browser showing a customized report for an easy and quick review of the instrument performance criteria (DFTPP ion ratios, tailing, and degradation) results fulfilling the EPA 8270E method requirements.

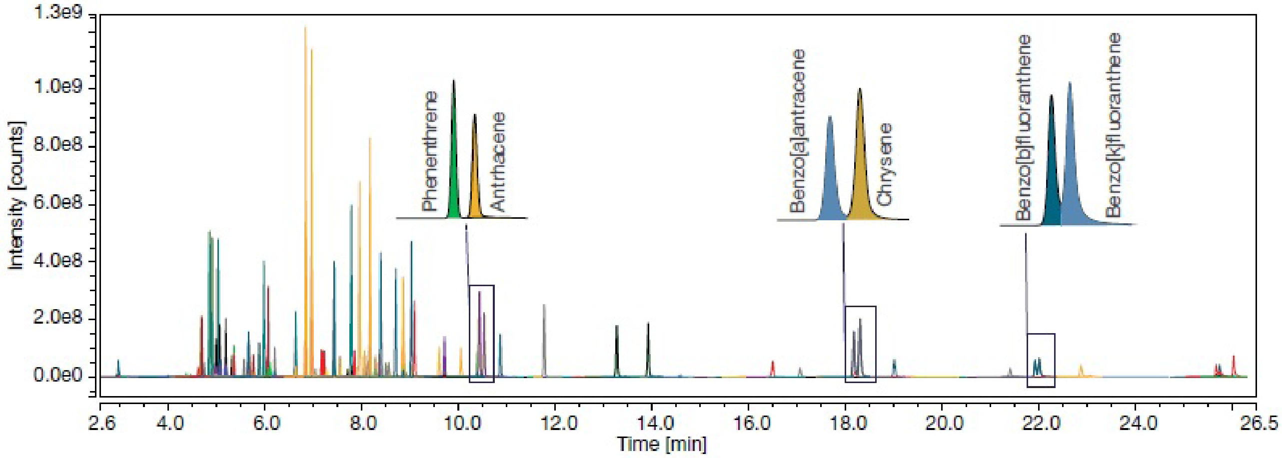


Figure 3. Example of chromatography achieved for a solvent standard spiked at 500 µg/L. The insets show examples of resolution for some critical pairs in compliance with the EPA 8270E method.

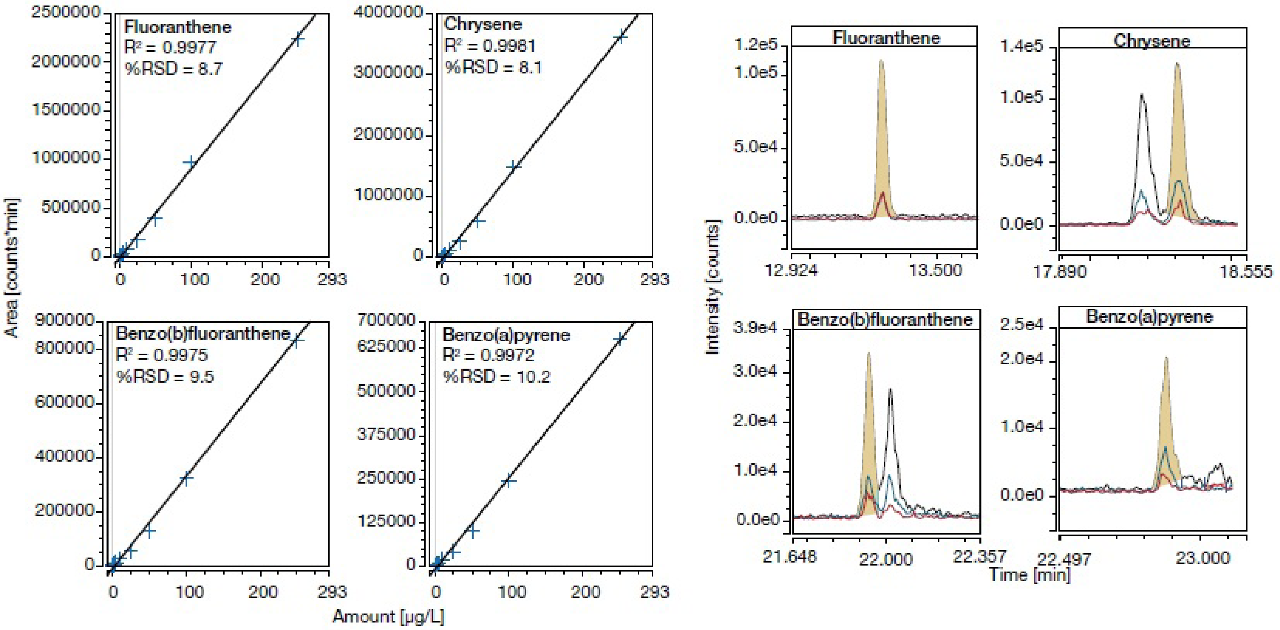


Figure 4. Example of calibration curves prepared in DCM (range: 0.5–250 µg/L) for some selected target analytes as well as quantifier and qualifier ions at 0.5 µg/L. Coefficients of determination (R2) and RF %RSD are annotated.

Therefore, the IDL is a statistically rigorous method that uses the precision of a measurement at low analyte levels and accurately reflects the true detection limit of an instrument, ultimately defining how sensitive an analytical system is.[9] The IDL was determined for all the target compounds by preparing n=7 solvent standard in DCM at 1 µg/L. IDLs were calculated using the Students t-test values for the corresponding n-1 degrees of freedom at 99% confidence, the amount of analyte on column, and the absolute peak area %RSD for each analyte as per Equation 2.[10] MDL calculation reports are already available for Chromeleon CDS.

$$\text{Equation 2: } IDL = t * Amount * \%RSD$$

t = Student t-value for one-tailed distribution
Amount = Amount of analyte (on-column)
%RSD = Relative standard deviation of the response

Calculated IDLs for selected compounds covering the entire volatility range are reported as an example in Figure 5. IDLs ranged from 5 to 45 µg/L with peak area RSD <10% for the majority of the target compounds. Details of the calculations are reported in **Appendix 2**.

EPA Method 8081B

U.S. EPA Method 8081B provides validated procedures for the determination of organochlorine pesticides (OCPs). OCPs are a group of synthetic chlorinated hydrocarbon derivatives, which were commonly used to protect crops, livestock, buildings, and households from the damaging effects of insects. OCPs have been banned in the United States and many other countries across the world because of their persistent presence in the environment and the threat they pose to food safety and animal health. EPA Method 8081B suggests the use of dual-column gas chromatography with electron capture detector (ECD) as this allows detection and measurement of electronegative chemical compounds (most notably halogens, organohalides, and nitrogen-containing compounds) with extremely high sensitivity. Despite the high sensitivity provided towards electronegative compounds, the ECD poses some concerns in terms of compound identification and laboratory safety and operations due to the use of a 63Ni radioactive source. Because of the complexity of an analog-style chromatographic separation, the second column is still needed to confirm IDs and discriminate between the target analytes and matrix interferents.

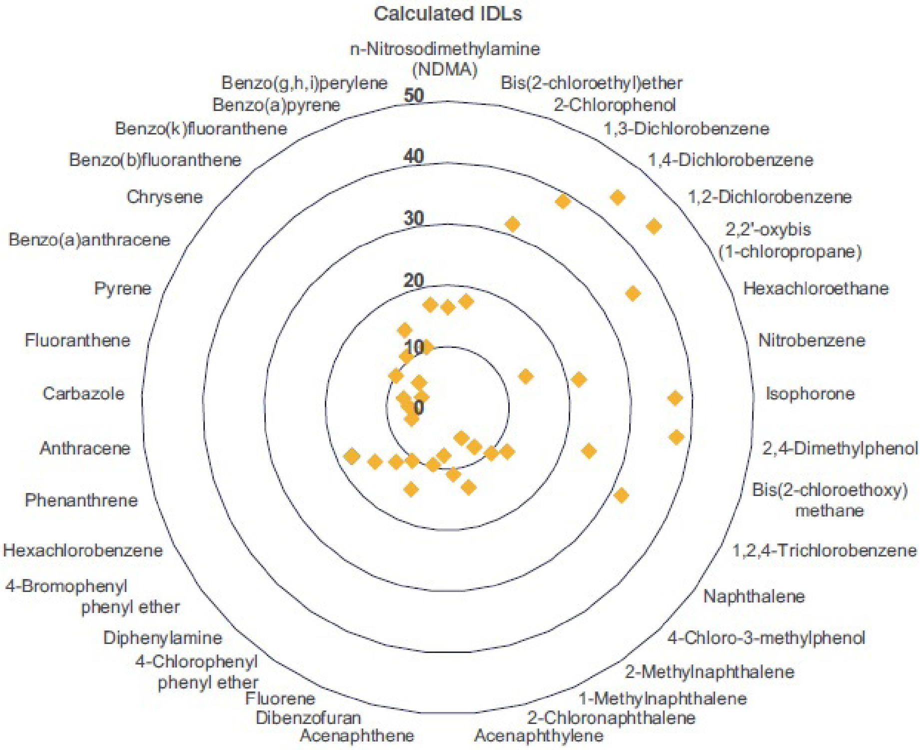


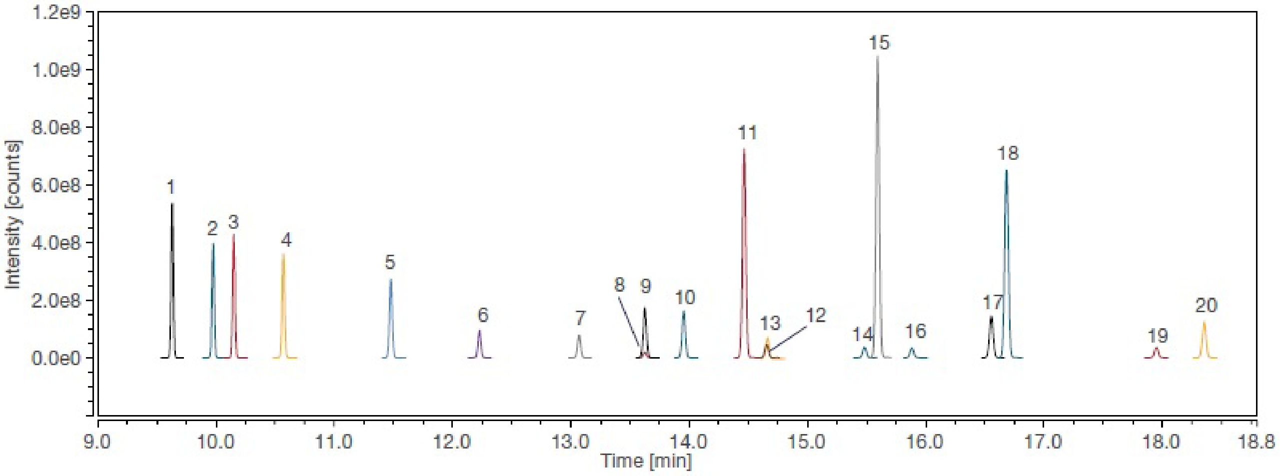
Figure 5. Examples of calculated IDLs for some selected compounds covering the whole volatility range. Calculated IDLs for solvent standard spiked at 1 µg/L resulted in the range from 5 to 45 µg/L with peak area %RSD <10 for the majority of the compounds.

The dual-column configuration also requires twice as much carrier gas, as well as an additional analytical column and unions, which makes continued operations costly from a consumable standpoint. Although ECD cells contain a small radioactive Ni63 and are generally considered safe to maintain and handle by trained operators, their use may require certain registrations and licensing fees on a yearly basis to maintain compliance with the radiation safety procedures stated in the regulations of the Nuclear Regulatory Commission (NRC) and state and local guidelines.

The use of GC-MS/MS can overcome challenges associated with using ECD as it is sensitive enough to provide equivalent detection limits but adds the advantage of selectivity, as compounds can be identified based on their unique mass and fragmentation pattern. These two features allow the end user to monitor unique ion transitions for each compound of interest, thus improving confidence in compound identification and quantitation, all while removing safety concerns related to the use of a radioactive source. An example of typical chromatogram for a solvent standard spiked at 1,000 µg/L obtained using GC-MS/MS with t-SRM is reported in Figure 6. Endosulfan I and γ-chlordane as well as endrin and dieldrin tend to coelute on the 5% phenyl 95% dimethylpolysiloxane stationary phase used for this application; therefore, the capability of selecting unique mass ions allowed the discrimination between two compounds that are not chromatographically resolved.

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

The TSQ 9610 NeverVent AEI is equipped with the XLXR detector, which is an electron multiplier that offers extended detector lifetime and dynamic range. Calibration curves in DCM were automatically prepared using an off-line TriPlus RSH autosampler by diluting a pesticide mix in the range from 0.5 to 1,000 µg/L. Linearity was evaluated using the internal standard method by calculating the calibration factor for each analyte at each concentration, the mean calibration factor, and the relative standard deviation (RSD) of the calibration factors. The calibration factor RSD were <20% for each analyte, therefore confirming the linear trend and demonstrated in Table 2. The advantage of using internal standard calibration is to account for routine change in response of the chromatographic system as well as variation in the volume of the introduced sample or sample extract.



1=BHC, Alpha; 2=BHC, beta; 3=BHC, gamma; 4=BHC, delta; 5=Heptachlor; 6=Aldrin; 7=Heptachlor epoxide; 8=Endosulfan peak 1; 9=Chlordane gamma-trans; 10=Chlordane alpha-cis; 11=4,4'-DDE; 12=Endrin; 13=Dieldrin; 14=Endosulfan peak 2; 15=4,4'-DDD; 16=Endrin Aldehyde; 17=Endosulfan sulfate; 18=4,4'-DDT; 19=Endrin-Ketone; 20=Methoxychlor

Figure 6. Typical chromatogram for a solvent standard spiked at 1,000 µg/L. The capability of monitoring typical transitions allowed for the confident identification of the coeluting peaks as shown in the insets.

Method detection limit and instrument repeatability were assessed for all the target compounds by preparing n=10 solvent standards at a concentration of 1 µg/L. IDLs were calculated by using Equation 2 and resulted within 0.10 to 0.68 µg/L with peak area %RSD for 10 replicated injections <20, with the only exception of endosulfan (peak 1) for which peak area %RSD was 24, as reported in Table 2. Overlaid chromatograms showing peak area repeatability obtained for n=10 replicated injections for aldrin are reported as an example in Figure 7.

The best-in-class t-SRM acquisition mode coupled to the ultra- sensitive AEI ion source delivered unprecedent sensitivity with improved S/N ratio. Figure 8 demonstrates the intensity signal obtained for alpha, beta, gamma, and delta BHC at the lowest calibration point (0.5 µg/L). The calculated S/N resulted in detectability far surpassing the minimum S/N > 3 threshold often reported, therefore suggesting that limits of detection could be potentially lowered even further for future proof analysis.

Table 2. Calculated IDLs, peak area %RSD, and average calibration factor %RSD for the investigated pesticides. IDLs ranged from 0.16 to 0.68 µg/L with average RF and peak area %RSD <20%, with the only exception of endosulfan (peak 1) for which peak area %RSD was 24.

Compound	RT (min)	Average RF %RSD	Calculated IDL (µg/L)	Peak area %RSD
BHC, alpha	9.63	5.2	0.18	6.5
BHC, beta	9.98	7.8	0.31	11.4
BHC, gamma	10.15	5.9	0.16	5.8
BHC, delta	10.58	9.1	0.12	4.2
Heptachlor	11.49	9.2	0.35	11.6
Aldrin	12.23	8.6	0.33	11.3
Heptachlor epoxide	13.08	8.7	0.32	11.3
Chlordane, gamma-*trans*	13.64	7.3	0.18	6.6
Endosulfan, peak1	13.64	17.7	0.68	23.7
Chlordane, alpha-*cis*	13.94	9.3	0.28	10.0
4,4'-DDE	14.48	9.4	0.1	3.7
Endrin	14.66	8.5	0.18	6.6
Dieldrin	14.68	14.4	0.35	16.4
Endosulfan, peak 2	15.5	15.9	0.43	12.5
4,4'-DDD	15.61	15.7	0.14	4.9
Endrin aldehyde	15.89	19.2	0.5	16.7
Endosulfan sulfate	16.57	9.8	0.16	6.5
4,4'-DDT	16.7	11.7	0.22	7.4
Endrin ketone	17.96	13	0.26	9.2
Metoxychlor	18.36	15.5	0.48	17.0

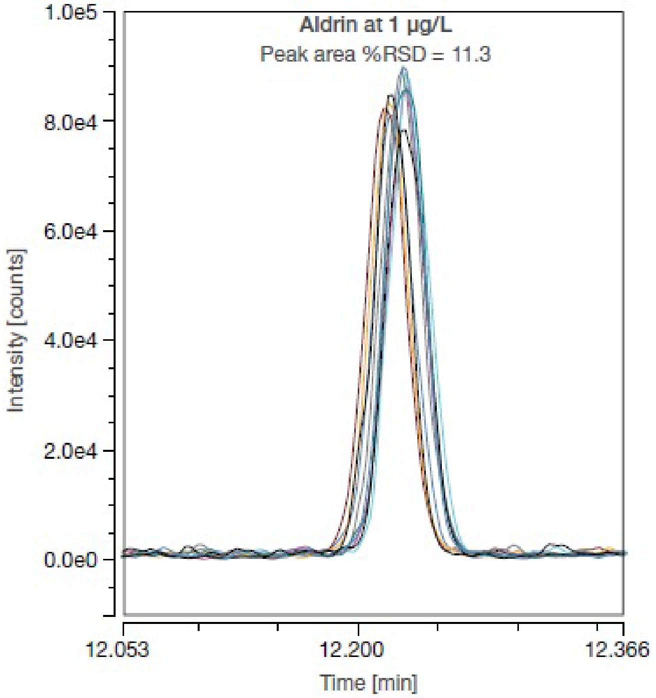


Figure 7. Overlaid chromatograms showing aldrin peak area repeatability obtained for n=10 replicated injections of solvent standard at 1 µg/L.

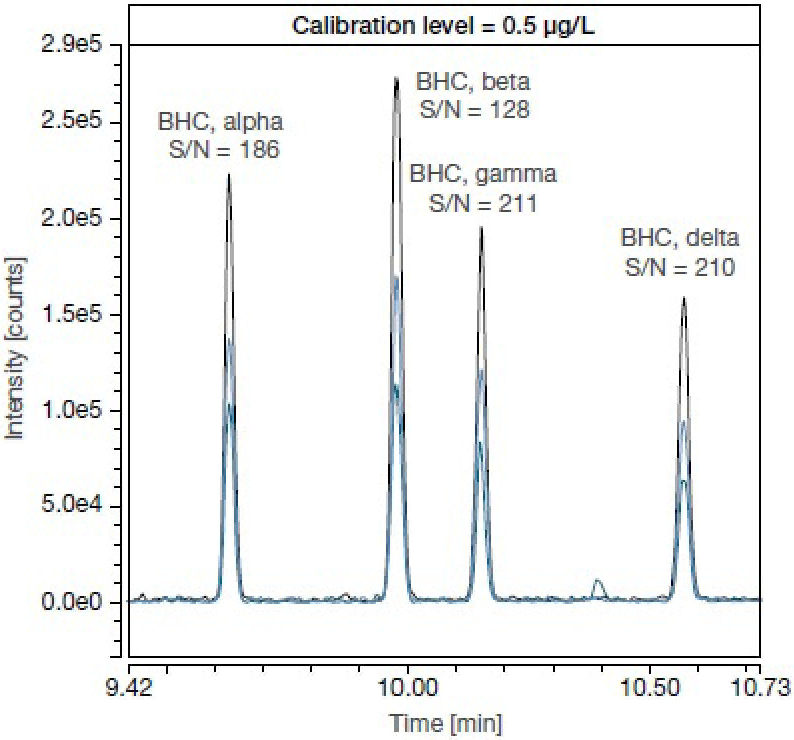


Figure 8. Intensity signal obtained for alpha, beta, gamma, and delta BHC at the lowest calibration point (0.5 µg/L). The best-in-class t-SRM acquisition mode coupled to the ultra-sensitive AEI ion source allowed for improved S/N ratio. Quantifier ion = black trace. Qualifier ions = blue and red traces.

CONCLUSIONS

Modern environmental laboratories benefit greatly from the next generation of gas chromatography-mass spectrometry instrumentation that allows analysts to be more productive with simpler to use, more rugged, and more sensitive instrumentation.

Advances in the Thermo Scientific line of GC-MS/MS allow for modernization of common environmental workflows for the analysis of SVOCs and organochlorine pesticides, as well as many more target analytes, all from a single, easy-to-use platform.

Modernizing instrumentation leads to simplified streamlined laboratory operations:

- Using a single hardware platform translates into increased sample throughput and the potential for consolidating multiple methods in a single GC run for streamlined operations.
- Harmonization of consumables and supplies, as well as decreasing the amount of expensive carrier gas, leads to more efficient lab operations and better ROI.
- A single software interface for acquisition, tuning, and reporting that can be used in an enterprise environment provides traceability and simplicity.
- Improved analyst's safety while reducing the risk of errors and cross-contaminations through the use of automated sample preparation benefits all ranges of lab staff.
- Accelerated routine maintenance operation through the NeverVent technology, allows a user to maintain the system without breaking the vacuum, and the modular concept of the TRACE 1610 GC allows for flexible configurations and reduced instrument downtime.
- Future-proof analysis with the GC-MS/MS timed-SRM acquisition and the AEI ion source for lower limits of detection and confident compound identification and quantitation, far surpassing current regulations.

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