

## **Integrated Solutions for GC/MS POP's Analysis**

Dwain Cardona  
Vertical Marketing - Environmental and Industrial  
Thermo Scientific, Austin, TX

**Sample prep /  
consumables**

**Gas  
Chromatograph  
(GC)**

**GC Mass  
spectrometry**

**Data analysis  
Software**



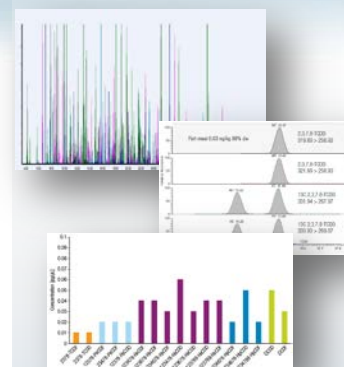
- Automation for sample preparation
- Pops consumables that simplify and improve results



- Accuracy Speed and Productivity.
- Innovating GC for routine / demanding applications



- Expect more productivity in POP's analysis



- Software for your specific Pop's analysis needs

***Workflow solutions for POP's analysis***

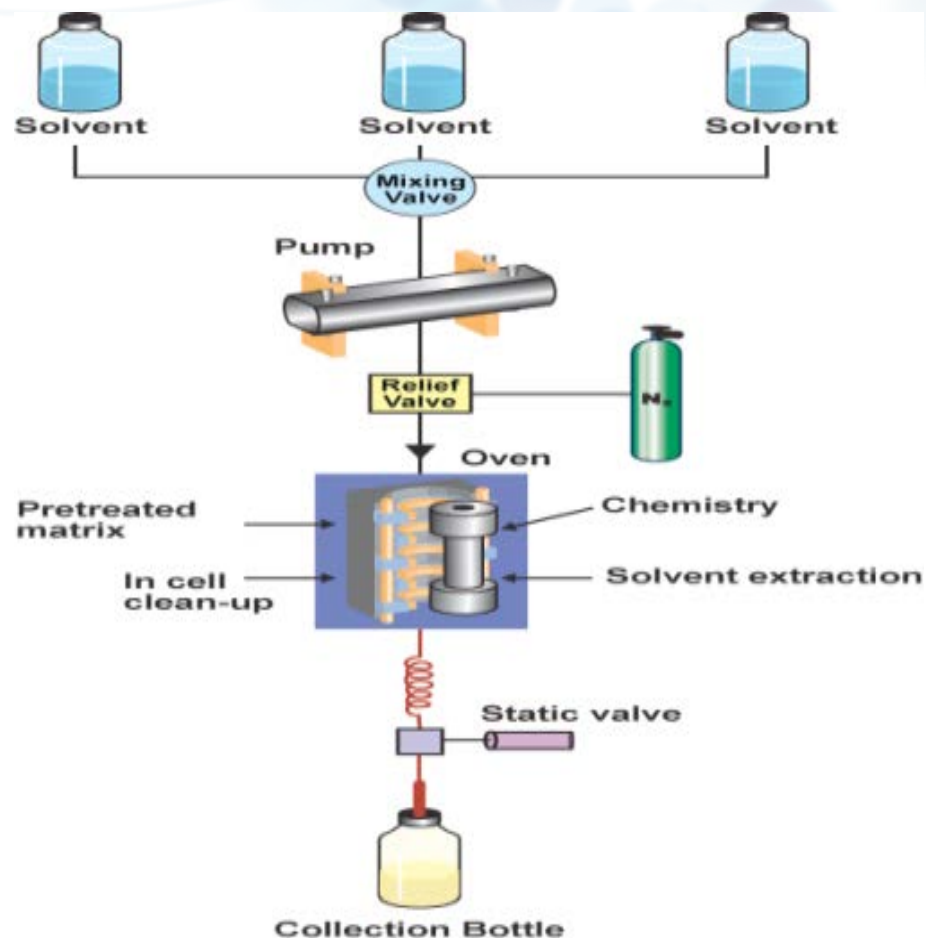
**Thermo Scientific™ Dionex™ ASE™  
350 Accelerated Solvent Extractor  
System**



# Accelerated Solvent Extraction

## Sample Extraction & Cleanup

- Extractions in minutes
- Dramatic solvent reduction
- Automated Extraction of up to 24 samples
- Sample Cell sizes: 1, 5, 11, 22, and 33 mL
- Collection bottle 40 or 60 mL
- Operating pressure 500–3000 PSI (35–200 Bar)
- Target compounds can be extracted from high fat content samples to high water content samples.



# Extraction of PAH's from Environmental Samples by Accelerated Solvent Extraction Technique

## Accelerated Solvent Extraction Technique Sample Extraction Conditions

- Solvents used
  - Dichloromethane , Acetone
- System Pressure:1500PSI
- Oven Temp: 100 ° C
- Sample Size: 7g.
- Oven heat-up time: 5 min
- Static Time:
- Solvent: 1Dichloromethane/1acetone (V/V)
- Flush Volume: 60% of the extraction cell volume
- Nitrogen Purge: 1 MPa (150 psi) for 60 s
- Extracts obtained by ASE were concentrated to 4 mL for analysis by U.S. EPA Method 8270

## GC/MS Analytical Conditions

- GC/MS 1 $\mu$ L on 30 m x 0.25 mm i.d. x 0.25  $\mu$ m
- Injector temp: 270 ° C
- Transfer line: 300 ° C.
- A three-ramp oven program was used:
  - 50 to 310 ° C at 10 ° C/min 3 min hold
  - 310 to 326 ° C at 4 ° C/min
  - 326 to 350 ° C at 10 ° C/min 10 min hold
- Carrier gas: He
- linear velocity: approximately 30 cm/s
- Scan range: 35 to 500 amu.

# Extraction of PAHs from Environmental Samples by Accelerated Solvent Extraction Technique

## Extraction analysis results

- Canadian marine sediment samples are presented
- Only four of the compounds are outside the 90% confidence interval (CI) for the certified values
- Average recovery for anthracene was lower than the certified value
- Results for , benzo[*b*]fluoranthene, benzo[*k*]fluoranthene, and dibenz[*a,h*]anthracene are higher than the certified values.
- The results indicate that the ASE technique provides equivalent or superior extraction of PAH compounds as compared to the traditional Soxhlet method.
- ASE meets the requirements for PAH analysis as described in U.S. EPA SW-846 Method 3545 (Proposed).

**Table 2. PAHs from Marine Sediment HS-3 (mg/kg)**

Compound	Average Recovery (n = 4)	Standard Deviation	Certified Value	90% CI <sup>a</sup>
Naphthalene	8.87	1.00	9.0	0.7
Acenaphthalene	ND <sup>b</sup>	NA <sup>c</sup>	0.3	0.1
Acenaphthene	4.89	0.51	4.5	1.5
Fluorene	10.09	1.26	13.6	3.1
Phenanthrene	68.80	6.44	85.0	20
Anthracene	7.73	0.57	13.4	0.5
Fluoranthene	54.73	4.82	60.0	9
Pyrene	33.70	2.83	39.0	9
Benz[ <i>a</i> ]anthracene	12.40	1.07	14.6	2
Chrysene	14.95	1.52	14.1	2
Benzo[ <i>a</i> ]pyrene	6.27	0.65	7.4	3.6
Benzo[ <i>b</i> ]fluoranthene	11.46	1.27	7.7	1.2
Benzo[ <i>k</i> ]fluoranthene	10.16	1.28	2.8	2
Benzo[ <i>ghi</i> ]perylene	4.14	0.69	5.0	2
Dibenz[ <i>ah</i> ]anthracene	2.58	0.33	1.3	0.5
Indeno[1,2,3- <i>cd</i> ]pyrene	4.30	0.77	5.4	1.3

<sup>a</sup> CI = Confidence interval of the mean

<sup>b</sup> ND = Not detectable at the level of detection (1.5 mg/kg)

<sup>c</sup> NA = Not applicable

**Thermo Scientific™ Dionex™  
AutoTrace™ 280 Solid-Phase  
Extraction (SPE) Instrument**





# Automated Solid-Phase Extraction (SPE) of Dioxins and Furans in Surface Water

- The addition of a 1% v/v isopropanol solution to the sample bottle reduces losses due to adhesion to glass and tubing.
- The use of HCL 0.1 M to acidify the sample to pH 2 prevents the humic acids often present in the water from allowing dioxins to pass through the Thermo Scientific™ Dionex™ SolEx™ SPE C18 Cartridge
- The instrument sample rack has six positions that can take volumes from 10 mL to 2000 mL and six sample collection positions for the eluent.

## Sample Preparation

- A 500 mL sample of river water is taken for the analysis and mixed with 5 mL of isopropanol to prevent the components from sticking to the glass bottle.
- The use of HCL 0.1 M is important to adjust the water to pH 2 to enhance recoveries
- A standard Dionex SolEx SPE C18 cartridge end capped SPE silica column, 6 mL, 1 g, can be used for the clean up. The elution solvent is ethanol/toluene (70:30) mL and six sample collection positions for the eluent.



# Automated Solid-Phase Extraction (SPE) of Dioxins and Furans in Surface Water

No.	Method: Estimated Time 1 h 30 min
1	Process six samples using the following method steps:
2	Condition column with 5.0 mL of CH <sub>3</sub> OH into solvent waste.
3	Condition column with 5.0 mL of water into aqueous waste.
4	Load 500.0 mL of sample into column.
5	Rinse column with 3.0 mL of CH <sub>3</sub> OH/water 40:60 into solvent waste.
6	Wash syringe with 5.0 mL of 70%EtOH/toluene.
7	Dry column with gas for 10 min.
8	Collect 5.0 mL fraction into sample tube using 70%EtOH/toluene.
9	Wash syringe with 5.0 mL of CH <sub>3</sub> OH.
10	End.

## Parameters

### Flow Rates

Cond Flow:	15.0 mL/min
Load Flow:	10.0 mL/min
Rinse Flow:	20.0 mL/min
Elute Flow:	5.0 mL/min
Cond Air Push:	15.0 mL/min
Rinse Air Push:	20.0 mL/min
Elute Air Push:	5.0 mL/min

### SPE Parameters

Push Delay:	5 sec
Air Factor:	1.0
Autowash Vol.:	1.00 mL

### Instrument Parameters

Max. Elution Vol.:	12.0 mL
Exhaust Fan On:	Yes
Beeper On:	Yes

**Thermo Scientific™ TriPlus RSH™  
Autosampler**



# Keypoints and solutions for the productive lab

- A **large number** of samples in the trays  
Up to **648 2-mL** vials and multiple 100 mL solvent bottles stations
- Unattended, **injection modes changes in a sequence**: liquid – liquid Large Volume - HS - SPME  
ATC (Automatic Tool change) Station for automatic recognition and syringe exchanges during operation
- **Reliable, reproducible** injections with microvolume samples using the **bottom sensing sensor**  
<2%RSD and up to 3 injections possible with 5 µl sample volume in vial.
- **Advanced sample handling** and sample preparation  
Dilution, derivatization, standard addition, internal standard additions, etc.
- **Barcode reading** for avoiding writing mistakes
- Set up possible for **two GC's**
- **Completely adaptable to your wishes:**
  - cooled/heated trays;
  - larger washing stations;
  - HS ovens;
  - vortex for mixing;
  - and more.....
  - **just ask us for implementation of your idea!**



## Thermo Scientific™ TRACE™ 1300 Series Gas Chromatograph

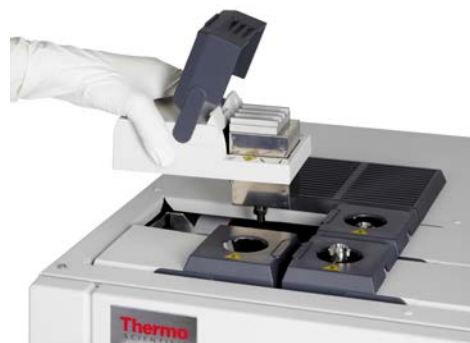


# TRACE 1300 Series - Ground-breaking **ease of use** and **performance!**

**TRACE 1310:** Touch screen interface provides instant access for ease of use and local control



**TRACE 1300:** Local built-in ultra-simplified user interface – **two buttons and four LEDs.**



## **“instant connect” modularity**

### **Modules available:**

INLETS: SSL - SSL backflush - PTV - PTV backflush

DETECTORS: FID - TCD - ECD - NPD - MS\*

OTHER OPTIONS: Oven Cryo - Aux carrier

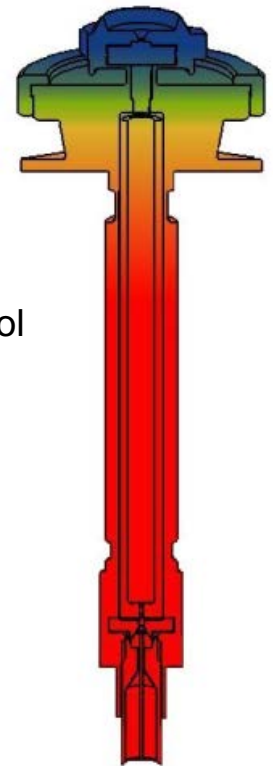
Software drivers: TraceFinder, Chromeleon CDS, Xcalibur, ChromQuest, ChromCard

\* Supported MS: ISQ; ITQ; TSQ8000; TSQ Quantum XLS Ultra; DFS; Delta V



# Gas Chromatograph for the POP's lab:

- **Modular** approach:
  - Change injectors and detectors in 3 minutes only
  - Easy maintenance -disassemble and sonicate
  - the injector arts
- **Fast cooling** of the oven and PTV for fast run to run times;
  - from 350C to 40C in approximately **4 minutes**
  - extra fast cooling with **cryo option** for oven and injector
- **Methodology is completely compatible with third party vendors**
  - **Same injection parameters, little RT difference**
  - Injector modules
  - Include injector body, valves, filters, electronics for temperature and carrier gas control
  - Cool head and septum
  - Less septum bleed
  - Increased column lifetime and MS sensitivity
- **Injection modes include:**
  - SSL, SSL with backflush, PTV, PTV with backflush
  - all are **compatible with Large Volume** without
  - any hardware change



# Organochlorine pesticides - EPA method 8081

## Recommended Conditions

### TRACE 1310 GC

Injection Volume: 1  $\mu$ L

Liner: Splitless with glass wool (P/N 453A1925)

Carrier Gas: Helium, constant flow, 1 mL/min

Column Type: 30 m, 0.25 mm, 0.25  $\mu$ m, TG-5MS (P/N 26098-420)

Column Oven: Initial 100  $^{\circ}$ C, hold 1.0 min. Ramp at : up to 180 $^{\circ}$ C. Ramp at 5.0  $^{\circ}$ C/min to : Ramp at 20.0  $^{\circ}$ C/min to 320  $^{\circ}$ C. Hold

### Instant Connect SSL Injector

Inlet Temperature: 250  $^{\circ}$ C

Mode: Splitless, 2 min; split flow 50 mL/min

### Instant Connect ECD

Temperature: 320  $^{\circ}$ C

Makeup Gas: Nitrogen, 15 mL/min makeup flow

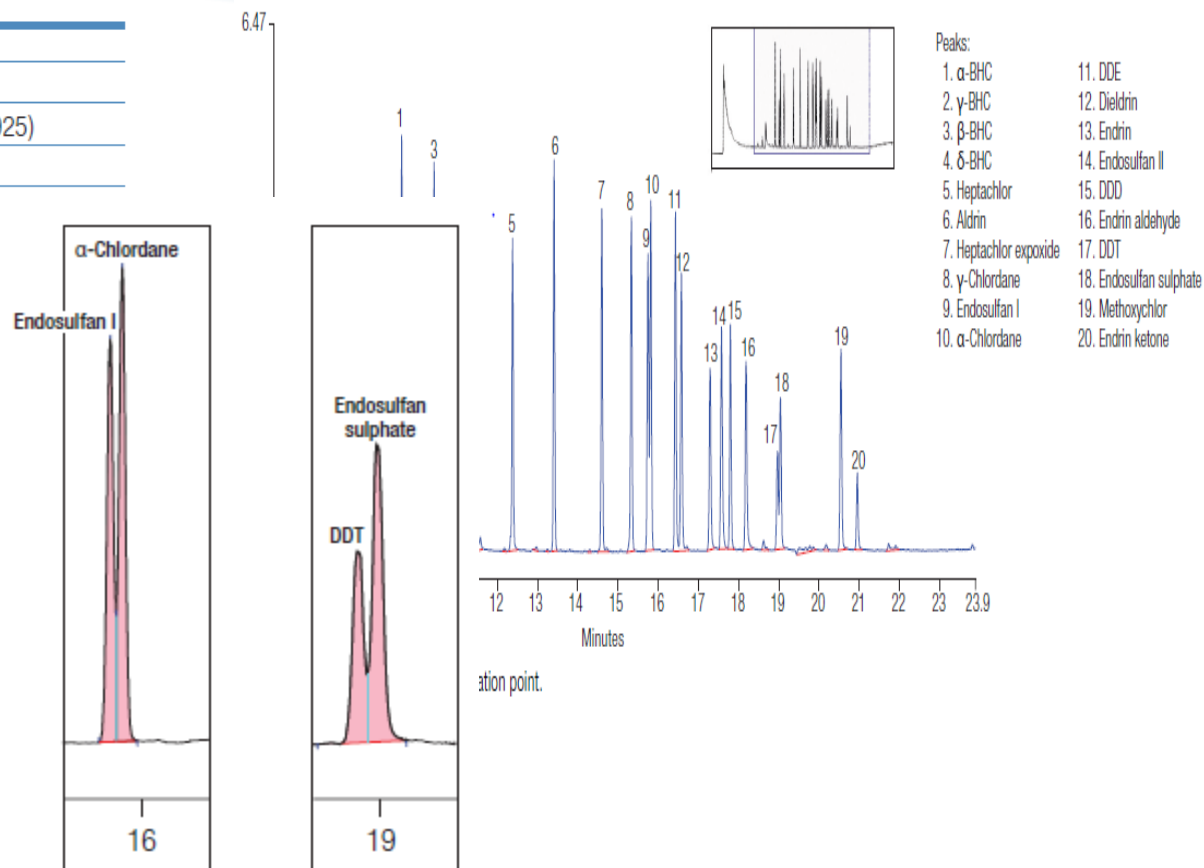


Figure 3. Resolution of "critical couples".



# Organochlorine pesticides - EPA method 8081

Table 2. Limit of detection.

	Std. Dev	No. of Repeats	t(14-1)	Calculated LOD (ppb)
$\alpha$ -BHC	0.009	14	2.650	0.023
$\gamma$ -BHC	0.009	14	2.650	0.025
$\beta$ -BHC	0.007	14	2.650	0.018
$\delta$ -BHC	0.007	14	2.650	0.019
Heptachlor	0.011	14	2.650	0.029
Aldrin	0.005	14	2.650	0.013
Heptachlor epoxide	0.008	14	2.650	0.021
$\gamma$ -Chlordane	0.073	14	2.650	0.194
Endosulfan I	0.013	14	2.650	0.034
$\alpha$ -Chlordane	0.019	14	2.650	0.050
DDE	0.008	14	2.650	0.020
Dieldrin	0.011	14	2.650	0.030
Endrin	0.018	14	2.650	0.049
Endosulfan II	0.023	14	2.650	0.062
DDD	0.009	14	2.650	0.025
Endrin aldehyde	0.01	14	2.650	0.026
DDT	0.008	14	2.650	0.020
Endosulfan sulphate	0.01	14	2.650	0.028
Methoxychlor	0.013	14	2.650	0.035
Endrin ketone	0.039	14	2.650	0.103

Table 3. Retention time and area repeatability (n = 10).

	Ret. Time RSD%	Peak Area RSD%
$\alpha$ -BHC	0.03	2.41
$\gamma$ -BHC	0.04	2.69
$\beta$ -BHC	0.03	2.02
$\delta$ -BHC	0.03	1.59
Heptachlor	0.03	2.40
Aldrin	0.02	2.16
Heptachlor epoxide	0.02	1.97
$\gamma$ -Chlordane	0.02	2.47
Endosulfan I	0.02	2.04
$\alpha$ -Chlordane	0.02	1.75
DDE	0.02	2.09
Dieldrin	0.02	2.18
Endrin	0.02	2.00
Endosulfan II	0.02	2.82
DDD	0.02	2.18
Endrin aldehyde	0.02	2.66
DDT	0.02	4.76
Endosulfan sulphate	0.02	1.71
Methoxychlor	0.02	2.25
Endrin ketone	0.02	4.14

## ● Chromatography Consumables



# Chromatography consumables



Find the best solution to your separation challenges: easily download one-click workflows for use with Chromeleon CDS, just search>filter>download>run -



**Sample**



## LC Columns & Consumables

Reversed phase, ion exchange, HILIC or normal phase chromatography.



## GC Columns & Consumables

Unrivalled GC column performance for multi-residue pesticide analysis and proven consumables for optimum system performance



## Sample Analysis Vials And Closures



## IC Columns & Consumables

Increase chromatographic efficiency and resolution with Dionex™ IonPac™ columns -





## **Gas Chromatography Mass Spectrometry**

# Step up to the next level of GC performance

TRACE 1300 series GC is part of the Thermo Scientific GC/MS solutions



ISQ QD™



DFS™



ISQ LT™



TSQ Duo™



TSQ Evo™

ISQ QD™ and ISQ LT™, *Single Quadrupole MS*  
TSQ Duo™ and TSQ Evo™ *Triple Quadrupole MS*  
DFS™, *Magnetic Sector high resolution MS*

# Full Source Removal...Under Vacuum!

## ExtractaBrite Source

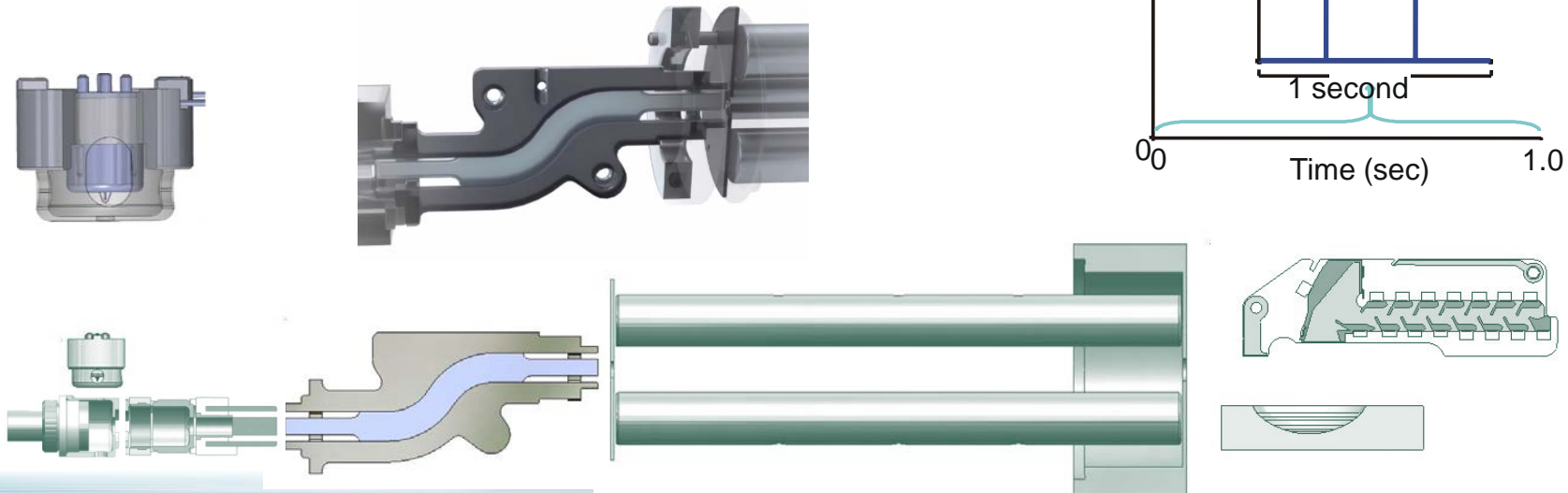
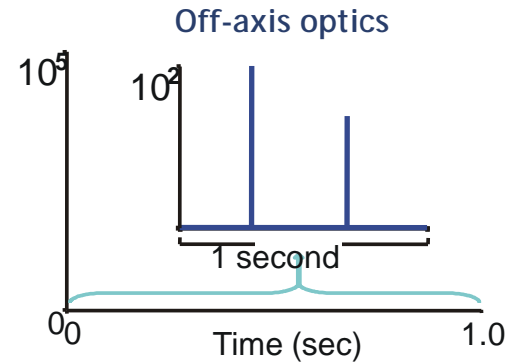
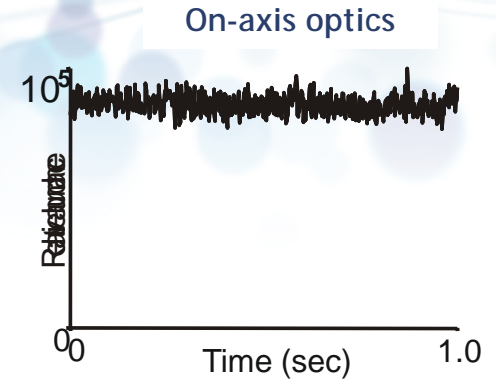


- Removes all parts needing periodic cleaning
- Includes first RF Source
- Eliminates approximately one day of down-time
- Important for dirty matrices often used with triple quads

**Thermo**  
SCIENTIFIC

# Designed for *Selectivity*

- S-Shaped *Flatapole* Ion Guide
  - Dramatic reduction in neutral noise
  - performance, even at very low concentrations
  - Peaks not riding on neutral noise background, making it easier for automated peak detection and review





# TRACE 1300/1310 ISQ QD and LT GC-MS



# Determination of Organochlorine Pesticides Using GC-MS with a Helium-conserving Injector

## Method Setup

### Conditions

#### TRACE 1310 GC

Injection volume:	1 $\mu$ L
Liner:	Splitless w/glass wool
Carrier gas:	Helium
Column type:	Thermo Scientific™ TraceGOLD™ TG-5 30 m, 0.25 mm, 0.25 $\mu$ m
Column oven:	Ready delay 1 min. Initial temperature 100 °C, hold 2 min. Ramp 15 °C/min to 160 °C, hold 5 min. Ramp 5 °C/min to 270 °C hold 2 min
SSL Injector:	225 °C; splitless mode for 2 min with a split ratio of 50:1. Helium delay 0.1 min
Column flow:	Constant flow at 1 mL/min

#### ISQ LT Mass Spectrometer

Source temperature:	270 °C
Transfer line temperature:	270 °C

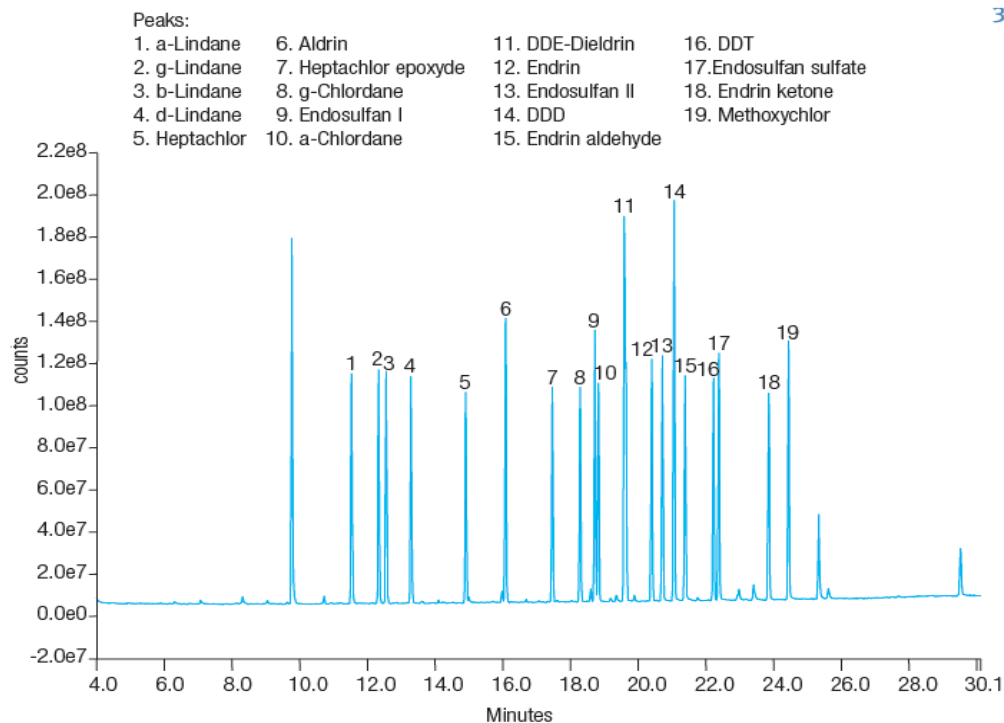


Figure 1. Analysis of organochlorine pesticides at 1 ppm in Full Scan mode.

# Determination of Organochlorine Pesticides Using GC-MS with a Helium-conserving Injector

Table 2. Calibration results.

Peak Name	Ret.Time	Cal.Type	Number of Points	Coeff. of Determination
a-BHC	11.565	Lin, WithOffset	6	0.999
g-BHC	12.362	Lin, WithOffset	6	0.998
b-BHC	12.585	Lin, WithOffset	6	0.998
d-BHC	13.322	Lin, WithOffset	6	0.997
Heptachlor	14.943	Lin, WithOffset	6	0.997
Aldrin	16.125	Lin, WithOffset	6	0.999
Heptachlor epoxyde	17.507	Lin, WithOffset	6	0.999
g-Chlordane	18.334	Lin, WithOffset	6	0.998
Endosulfan I	18.767	Lin, WithOffset	6	0.998
a-Chlordane	18.875	Lin, WithOffset	6	0.998
DDE	19.637	Lin, WithOffset	6	0.997
Dieldrin	19.684	Lin, WithOffset	6	0.997
Endrin	20.445	Lin, WithOffset	6	0.998
Endosulfan II	20.760	Lin, WithOffset	6	0.997
DDD	21.102	Lin, WithOffset	6	0.996
Endrin aldehyde	21.435	Lin, WithOffset	6	0.998
Endosulfan sulfate	22.272	Lin, WithOffset	6	0.996
DDT	22.431	Lin, WithOffset	6	0.996
Endrin ketone	23.907	Lin, WithOffset	6	0.997
Methosychlor	24.488	Lin, WithOffset	6	0.995

Table 3. Area repeatability.

Compound	RSD %
a-BHC	2.62
d-BHC	3.40
b-BHC	2.35
g-BHC	2.42
Heptachlor	2.42
Aldrin	2.56
Heptachlor epoxyde	2.57
g-Chlordane	2.53
Endosulfan	2.50
a-Chlordane	2.67
DDE	2.71
Dieldrin	2.32
Endrin	2.54
Endosulfan II	2.83
DDD	2.61
Endrin aldehyde	2.24
DDT	8.32
Endosulfan sulfate	2.64
Endrin ketone	2.17
Metoxychlor	2.89

# GC/MS features SIM (and SRM) Bridge

Truly **Simple**

## Simplify your transition to triple quadrupole GC-MS/MS

The TSQ Duo GC-MS/MS enables truly simple operation whether you choose to use it in single or triple quadrupole mode. It also bridges the gap between single and triple quadrupole within the same instrument to allow easy adoption of powerful MS/MS workflows when required.

Using the instrument in single quadrupole GC-MS mode allows you to continue running your current set-up and established methods. When the time is right, integrated software tools will walk you through a step-by-step process to manage the transition to powerful triple quadrupole methods.

**TSQ Duo SIM Method**

Option 1: Continue with SIM method

**Current Method**

Whether you are new to triple quadrupole GC-MS/MS or not, all you need is your current compound list and/or method.

Once you are up and running with SRM methods, optional software tools such as timed SRM (t-SRM) are available to keep your method optimal in the easiest way possible – no more complex time window set-up and extended time for running samples.

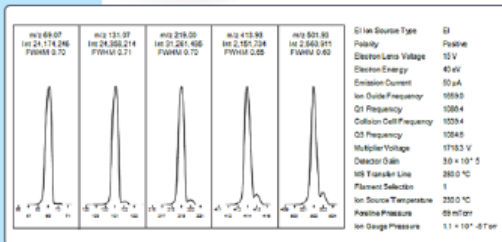
**TSQ Duo SRM Method**

Option 2: Straight to MS/MS method

**AutoSRM**

Ready to move to MS/MS

Fully optimized SRM transitions

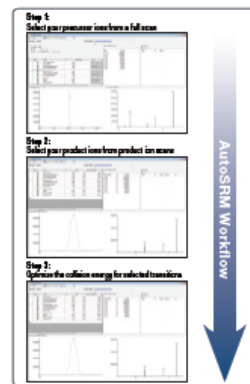


▲ The TSQ Duo GC-MS/MS is as easy to operate routinely as a single quadrupole instrument, including tuning. Simple, fully automated tuning is available in both single and triple quadrupole modes, including leak checking.

### SIM Bridge

The SIM Bridge tool allows SIM methods exported from other sources to be translated to the TSQ Duo method. Those SIM methods can be immediately

run on the TSQ Duo system or through AutoSRM to translate the SIM information into a powerful SRM method.



AutoSRM is your very own mass spectrometer method development expert integrated into your system. This software walks you through the development of full optimum SIM target ions or SRM transitions in a very simple and efficient workflow. If you like to develop from your current SIM method, SIM Bridge streamlines the workflow by importing your method details. All together, it is full MS and MS/MS method development independence even for the less experienced user.

# TSQ Duo and Evo GC-MS/MS

**TSQ Duo**  
*Mass Spectrometer*

**A Simply Unique  
GC-MS/MS**



**TSQ 8000 EVO**  
*Triple Quadrupole Mass Spectrometer*

Expect **More**  
Productivity





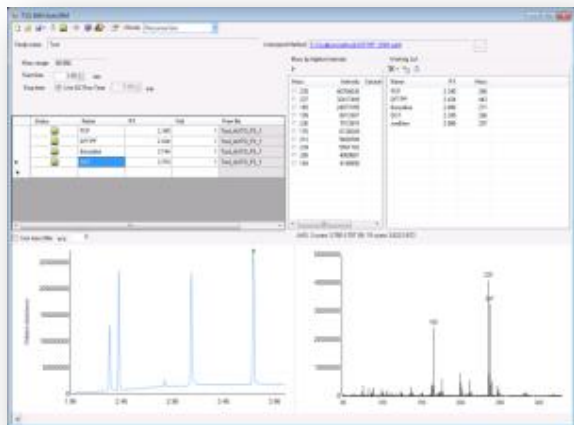
# Compliance with New EU Dioxin Regulation

European Commission GC-MS/MS Confirmatory Performance Criteria	TSQ 8000 Evo GC-MS/MS Capabilities	Compliance Confirmed
Two specific precursor ions with two specific production ions	All recommended methods developed <b>as defined in criteria</b> Fully optimized by AutoSRM	<b>Yes</b>
Tolerance of ion ratios within $\pm 15\%$	<b>&lt; 10%</b> measured at EPA 1613 CSL level (n=14)	<b>Yes</b>
Resolution of each quadrupole equal to or better than unit mass resolution	All recommended methods developed <b>Q1 and Q3 at 0.7 Da</b>	<b>Yes</b>
The % RSD of the five (or more) Relative Response Factors (RRFs) for each unlabeled PCDD/PCDF and labelled internal standards must not exceed 20%	6 point curve EPA 1613 CSL-CS4 <b>2%</b>	<b>Yes</b>

Expect **More**  
Performance

# AutoSRM : Automated Optimization of SRM Methods

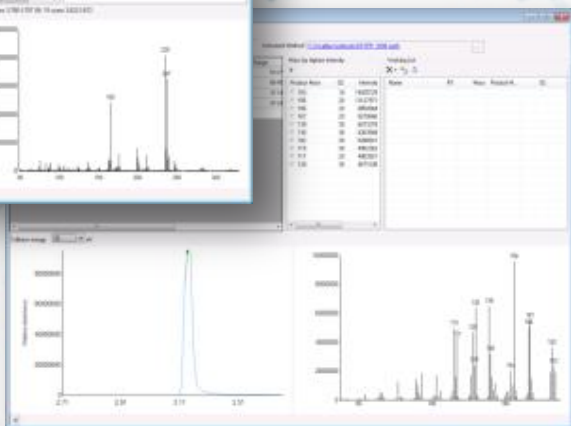
## 1) Precursor ion selection



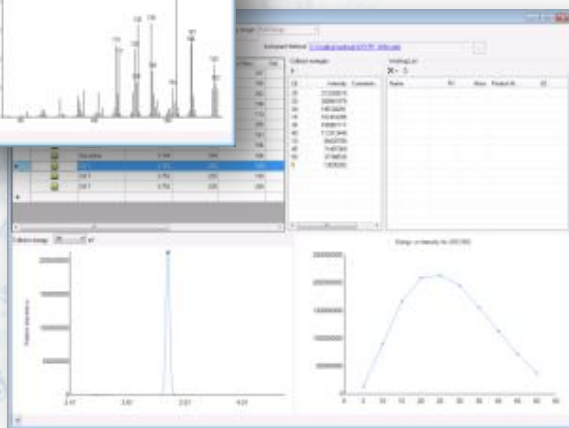
Expect **More**  
Simplicity

AutoSRM automates  
the development of  
SRM methodology

## 2) Product ion selection

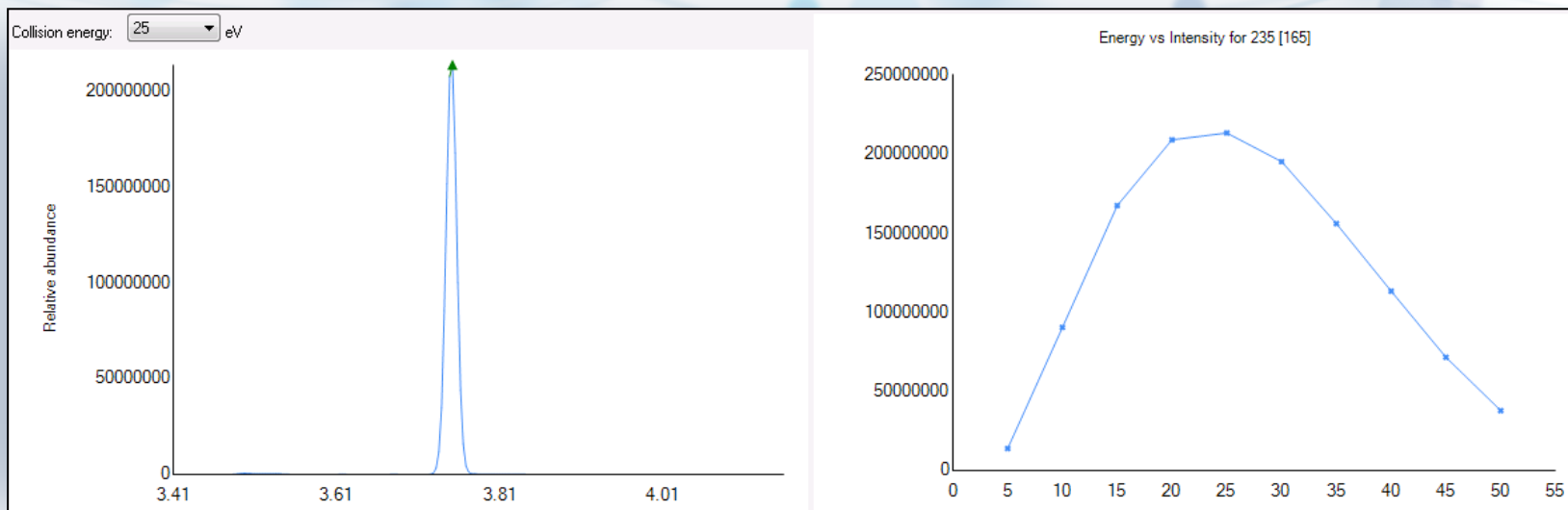


## 3) Collision energy optimization





# Highlights of AutoSRM



*End result showing optimized transition*

- **Automates the following:**

- Creation of fullscan, product ion scan and SRM methods
- Creation of sample sequences
- Creation of data layouts for analyzing results
- Selection of precursor, product and collision energies

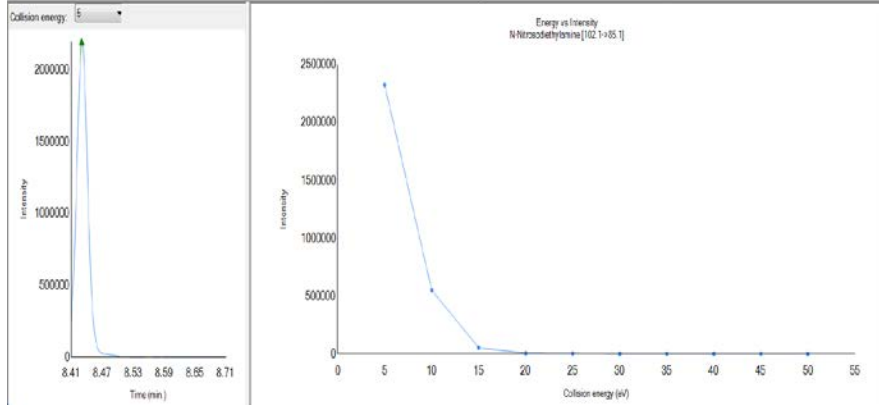
# SRM development output

- Put the magnifying glass on areas where we can improve your analysis

Status	Name	RT	Mass	Product Mass	Val Position
	N-Nitrosodimethylamine	8.194	71.1	45.1	1
	N-Nitrosodethylamine	8.56	102.1	42.1	1
	N-Nitrosodethylamine	8.56	102.1	44.1	1
	N-Nitrosodethylamine	8.56	102.1	56.1	1
	N-Nitrosodethylamine	8.56	102.1	57.1	1
	N-Nitrosodethylamine	8.56	102.1	85.1	1
	N-nitrosod-n-propylamine-d14	9.594	80.2	70.1	1
	N-nitrosod-n-propylamine-d14	9.594	110.1	46.1	1
	N-nitrosod-n-propylamine-d14	9.594	144.2	46.1	1
	N-nitrosod-n-propylamine-d14	9.594	144.2	50.1	1
	N-nitrosod-n-propylamine-d14	9.594	144.2	70.1	1
	N-nitrosod-n-propylamine-d14	9.594	144.2	120.2	1

CE	Intensity	Comments
5	232299	
10	56203	
15	54544	
20	8231	
25	4182	
40	1096	
45	1163	
30	1372	
35	1353	
50	225	

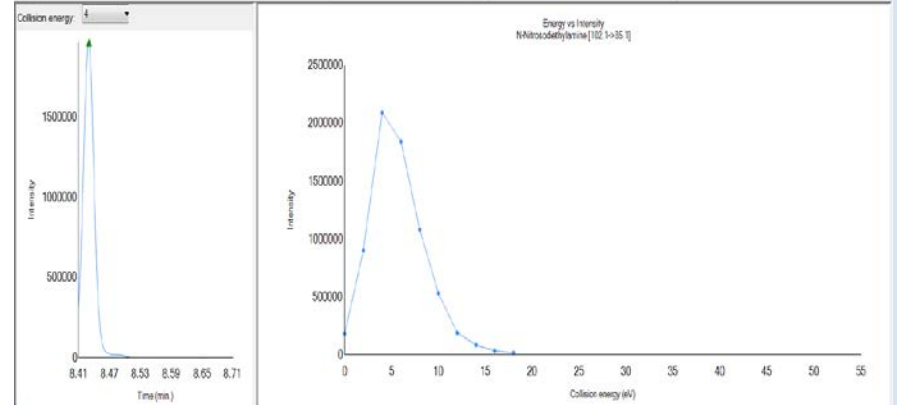
Name	RT	Mass	Product	CE
N-Nitrosop...	11.698	114.1	42.1	15
N-Nitrosop...	11.698	114.1	55.0	15
N-Nitrosop...	11.698	114.1	56.1	10
N-Nitrosop...	11.698	114.1	84.1	5
N-Nitrosop...	11.698	114.1	97.1	5
N-Nitrosop...	11.900	114.1	41.1	10
N-Nitrosop...	11.900	114.1	55.1	15
N-Nitrosop...	11.900	114.1	83.1	10
N-Nitrosop...	11.965	100.1	41.1	15
N-Nitrosop...	11.965	100.1	43.1	10
N-Nitrosop...	11.965	100.1	55.1	5
N-Nitrosop...	11.965	100.1	68.1	10
N-Nitrosop...	11.965	100.1	70.1	5



Status	Name	RT	Mass	Product Mass	Val Position
	N-Nitrosodimethylamine	8.194	71.1	45.1	1
	N-Nitrosodethylamine	8.56	102.1	42.1	1
	N-Nitrosodethylamine	8.56	102.1	44.1	1
	N-Nitrosodethylamine	8.56	102.1	56.1	1
	N-Nitrosodethylamine	8.56	102.1	57.1	1
	N-Nitrosodethylamine	8.56	102.1	85.1	1
	N-nitrosod-n-propylamine-d14	9.594	80.2	70.1	1
	N-nitrosod-n-propylamine-d14	9.594	110.1	46.1	1
	N-nitrosod-n-propylamine-d14	9.594	144.2	46.1	1
	N-nitrosod-n-propylamine-d14	9.594	144.2	50.1	1
	N-nitrosod-n-propylamine-d14	9.594	144.2	70.1	1
	N-nitrosod-n-propylamine-d14	9.594	144.2	120.2	1

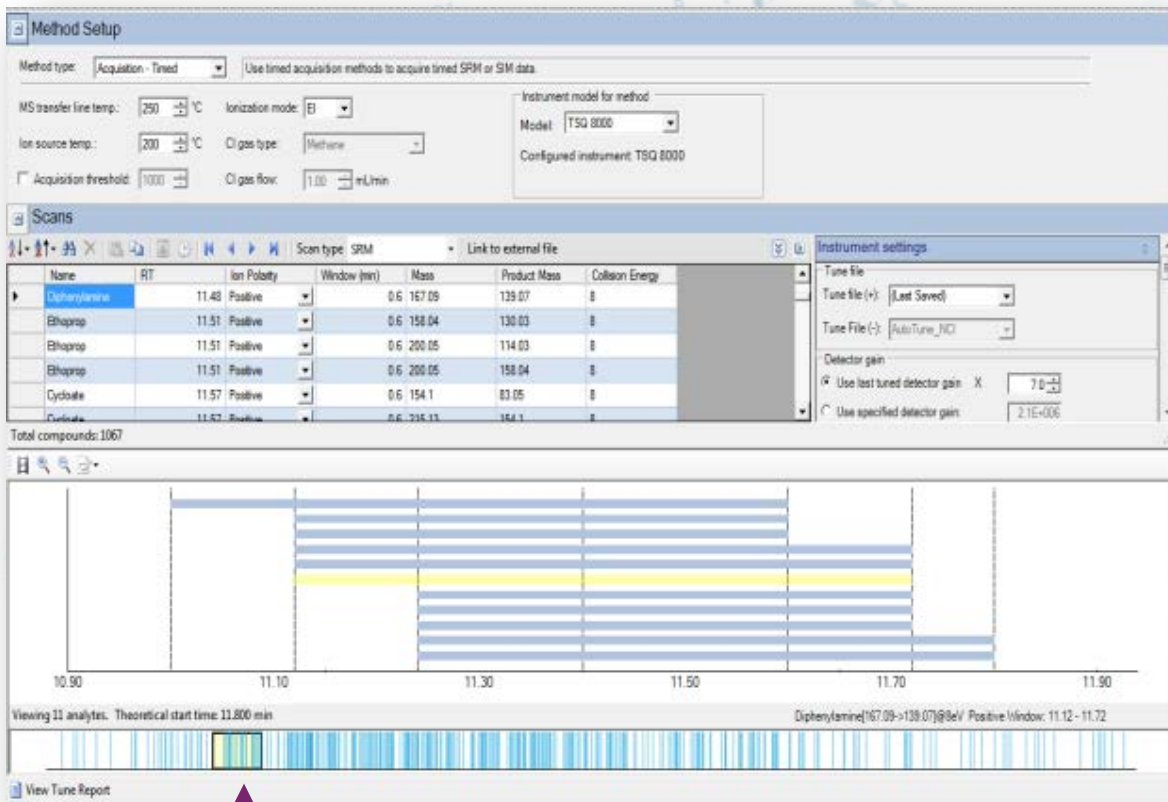
CE	Intensity	Comments
4	203217	
6	134148	
8	109120	
2	90100	
10	53072	
12	19997	
8	181796	
14	8528	
16	33658	
18	15705	

Name	RT	Mass	Product	CE
N-Nitrosop...	11.698	114.1	42.1	14
N-Nitrosop...	11.698	114.1	55.0	18
N-Nitrosop...	11.698	114.1	56.1	12
N-Nitrosop...	11.698	114.1	84.1	6
N-Nitrosop...	11.698	114.1	97.1	6
N-Nitrosop...	11.900	114.1	41.1	10
N-Nitrosop...	11.900	114.1	55.1	16
N-Nitrosop...	11.900	114.1	83.1	12
N-Nitrosop...	11.965	100.1	41.1	18
N-Nitrosop...	11.965	100.1	43.1	8
N-Nitrosop...	11.965	100.1	55.1	6
N-Nitrosop...	11.965	100.1	68.1	8
N-Nitrosop...	11.965	100.1	70.1	6



# AutoSRM : Automated Optimization of SRM Methods

Expect **More**  
Simplicity

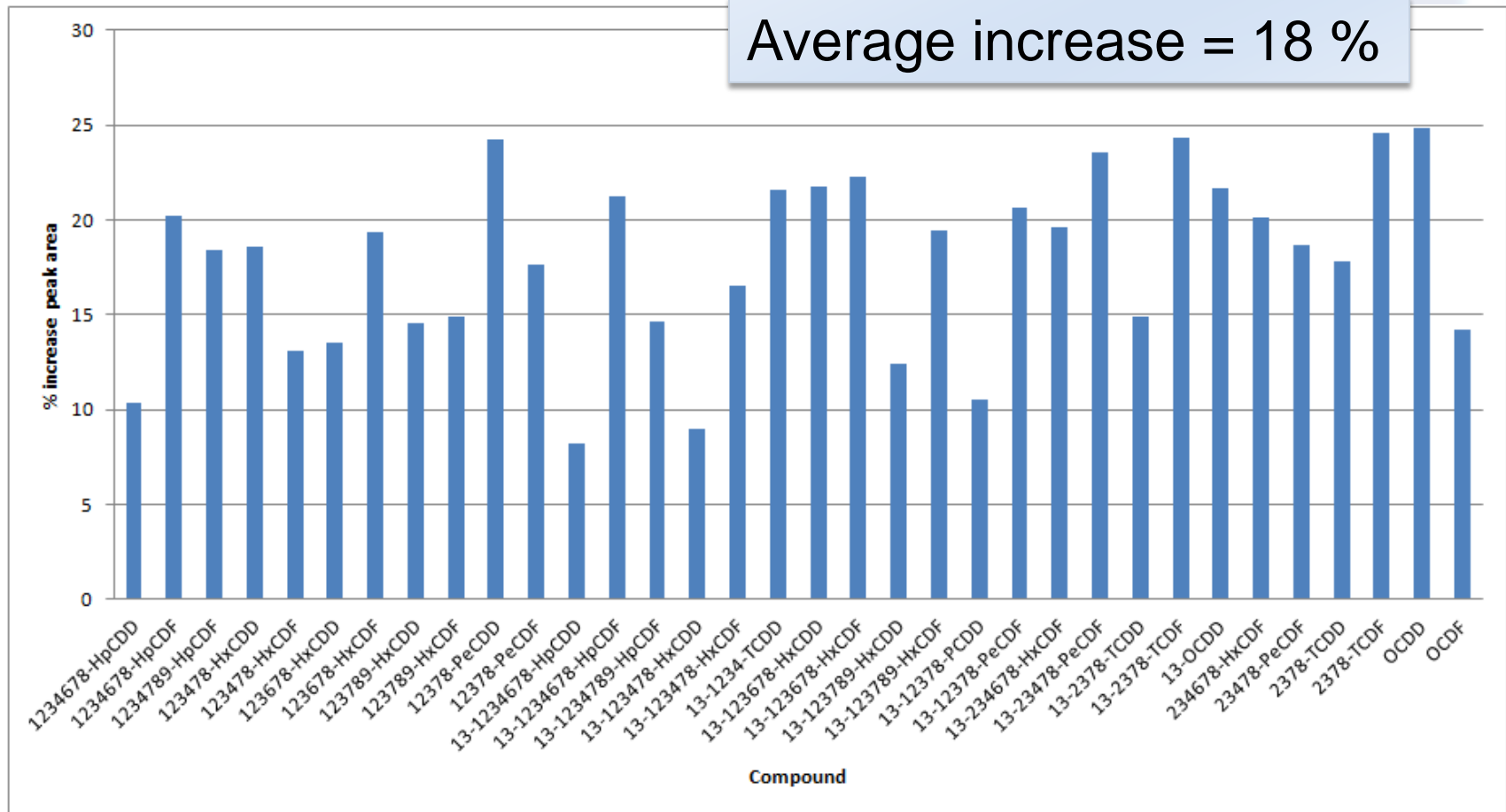


Method navigation using SRM density map

- Evolution of instrument method GUI to promote speed and ease of use
- Additional tools like SRM density map to help navigate complex methods

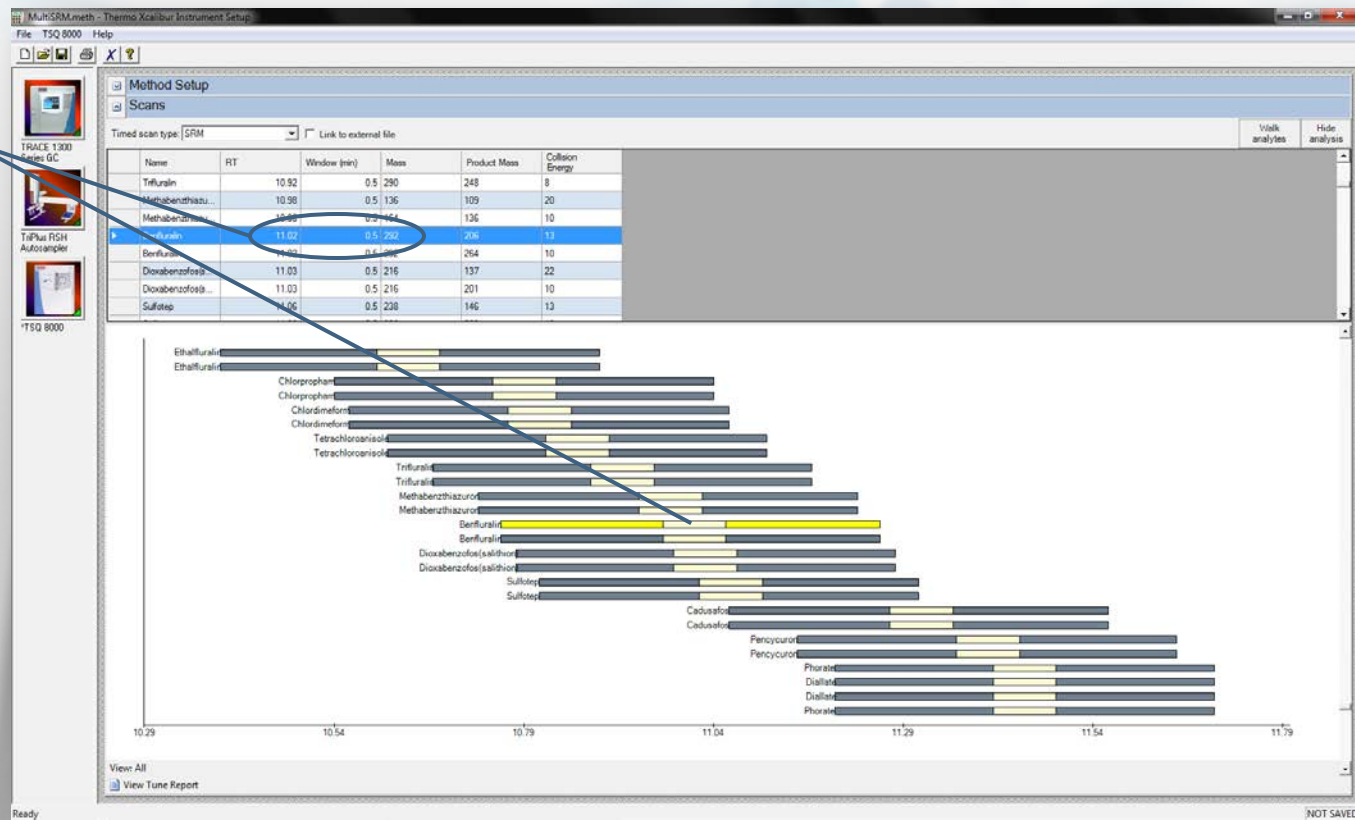
# Auto SRM Optimized CE(V) for Dioxin Analysis

- Optimized CE vs. 'generic' 22 eV

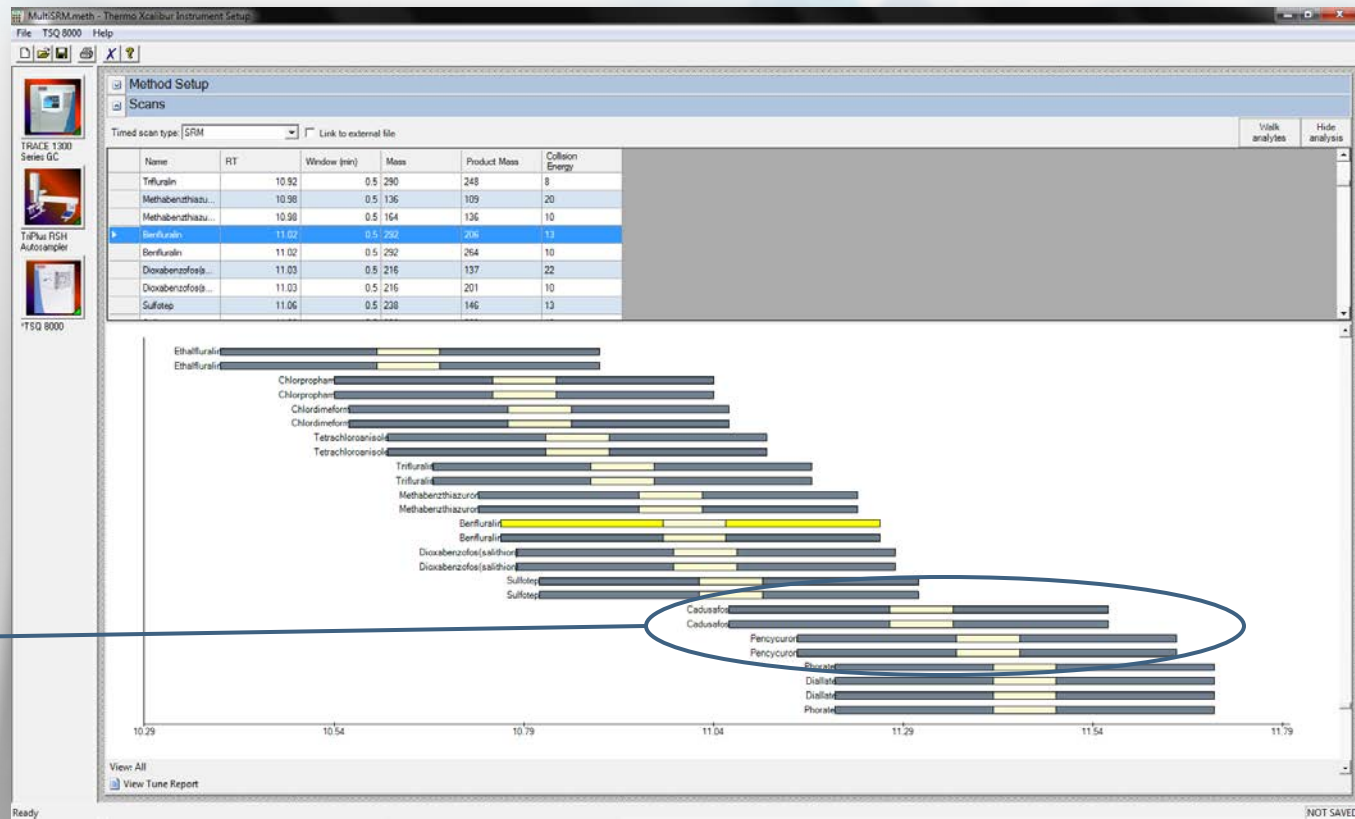


# Timed-SRM Method Overview

Acquisition windows centered around retention time



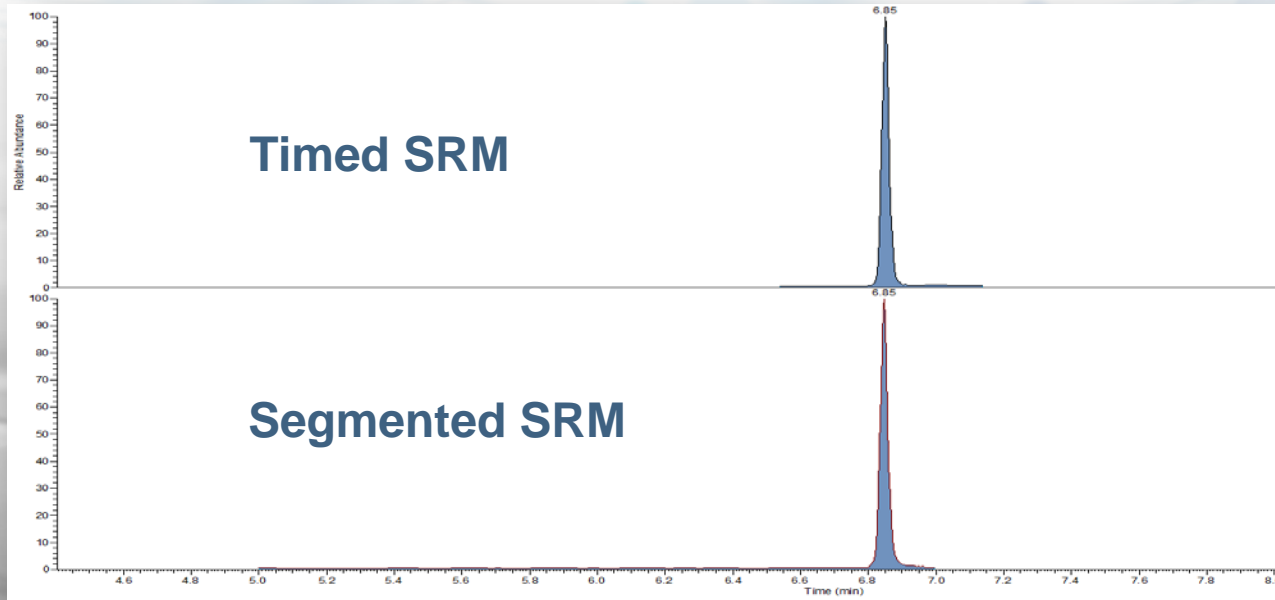
# Timed-SRM Method Overview



Acquisition windows allowed to overlap

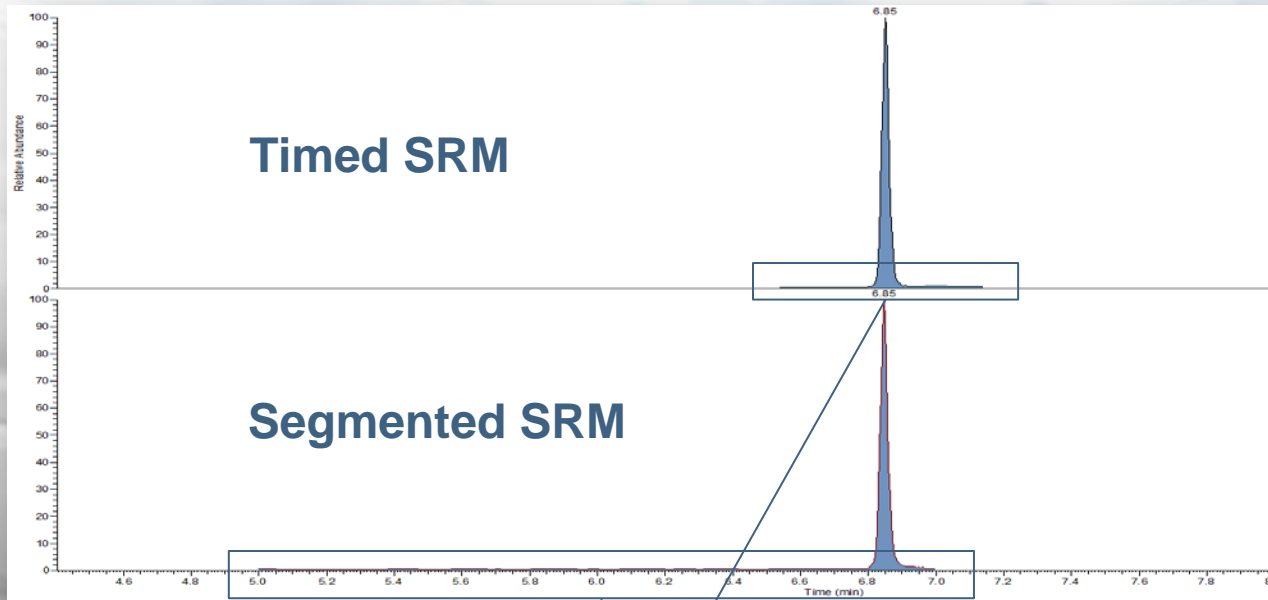


# Timed-SRM Advantages



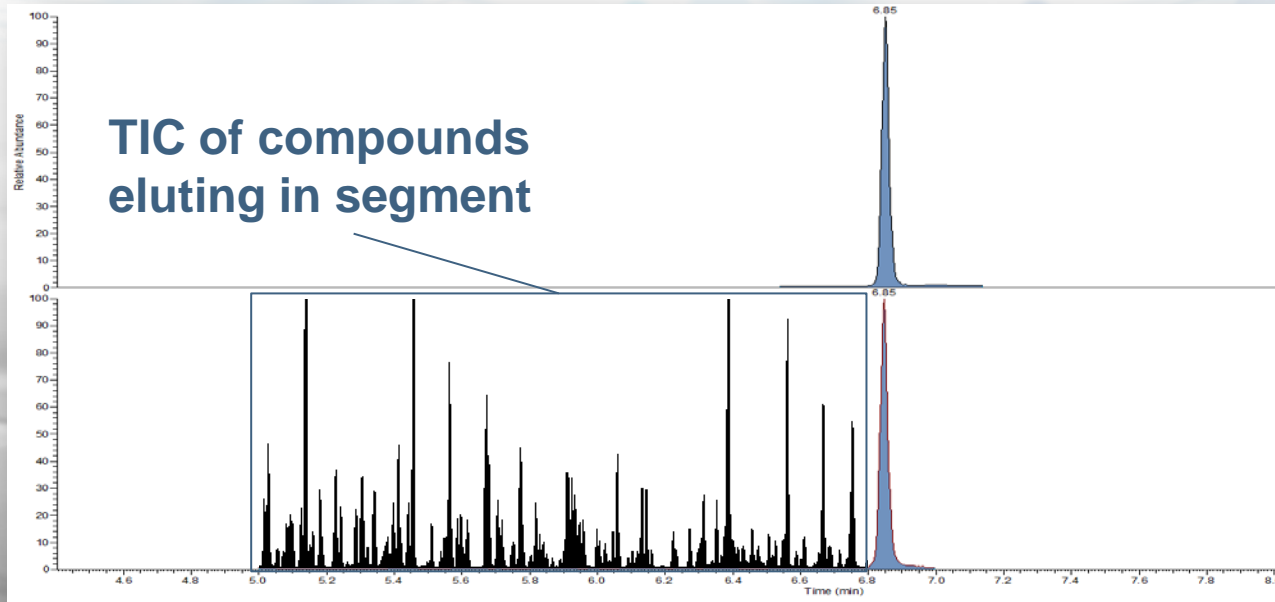


# Timed-SRM Advantages

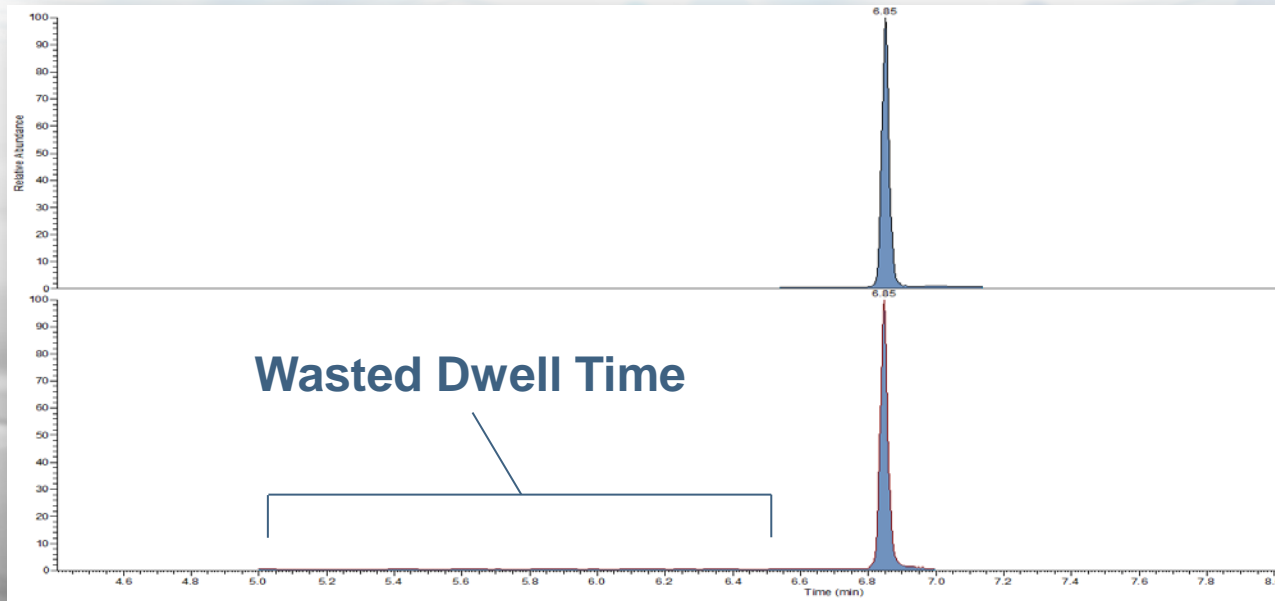


**Acquisition Windows**

# Timed-SRM Advantages

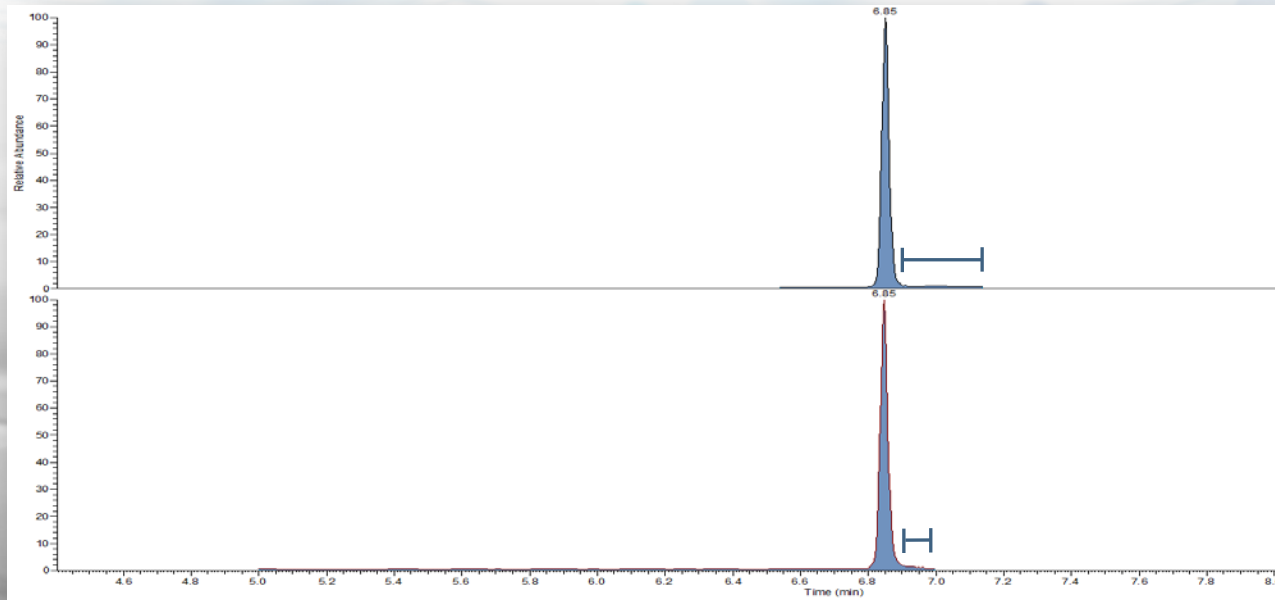


# Timed-SRM Advantages



- **Removes wasted dwell time**
  - Allow higher overall dwell times
  - Leads to higher sensitivity

# Timed-SRM Advantages

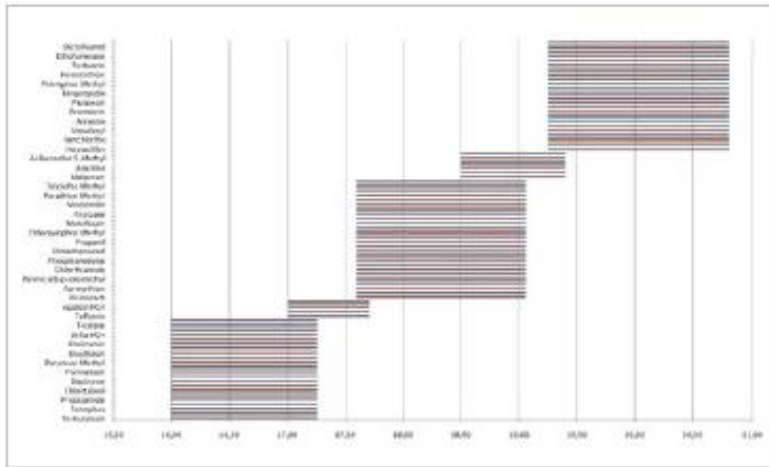


- **Timed-SRM peaks centered in acquisition window**
  - No peak elutes near acquisition break
  - Allows for retention time shift (e.g. due to heavy matrix)

# Truly Powerful Methods Use Speed Efficiently

## Traditional Segmented SRM

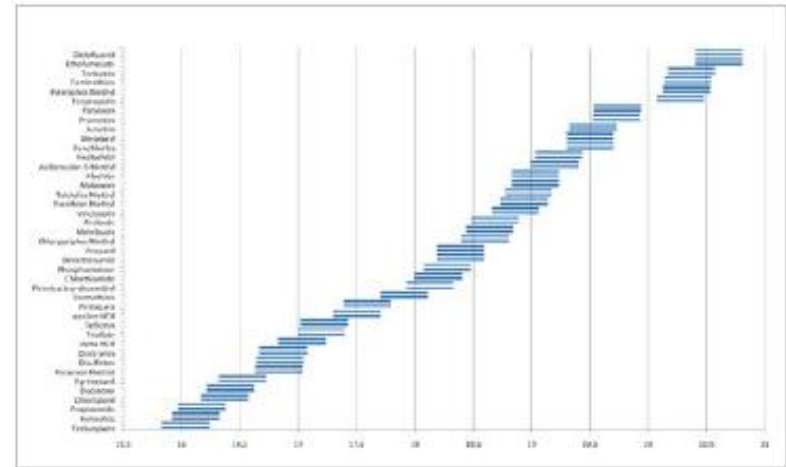
- Complicated set-up
- Wasted dwell time
- Reduced sensitivity
- Reduced tolerance to RT shifts



Traditional Segmented SRM

## TSQ 8000 Evo GC-MS/MS Timed SRM

- Automated set-up
- Optimized dwell time
- Maximized sensitivity
- Increased resistance to RT shifts

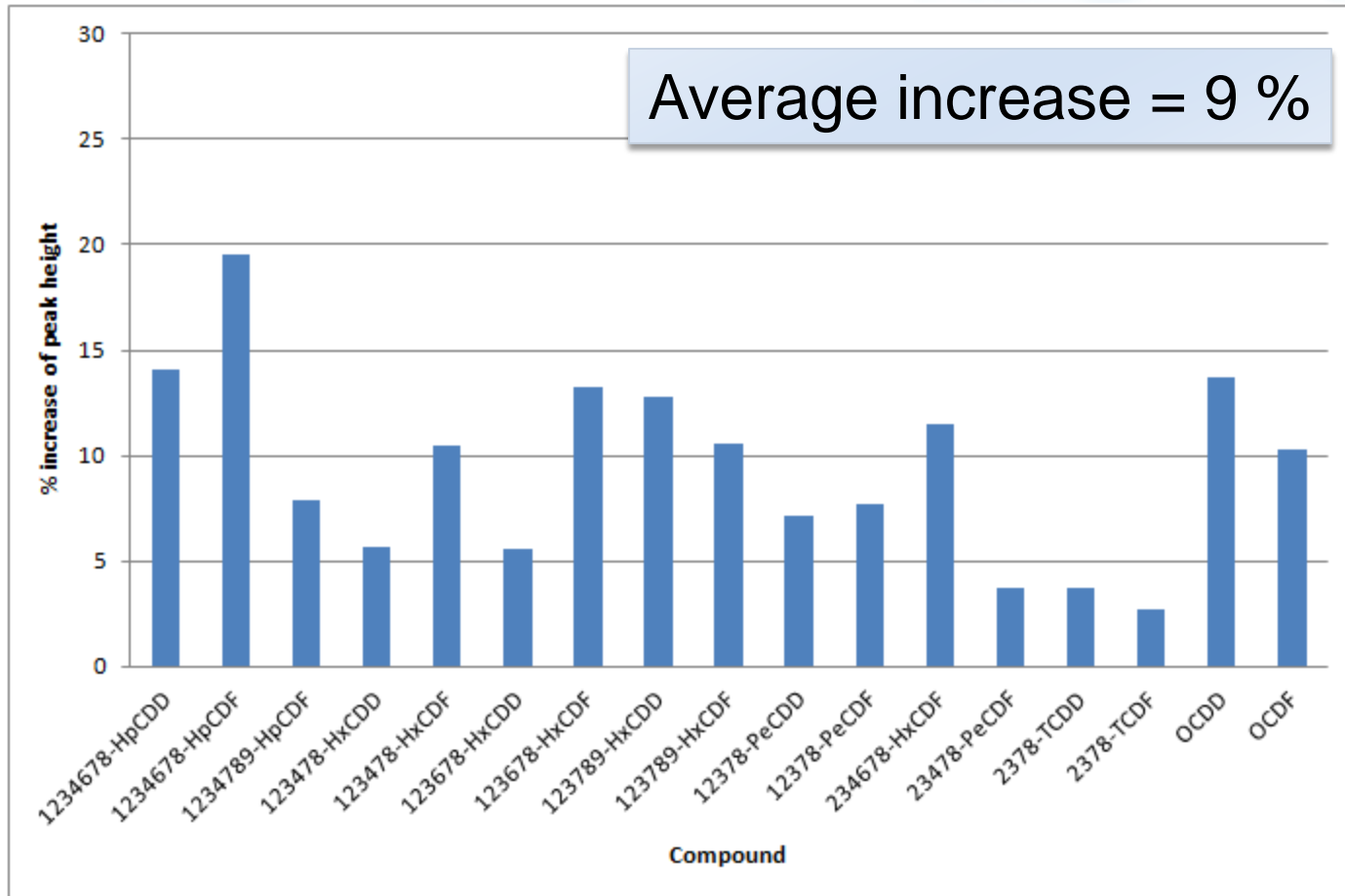


TSQ 8000 Evo GC-MS/MS Timed SRM

Expect **More**  
Capacity

# Timed-SRM Method Setup for Dioxin Analysis

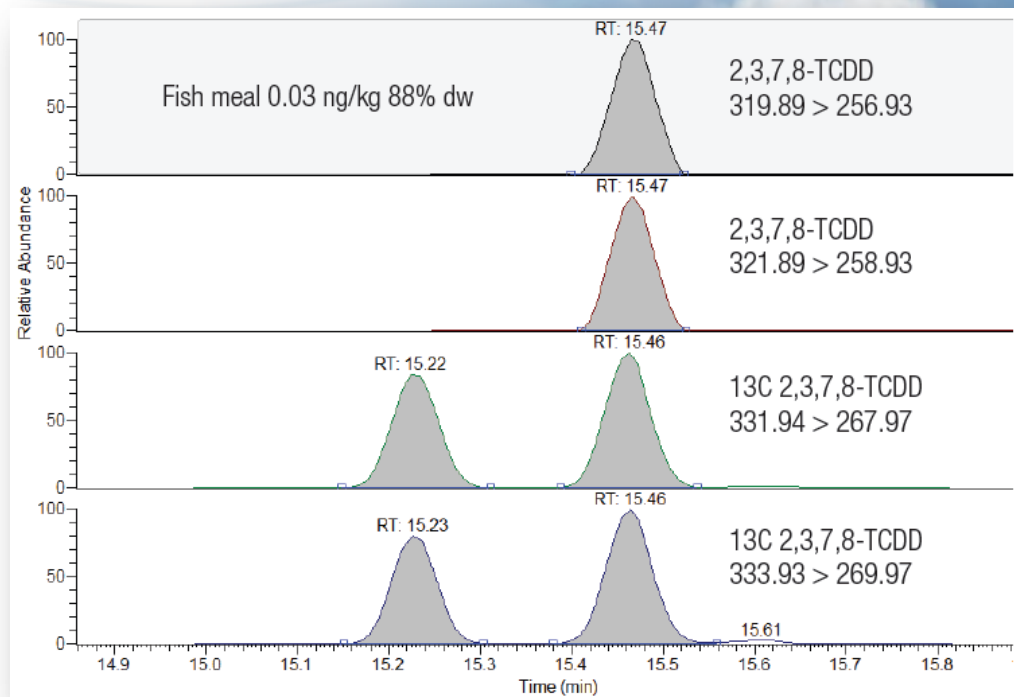
- Sensitivity increase (%) for data acquired in timed-SRM versus segmented SRM. Peak height (counts per second) of each PCDD/F congener was compared.





# Ultimate Sensitivity SRM - Dioxins and Furans

- 2,3,7,8- TCDD
- Superb ion ratio performance
- Excellent matrix selectivity

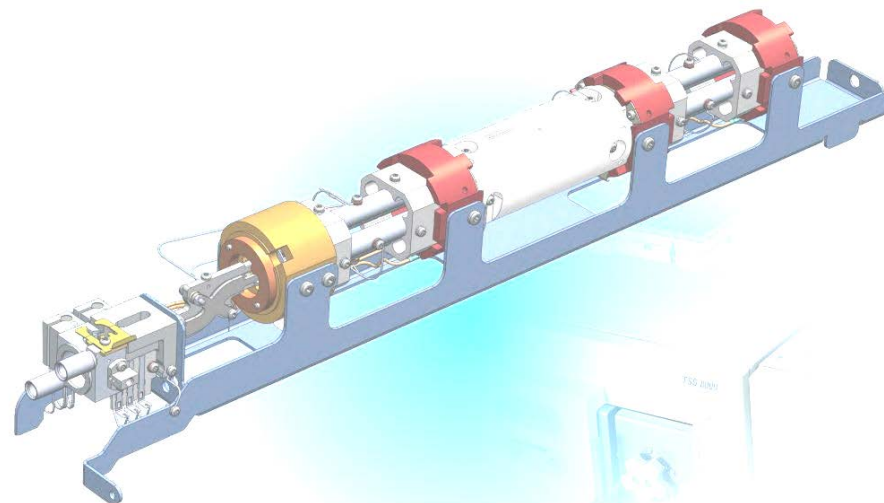
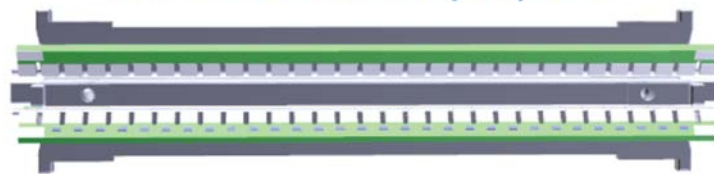


Expect **More**  
Performance

# Introducing EvoCell Technology

- EvoCell
  - Rapid, innovative collision cell technology
- Increased method capacity
  - More compounds
  - More SRM transitions
  - More results

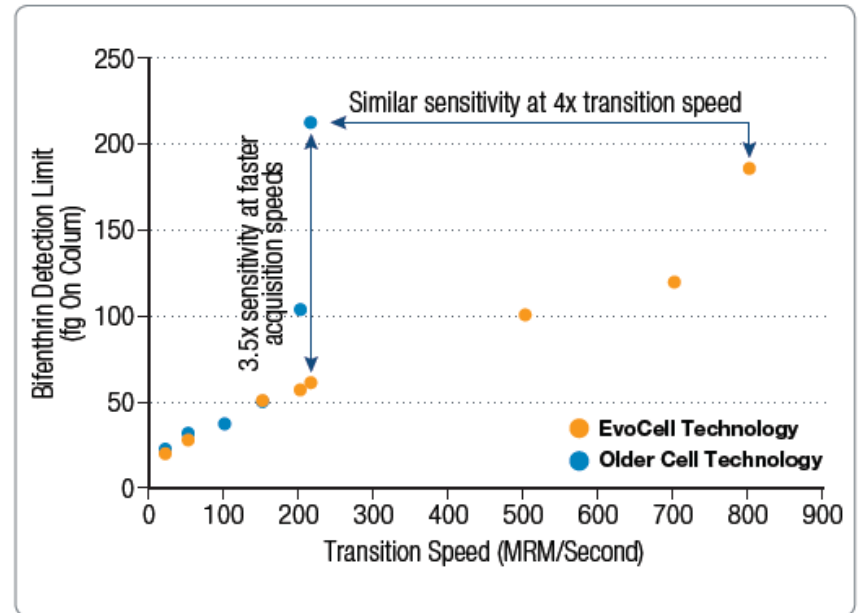
Enhanced Velocity Optics



Expect **More**  
Capacity

# More Sensitivity / More Speed

- Enjoy higher sensitivity at faster SRM speeds
- Up to 4 x more transitions whilst maintaining method sensitivity within the very low concentration ranges



Increased sensitivity at fast transition speeds allows the use of up to 4x transition speeds of standard collision cell technology

Expect **More**  
Capacity



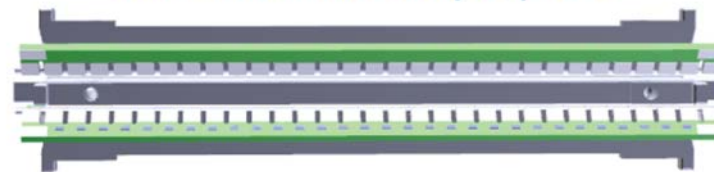
# Applying Speed into Methods

## EvoCell Collision Cell Technology

Features	Benefits	Impact
Increased number of transitions per compound	More points of confirmation More resistance to matrix interference	Higher confidence More on-time results
Increased number of compounds	Higher capacity methods	More method consolidation More efficiency in result production
Fast GC compatible	Faster run times	Faster turnaround More on-time results
Wider SRM windows	More resistance to the effects of RT shift caused by matrix	Faster turnaround More on-time results

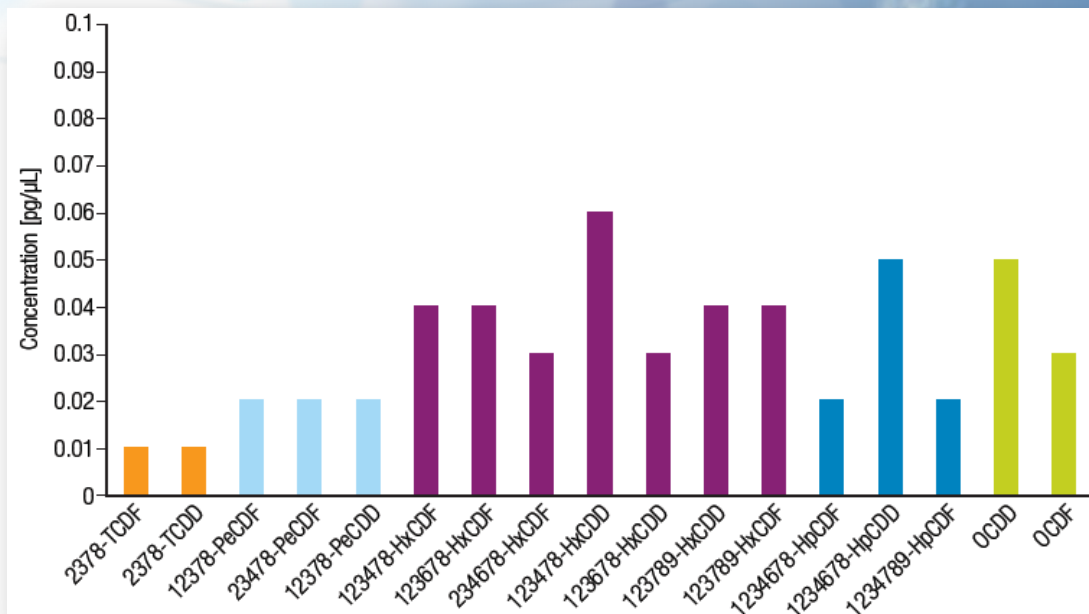
Expect **More**  
Capacity

### Enhanced Velocity Optics



# Ultimate Sensitivity SRM - Dioxins and Furans

- PCDD/Fs confirmatory analysis to ppt levels
- Superb ion ratio performance
- Excellent matrix selectivity



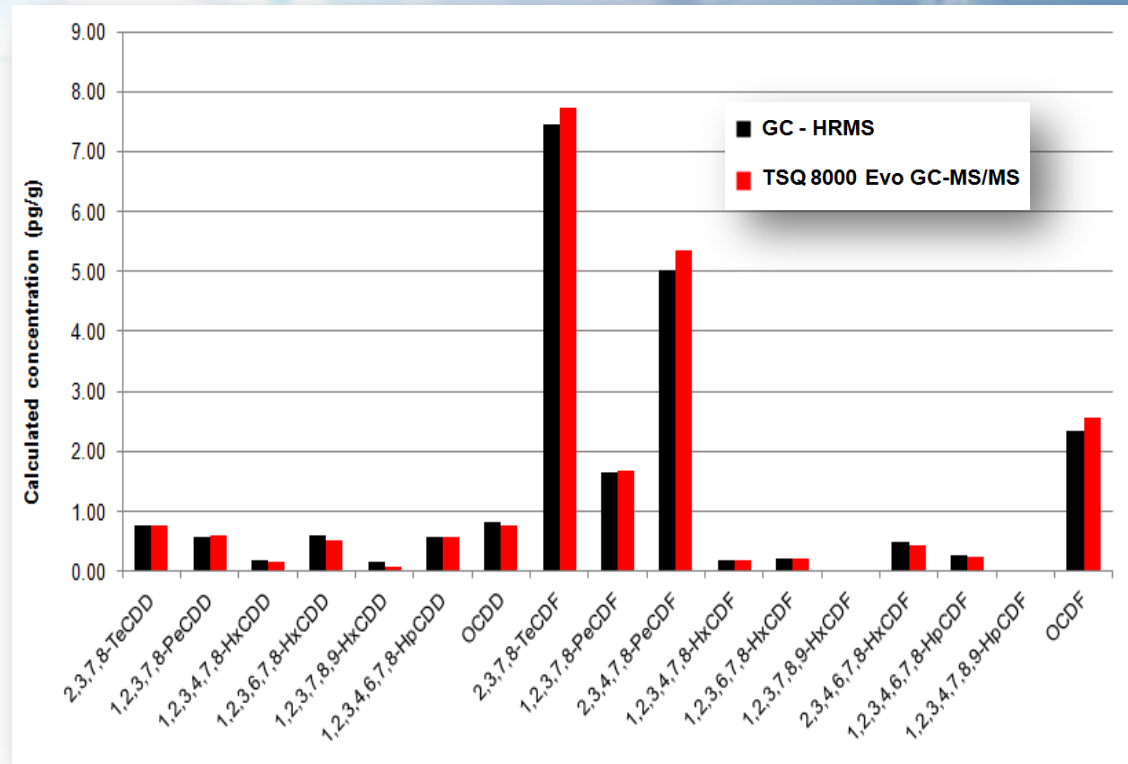
Instrument detection limit (IDL) for PCDD/Fs when satisfying all confirmatory criteria CSL x 5 dilution (n=10) injected using splitless mode

Expect **More**  
Performance



# Ultimate Sensitivity SRM - Dioxins and Furans

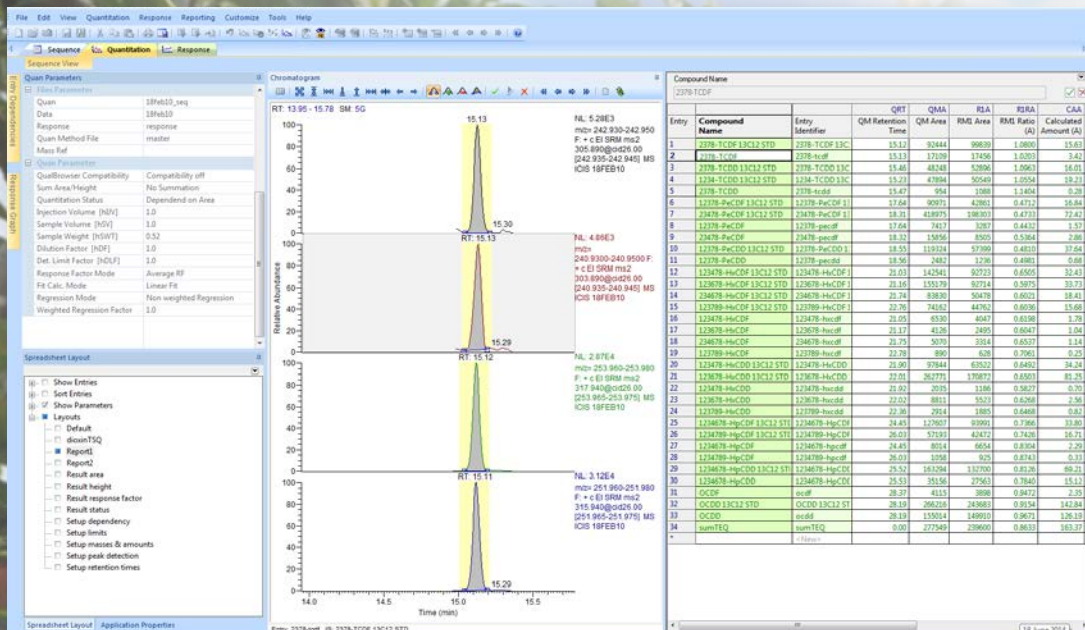
- Individual contribution of each PCDD/F congener to fish sample dioxin content (as TEQ pg/g)
- Comparison of TSQ 8000 EVO GC-MS/MS results with the GC-HRMS values.



Expect **More**  
Performance



# TargetQuan POPs Quantitation



- Data processing built for POPs
- Quantitation, based on relative response factors (RRF)
- Incorporation of Toxic Equivalence Factors (TEFs) to automatically calculate Toxic Equivalent Quotient (TEQ)
- Flagging of out-of-range ion ratios
- Totals calculations
- Lower, medium, and upper bound value calculations

Leading the way in regulatory  
**POPs quantification**

# Analyte Guru

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Thank You for Your Attention!

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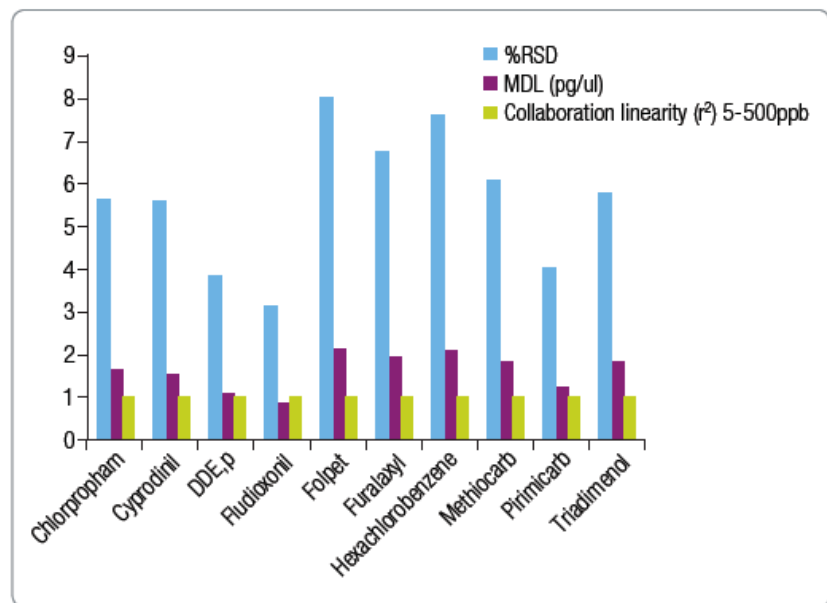
Questions?



# 500 $\mu$ s Dwell Time Performance

- Excellent quantitative performance at very low dwell times/high SRM speeds

- Precision
- Sensitivity
- Linearity

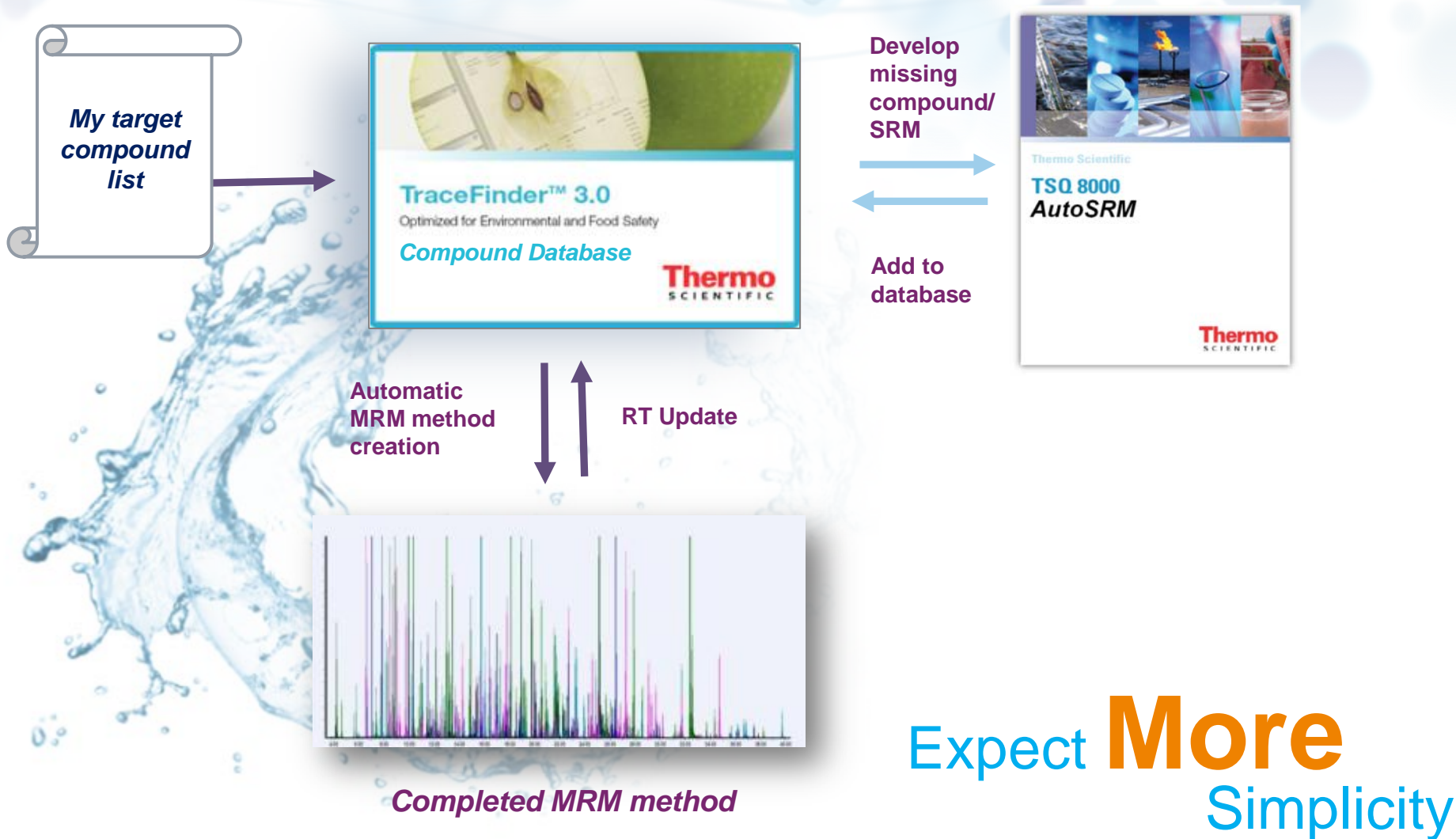


▲ Analysis of pesticides in rice (10  $\mu$ g/kg) with the EvoCell collision cell at 500  $\mu$ s dwell time, acquiring 800 transitions per second

Expect **More**  
Capacity

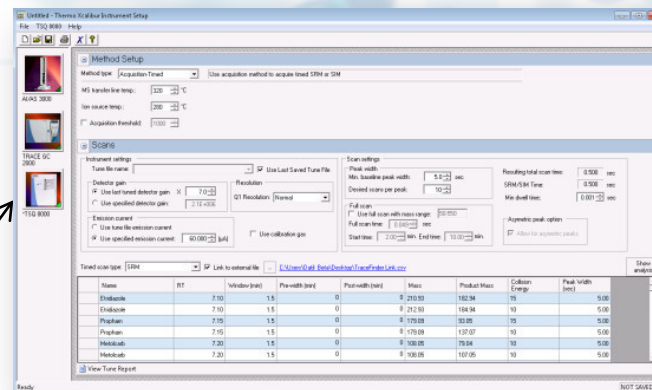
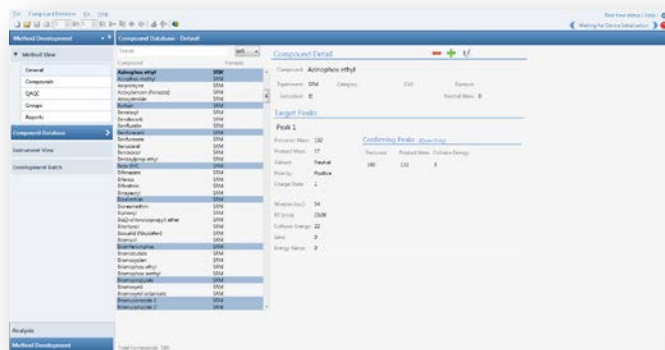


# Simple Method Creation and Management Workflows

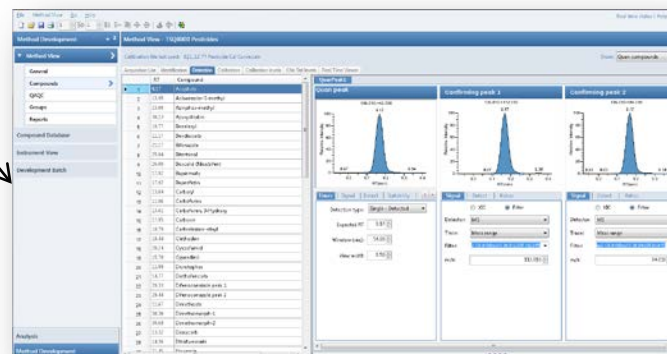


# Creating Your Compound Acquisition List

Selecting your compounds from the CDB...



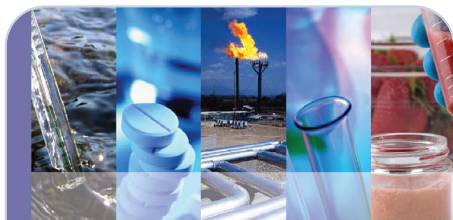
populates your acquisition...



and processing methods



# Adding New Compounds

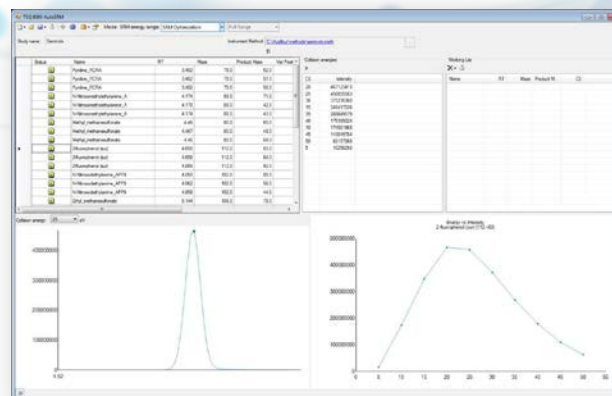


Thermo Scientific

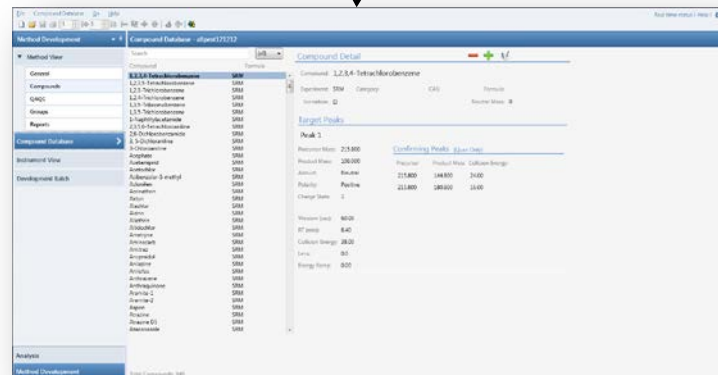
**TSQ 8000**

Pesticide Analyzer Installation Guide

Step-by-step instruction make adding new compounds to the Compound Database easy.



Step 1. Automated SRM development through AutoSRM



Step 2. Easy import into TraceFinder CDB