

Unstoppable Confidence with Thermo Scientific GCMS

ISQ 7610 & TSQ 9610

Thermo Scientific's 2022 GCMS Product Portfolio
Food Safety Seminar Bangkok

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Regional Application Leader – SEA & Taiwan

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 The world leader in serving science



Main challenges for trace analysis in food

- Sensitivity to consistently meet the regulations
- Multi-class and multi-matrix analysis
- Multiresidue methods
- High sample throughput
- Fast turnaround
- Low cost of analysis



New GCMS line up from Thermo Scientific

Thermo Fisher Scientific's GC and GC-MS Portfolio

- **Trace 1600/1610 GC**
 - A flexible, workhorse GC providing day-in, day-out performance
- **ISQ 7610 – Single Quadrupole GC-MS**
 - Robust and reliable for routine mass spec analysis
- **TSQ 9610 – Triple Quadrupole GC-MS/MS**
 - Sensitivity and selectivity for the most demanding research
- **Orbitrap Exploris GC**
 - High resolution, accurate mass for untargeted analysis and identification of unknowns
- **Autosamplers**
 - **AI/AS 1610 Liquid Autosampler** Cost effective and simple solution for liquid sample injections
 - **TriPlus RSH SMART** for enhanced sampling techniques capability and automation for sample preparation workflows



TRACE 1610



ISQ 7610



TSQ 9610



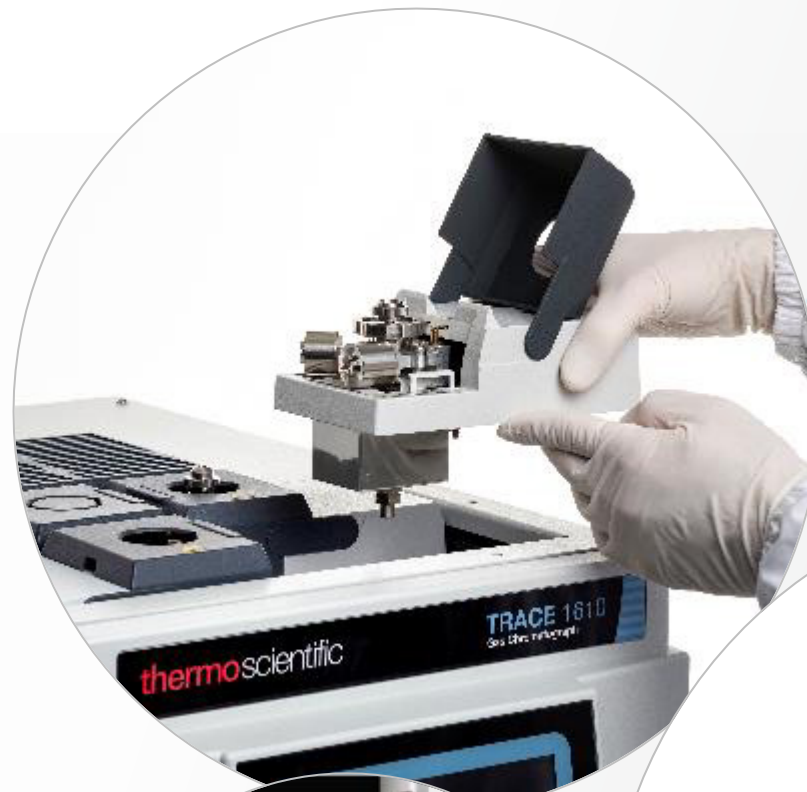
Orbitrap Exploris GC



TRACE 1600 Series GC

Efficient use of the resources

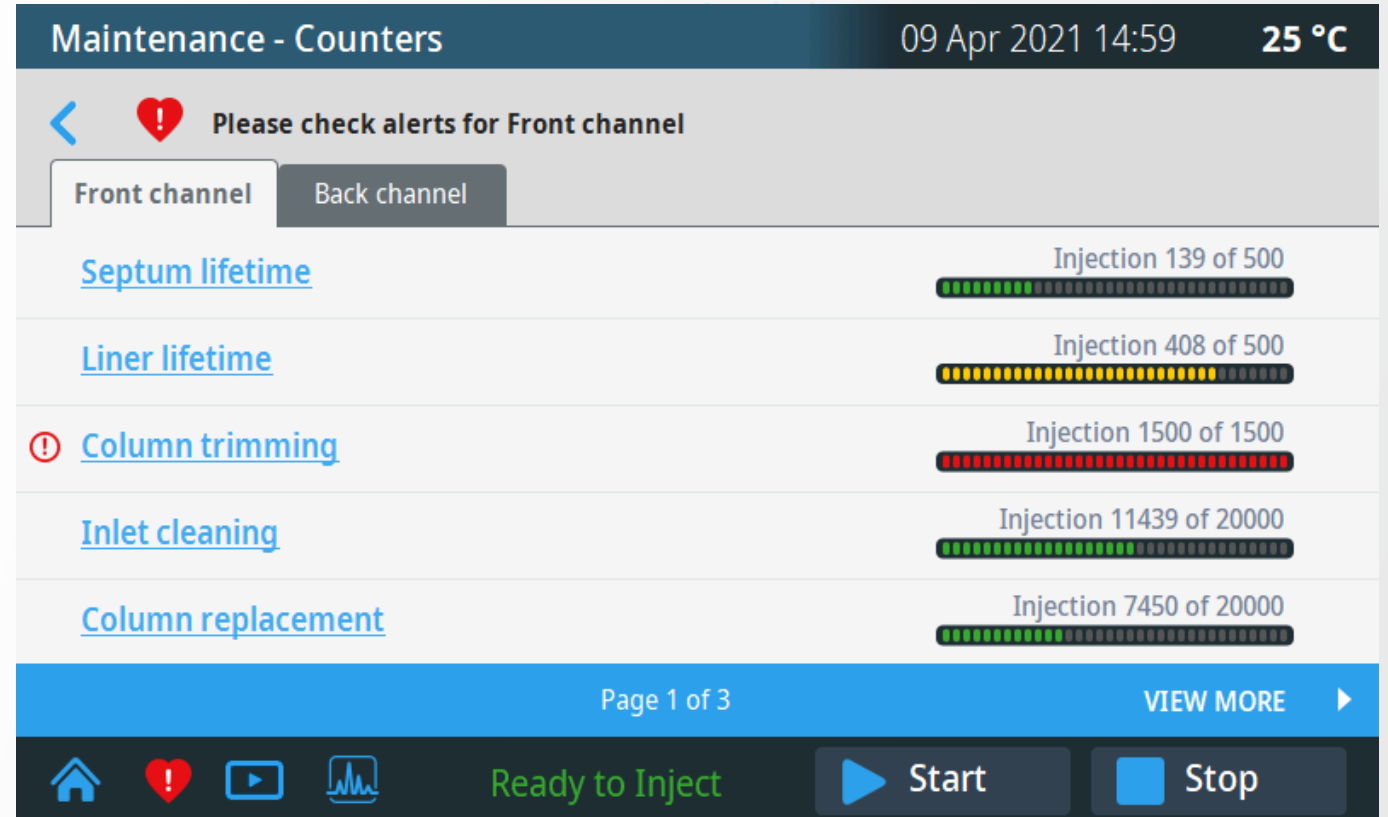
- Unique modular design for injectors and detectors
- Off-line maintenance possible
- Spare back up modules instead of full GC systems
- Interchangeable modules on existing TRACE GC systems
- Compact design for a better use of the bench space
- Patented carrier gas saving during operations



TRACE 1610 GC

Better consumables usage management

- Instrument health icon notification
- Consumables' usage counters with customizable limits
- Avoid unnecessary replacement
- Avoid unplanned downtime
- Instrument health view in CM and link to the audit trail for GLP compliance



Helium Saver Module Example



GC Flow conditions		EPA 8270 Standard
He carrier gas flow	mL/min	1
He split flow	mL/min	60
Gas saver flow	mL/min	20
Gas saver on	min	3
Purge flow	mL/min	5
Run time	min	25
He volume in cylinder	L	7,300
Runs per Day		57
He cylinder cost	USD	\$300
N ₂ cylinder cost	USD	\$60

- **Example:** U.S. EPA Method 8270 (semi-volatiles analysis with GC-MS)
- **Total Analysis Time:** 25 minutes
- **Around the Clock Analyses per Day:** 57

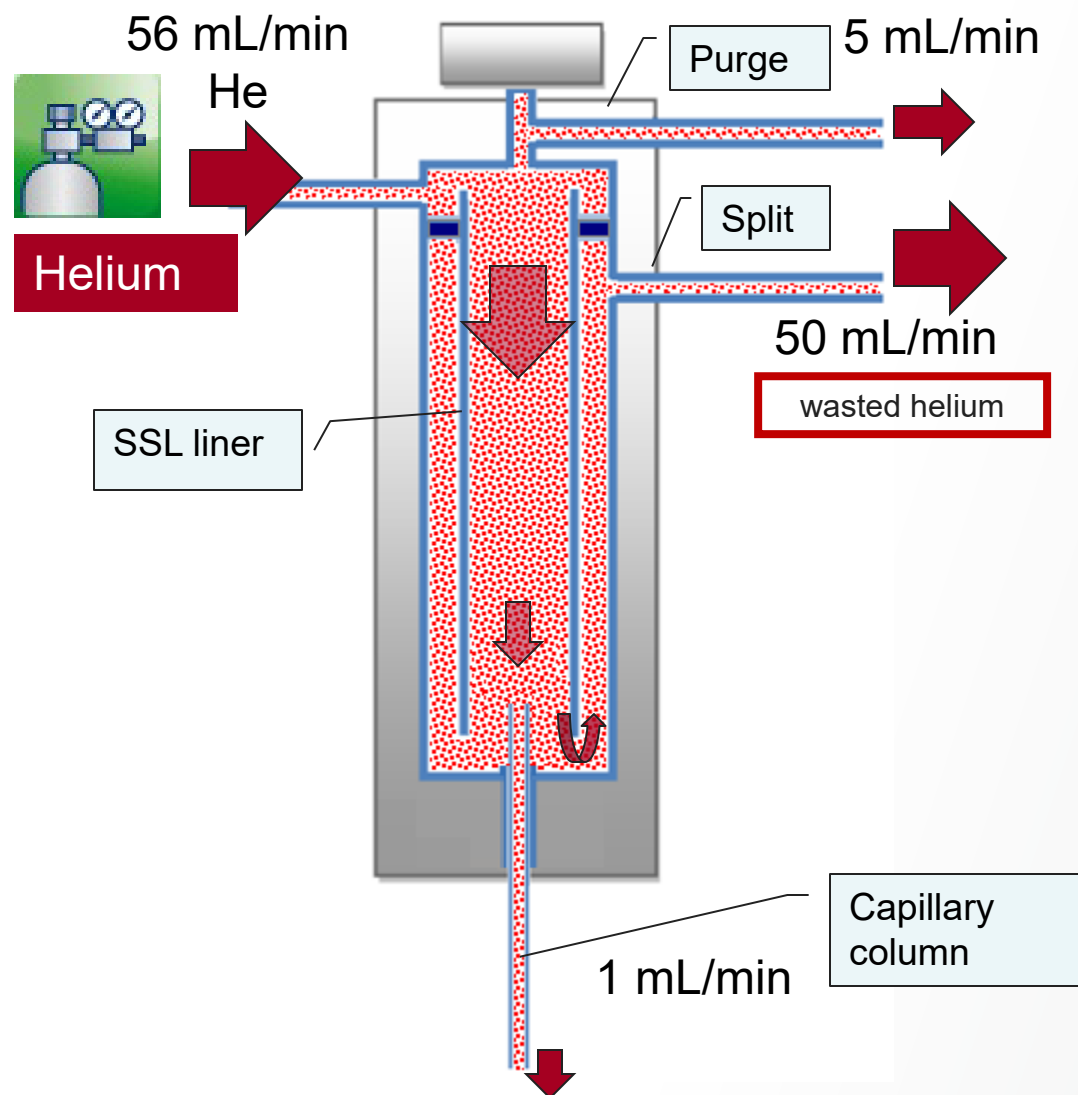
Helium cylinder lifetime was extended from 5 months to 3.5 years of continuous uninterrupted use

Helium Savings: 7 times
(continuous uninterrupted use)

Monetary Savings: 3 times

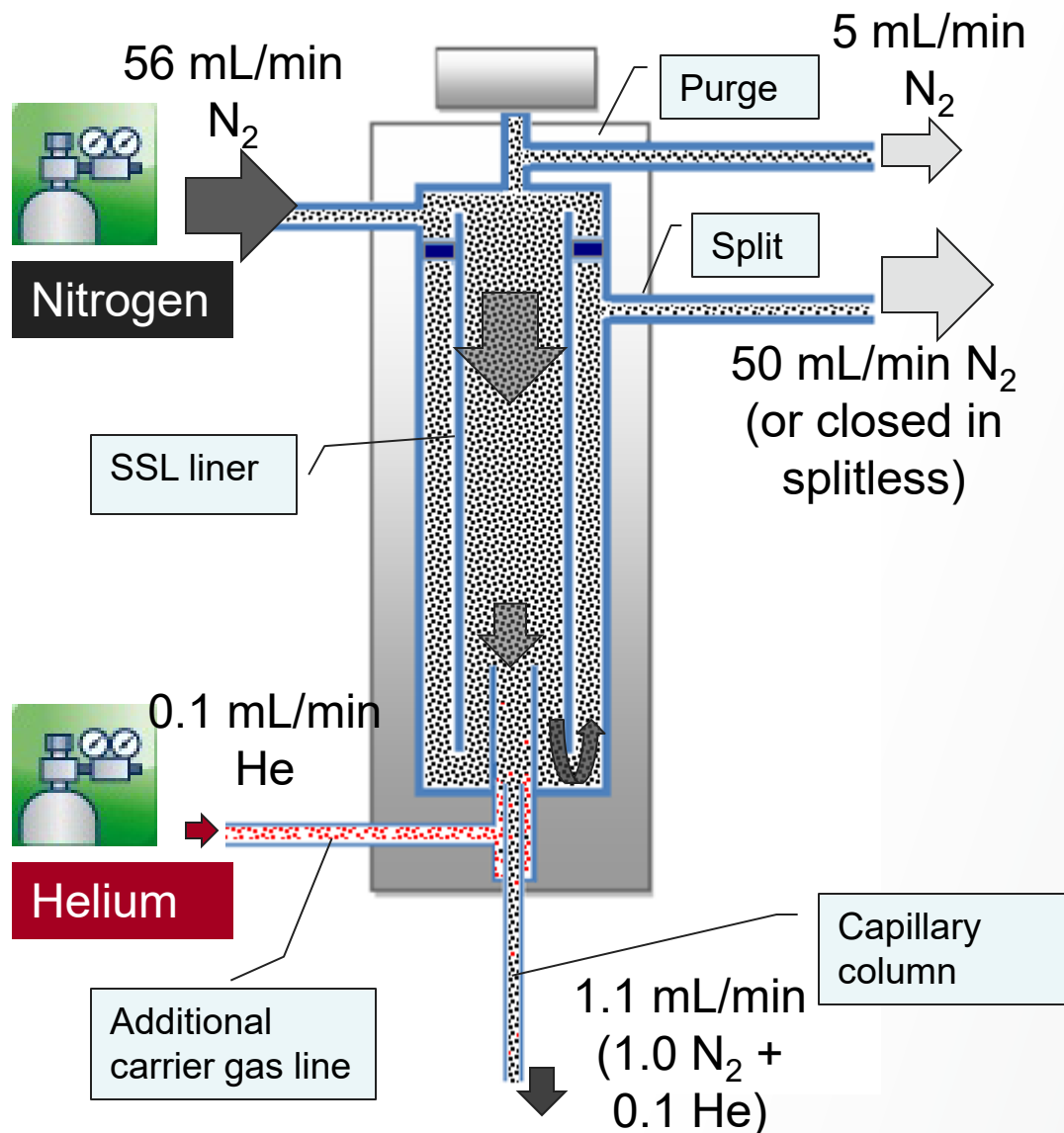
		Standard He Consumption	Helium Saver Consumption
Daily He usage	L	46.56	5.76
He cylinder life	Days	157	1,267
Daily N ₂ usage	L	0	40.8
N ₂ cylinder life	Days	0	179
Total Annual Cost		\$688	\$205

How Helium Saver Module Works: Standard SSL Injector



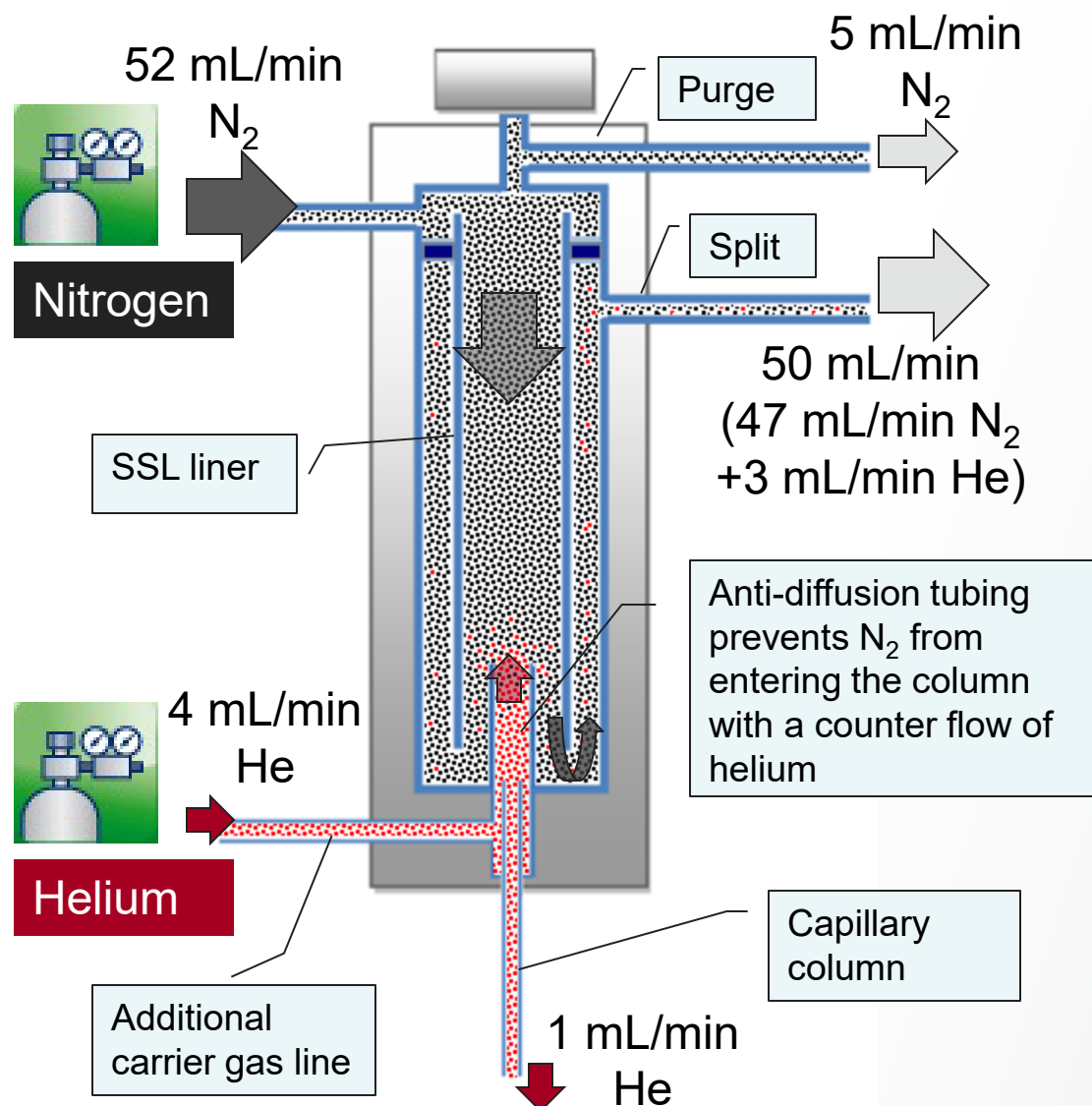
- The same gas is used in the carrier path, septum purge path, and split path.
- Typically, only ~1/10...1/50 of the total flow is used for the analytical column carrier flow.
- Purge and split flows cannot be reduced beyond a certain limit without introducing contamination into column/detector (sample matrix accumulated in liner and lines, septa particles, air diffusing from septa, seals off gassing.)

How Helium Saver Module Works: Injection



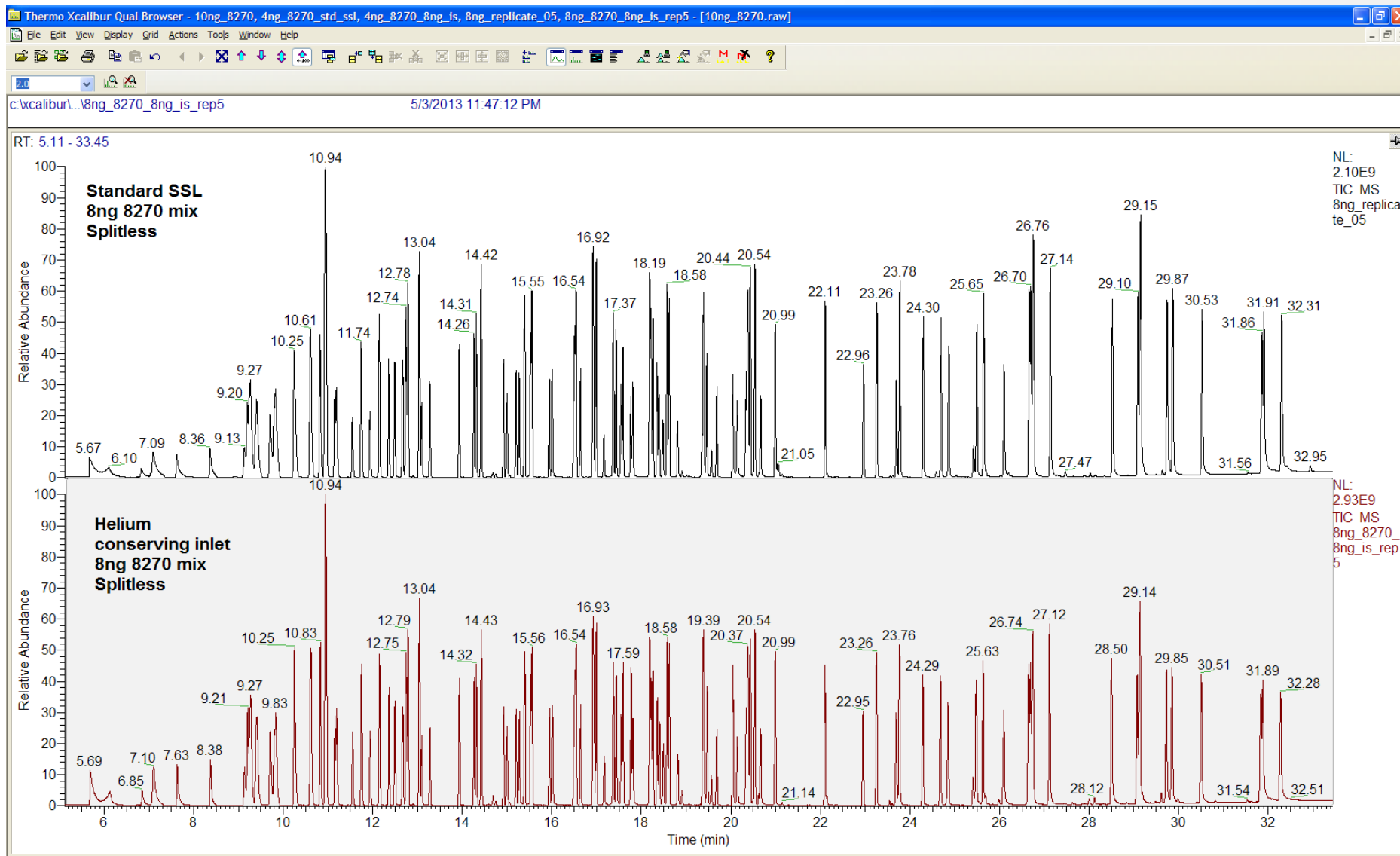
- During injection period, Helium is (almost) closed off and nitrogen flows into the column for sample introduction
- Helium is supplied at a bare minimum flow of 0.1 mL/min only to keep the connection swept and avoid dead volume negative effects during injection
- When GC is in stand-by (not running samples) it can be left in this condition with practically zero consumption of Helium

How Helium Saver Module Works: Operation



- Inlet is supplied with **2 different gases: Nitrogen and Helium**
- Nitrogen is used for septum purge and split flows, while Helium only feeds the analytical column flow
- During all “non-injection” periods, Helium is supplied with a flow that is just slightly higher than the column flow
- Helium consumption is only 1/15 – 1/20 of standard-plumbed SSL

Helium Saver Module: Retention Times Unchanged



Helium Saver Hydrogen Safer

- Occupied one injector slot
- Two HeSaver-H2Safer upgrades can be used on one GC fitted with two SSL and two detectors
- User upgradeable – the gas net is already built into the TRACE 1600 Series GC, all that is required is an easy and quick modification of the SSL module (it can be reverted to a standard SSL any time)
- Works either with helium or hydrogen as carrier gas
- When working with hydrogen as a carrier gas, there is **NO LONGER** need a H2 sensor due to safety improvements in the design



Standard iConnect SSL

www.thermofisher.com/helium-saver

Source Plug

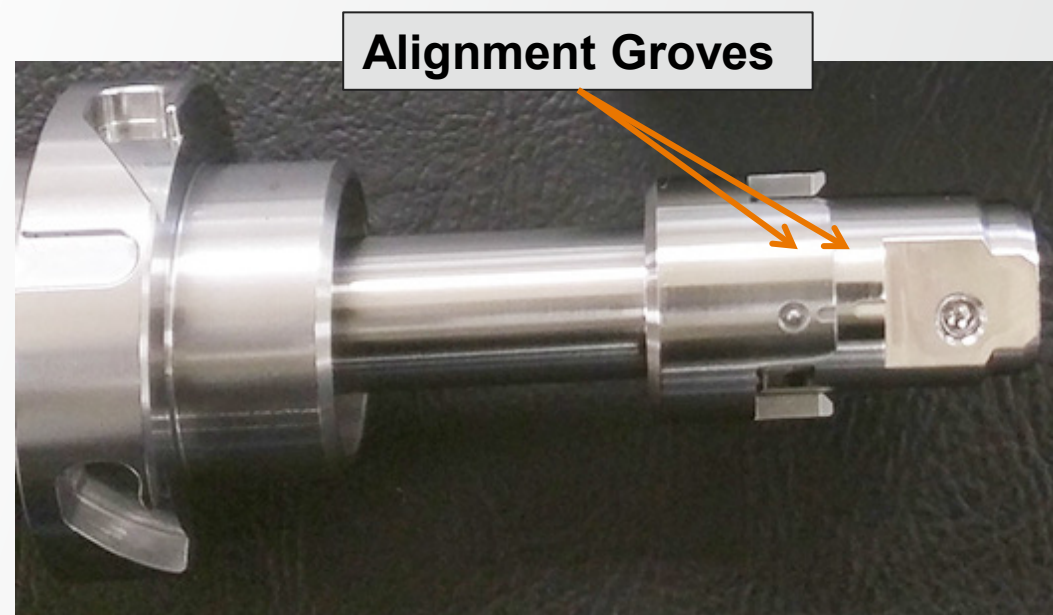
NeverVent Technology

- VPI is used to remove the Source without venting the system and save time during source maintenance, troubleshooting, and switching between EI and CI
- With the new Source Plug the column can now be removed from the Mass Spec system without venting. This will save time during column maintenance, troubleshooting, and switching between different columns



Source Plug Installation Tips

- Lower the temperatures to prevent injury, damage and contamination
 - GC Oven to 40C Source to 175C Transfer Line to 40C
- When Used to Change Column, the end of the column is inserted until it reaches the Source Plug instead of using Column Measuring Tool
- If column is not cut properly the tip of the column can break when pushed against the Source Plug causing Injection Intensity Issues
- Use the Alignment Groves to ensure the Source Plug is installed onto the Source Removal Tool Properly



Increasing instrument uptime







NeverVent Technology



Thermo Scientific™ NeverVent™ technology allows analytical laboratories to perform maintenance without interrupting their workflow



Available on the TSQ 9610 with the ExtractaBrite and Advanced Electron Ionization (AEI) source

		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%

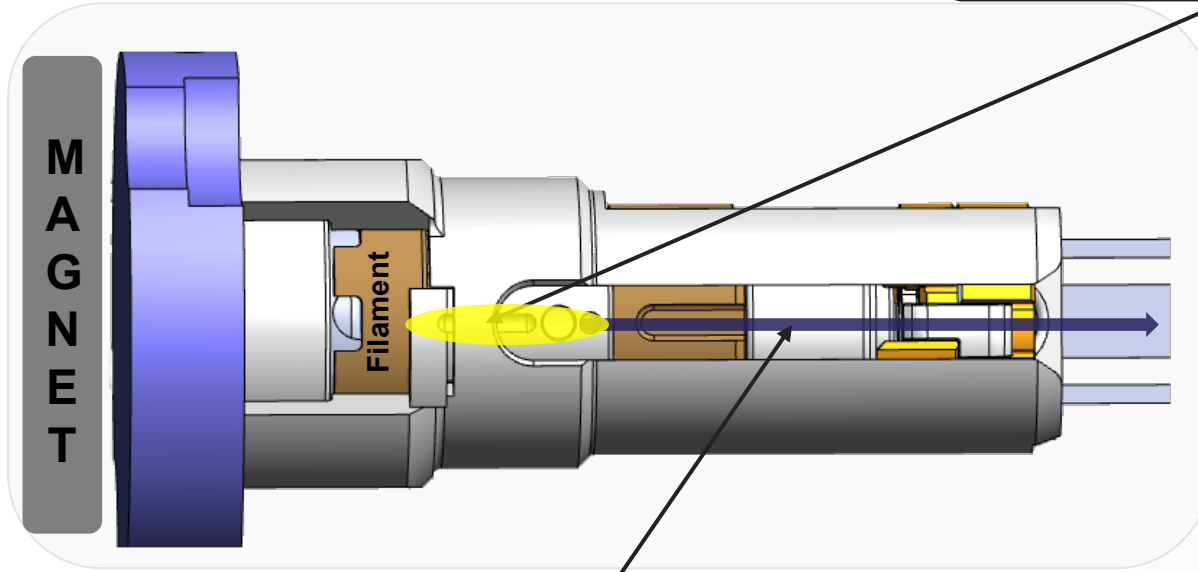


AEI vs. EI Comparison

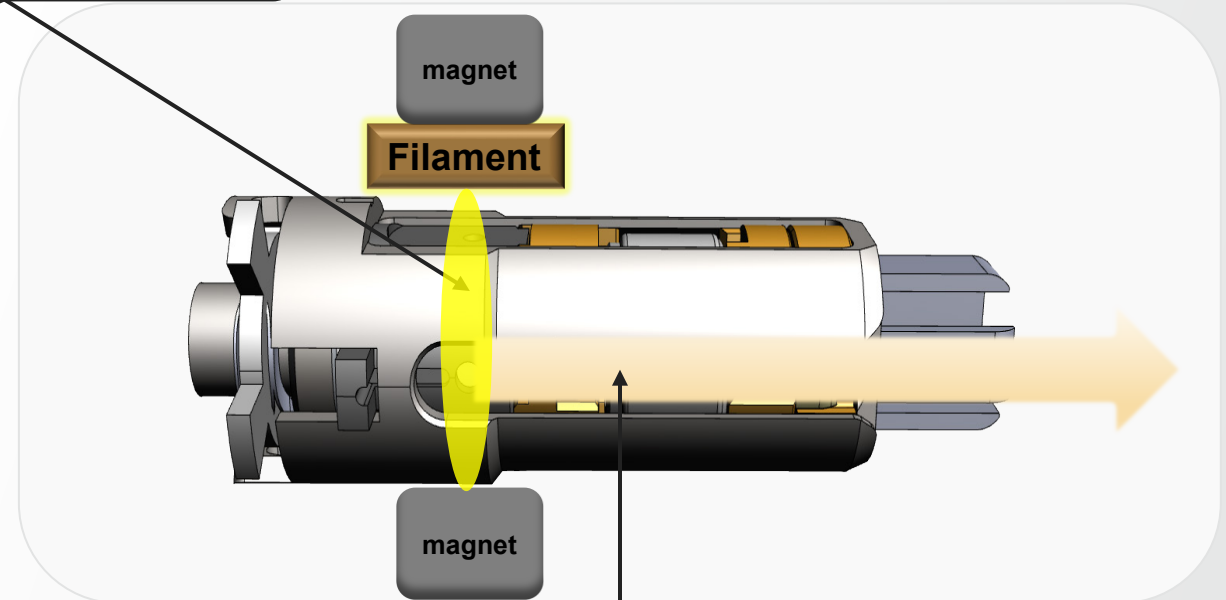
AEI

EI

Electron Beam
from Filament



Stronger Magnets and In line Design
produce a tight narrow Ion Beam for improved
Efficiency, Robustness & Sensitivity



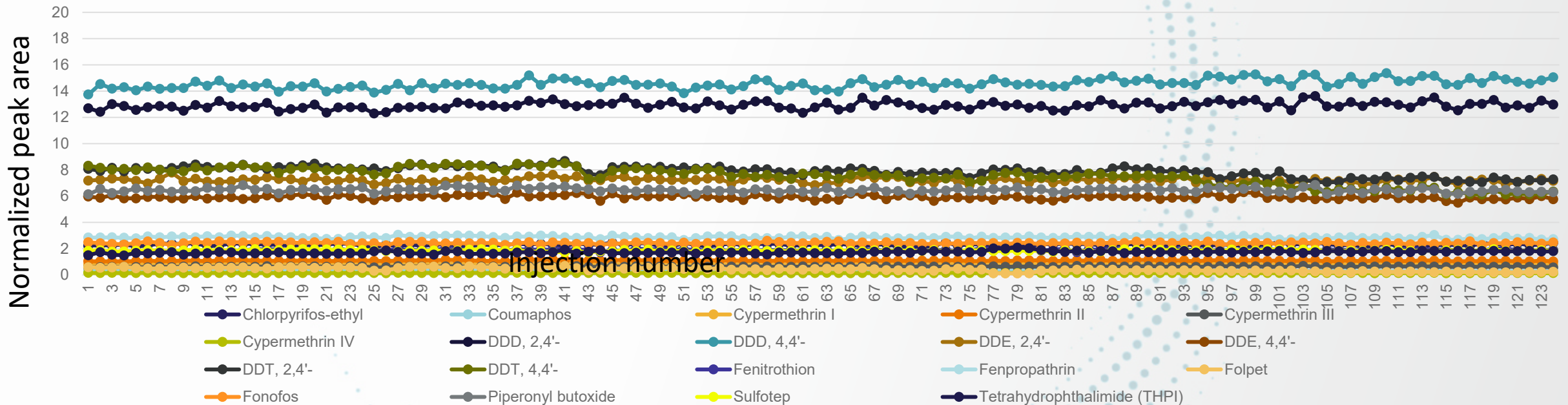
Diffused Ion Beam

Increasing instrument uptime

Consistent results at low levels



Consistent results delivered due to inherent robustness of the ExtractaBrite and Advanced Electron Ionization (AEI) source



Normalized peak area response (analyte peak area / ISTD peak area) obtained for n=124 consecutive injections of matrix samples spiked at 50 µg/kg

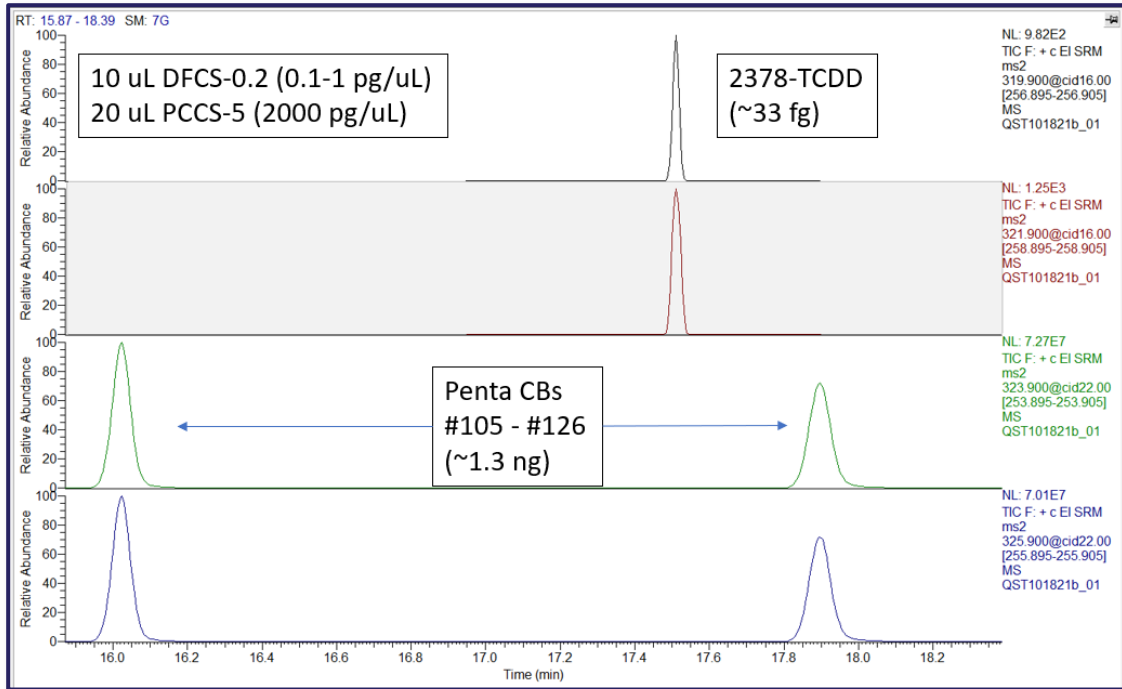


Maximizing sample throughput

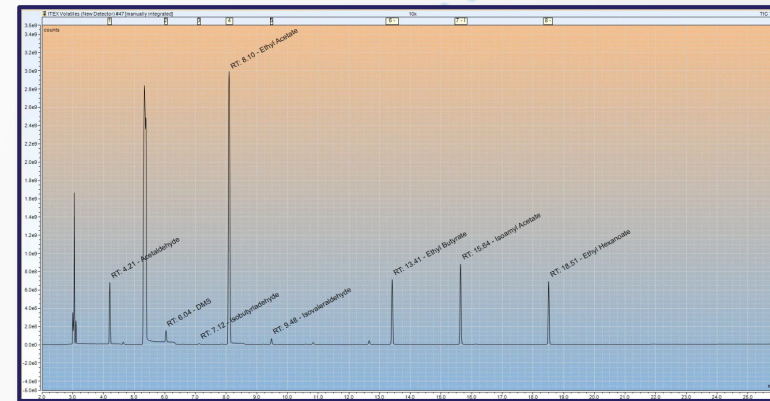
Extended dynamic range and lifetime detector



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



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



Combined methods for Beer 29, Beer 44, and Beer 48 on ISQ 7610



7x longer between
detector replacements



Providing a rapid return on investment

Compliant-ready tuning



Native instrument tuning provides compliant-ready software and in-sequence tuning, allowing rapid implementation for a regulated environment

Ensure optimal performance for every user

Tuning is complete.

- Ready to run samples
- PASS
- Check width passed
- For mass 502.0, FWHM=0.69
- For mass 414.0, FWHM=0.69
- For mass 219.0, FWHM=0.69
- For mass 131.0, FWHM=0.69
- For mass 69.0, FWHM=0.69

The tune file on the instrument is for an EI ion source.

Native tuning for compliance

Date	Time	Retention Time	Device	User
11/12/2021	10:39:07 AM -06:00	5.207		User ISQ
11/12/2021	10:37:25 AM -06:00	3.500	ISQ ISQ_MethodSettings	ISQ ISQ = Positi
11/12/2021	10:37:25 AM -06:00	3.500	ISQ ISQ_MethodSettings	ISQ ISQ Electros
11/12/2021	10:34:55 AM -06:00	1.000	GC	GC.Ten
11/12/2021	10:34:17 AM -06:00	0.368	Sampler	Log Rec
11/12/2021	10:34:17 AM -06:00	0.368	Sampler	Firmwa
11/12/2021	10:33:56 AM -06:00	0.019	ISQ	OverallStatus: Running
11/12/2021	10:33:56 AM -06:00	0.019	ISQ	DeviceStatus: Running



Confident analysis of ultra-trace pesticides residues in baby food using triple quadrupole GC-MS

- Pesticides are commonly used in agriculture to control various pests during cultivation, storage, and transportation
- To ensure food safety for consumers and protect the environment, many organizations and countries around the world have established maximum residue limits (MRLs), which for the majority of pesticide-commodity combinations are set at the default level of 10 µg/kg.
- the European Union (EU) has established LOD MRLs between 3–8 µg/kg for specific pesticides prohibited in baby foods.



Sample preparation with QuEChERS

10 g
baby
food

10 mL
ACN

Shake
(4 min)

Add :
4gr MgSO_4 (4g),
NaCl (1g),
 $\text{Na}_3\text{Citrate}\cdot 2\text{H}_2\text{O}$
(1g),
 $\text{Na}_2\text{Citrate}\cdot 1,5\text{H}_2\text{O}$
(0,5g)

Shake
(4 min)

Centrifuge
(4000
rpm,
5 min)

Take 1 mL
supernatant and
add:
 MgSO_4 (750 mg)
PSA (125 mg)

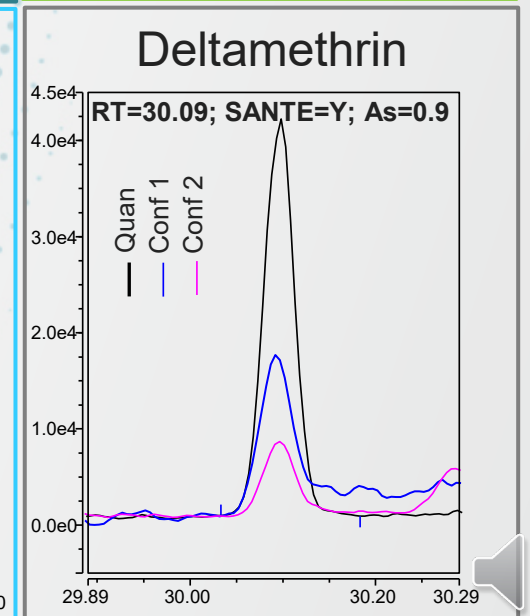
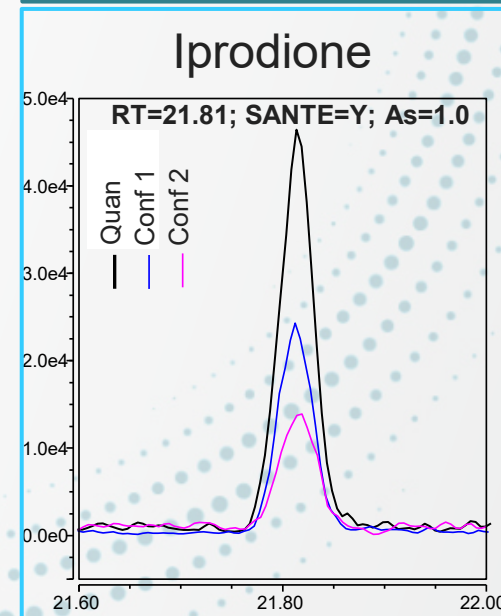
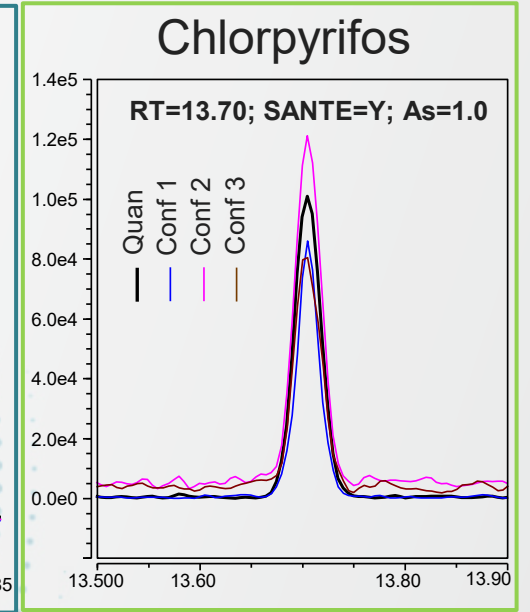
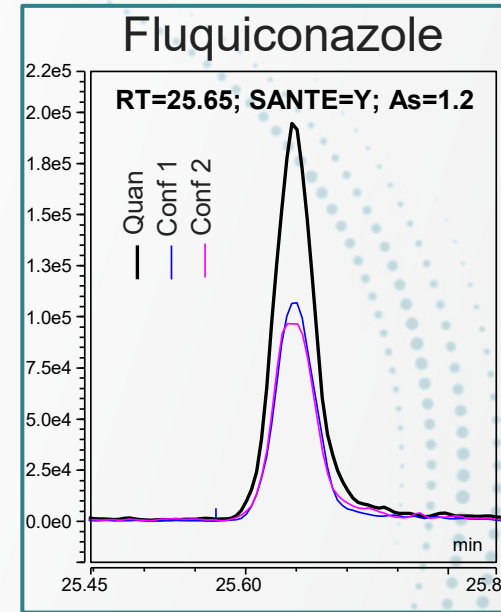
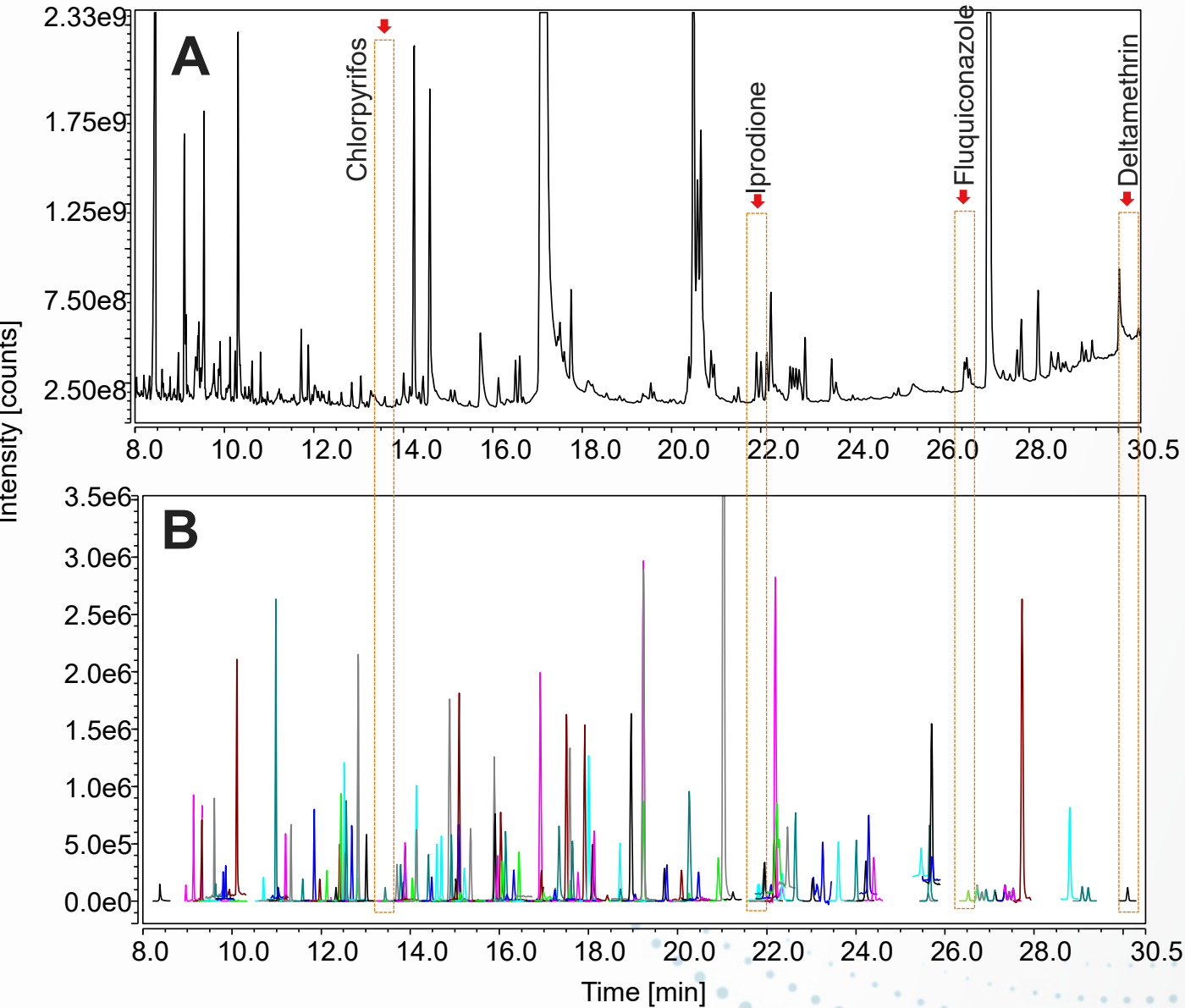
Vortex
(30s)

Centrifuge
(4000
rpm,
5 min)

Take 4 mL
supernatant and
acidify with 40 μl of
5% formic acid in
ACN (v/v)

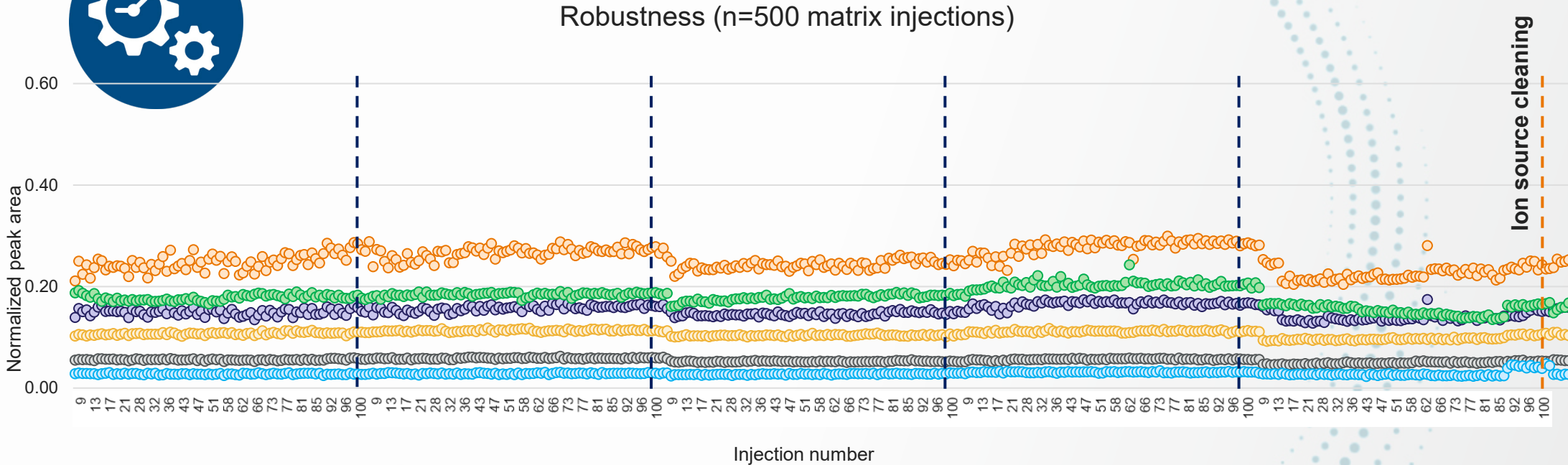


t-SRM for improved selectivity



Increasing instrument uptime: Assessment of robustness

Consistent results at low levels



○ BHC, Alpha (%RSD=7)

○ Hexachlorobenzene (%RSD=9)

○ Aldrin (%RSD=6)

○ Isodrin (%RSD=6)

○ Triflumizole

○ Permethrin peak (%RSD=10)

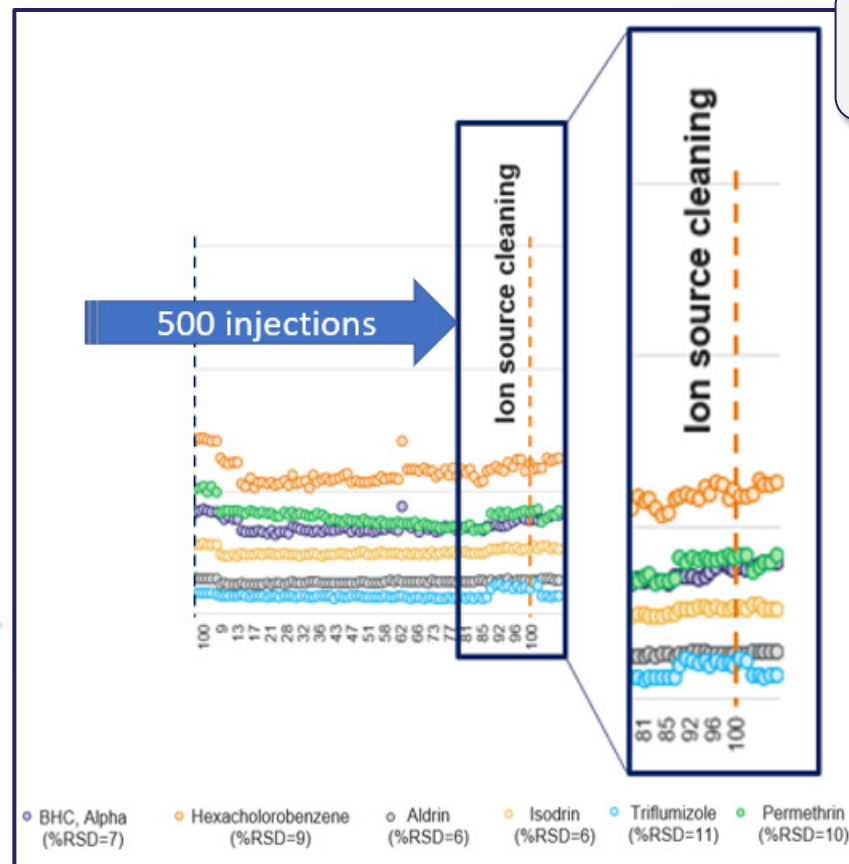


Increasing instrument uptime

Consistent results and NeverVent Technology



Even when maintenance is performed on the ionization source, the instrument produces consistent results at low levels



Maintenance performed to demonstrated stability after source clean



Instrument delivering consistent results again in under 2 hours



Summary and further information

Application note | 000437

ThermoFisher
SCIENTIFIC

Food safety

Confident analysis of ultra-trace pesticides residues in baby food using triple quadrupole GC

Authors
Customer's name¹, Giulia Riccardino², Adam Ladak³, and Paul Silcock⁴

Goal
The aim of this application note is to demonstrate the performance of the Thermo Scientific™ TSQ™ 9610 triple quadrupole mass spectrometer coupled to the Thermo Scientific™ TRACE™ 1610 GC equipped with programmable temperature vaporizing injector for the determination of trace level pesticide residues in baby food.

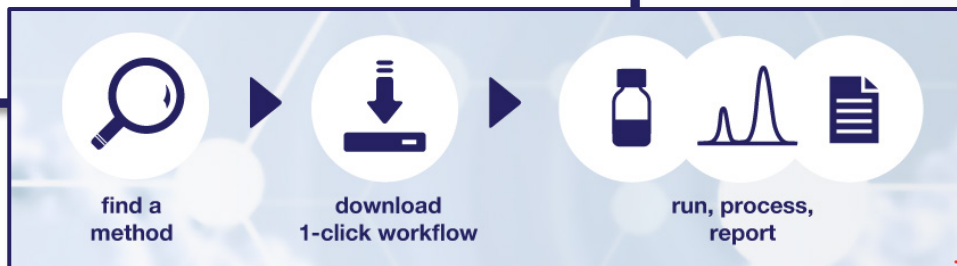
Introduction
Pesticides are commonly used in agriculture to control various pests during cultivation, storage, and transportation.¹ The application of pesticides can result in residues at detectable concentrations in food. To ensure food safety for consumers and protect the environment, many organizations and countries around the world have established maximum residue limits (MRLs), which for the majority of pesticide-commodity combinations are set at the default level of 10 µg/kg.^{2,3} However, the European Union (EU) has established LOD MRLs between 3–8 µg/kg for specific pesticides prohibited in baby foods.⁴

Keywords
Pesticides, baby food, gas chromatography-mass spectrometry, GC-MS, triple quadrupole, TSQ 9610 mass spectrometer, NeverVent Advanced Ionization Ion source (AEI), Trace 1610 GC, programmable temperature vaporizing injector, PTV, AI/AS 1610

The main challenge of pesticide analysis relates to the sensitivity required to meet strict regulatory limits. Moreover, analytical testing laboratories need to have multiclass, multiresidue methods that can be applied for the analysis of a large number of diverse pesticides in a high number of different sample types. These laboratories must also ensure high sample throughput, fast turnaround, and a low cost of analysis to offer a competitive service to their customers.



- Wide linear response and accurate quantitative performance for the investigated pesticides was obtained with a coefficient of determination of $R^2 > 0.99$ and AvCF %RSDs < 20 in spiked matrix over a concentration range of 0.05 to 500 µg/kg.
- High recovery (70–120%) and precision (RSD $\leq 10\%$) were demonstrated for pre-spiked QuEChERS extracts of at 3 µg/kg.
- Low instrument detection limits ranging from 6 to 650 fg on column corresponding to 0.006 to 0.65 µg/kg were achieved. The average calculated IDL for all compounds was 0.073 µg/kg.



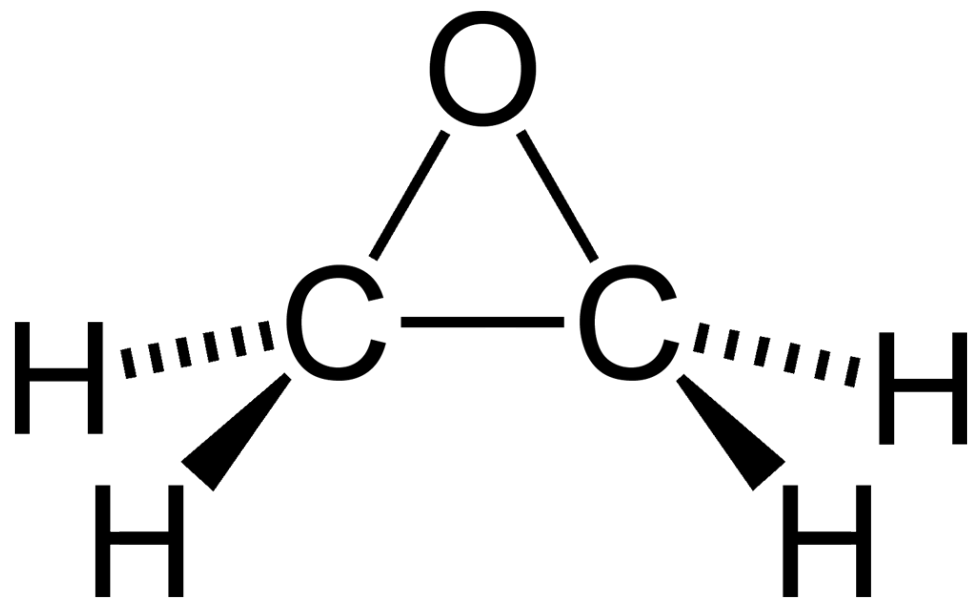
Analysis of ethylene oxide and 2-chloroethanol residues in food using GC-MS/MS

- Ethylene oxide (EO) is a substance of a broad spectrum of applications including preservation of dry food
- Upon consumption, ethylene oxide can negatively affect human health
- Residues of EO and its derivative product 2-chloroethanol (2CE) must be monitored closely
- High number of notifications published in the Rapid Alert System for Food and Feed (RASFF)

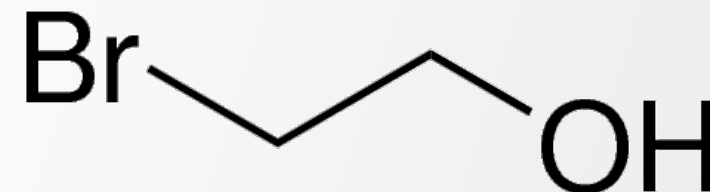


Ethylene oxide

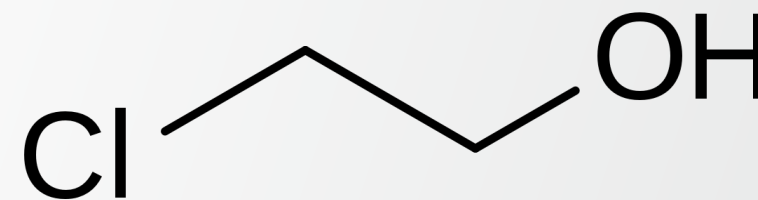
EO and its degradation products



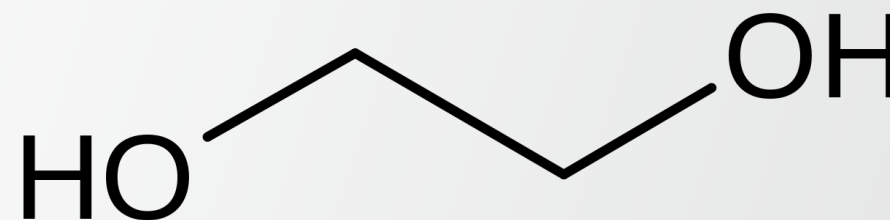
Ethylene oxide



2-bromoethanol



2-chloroethanol

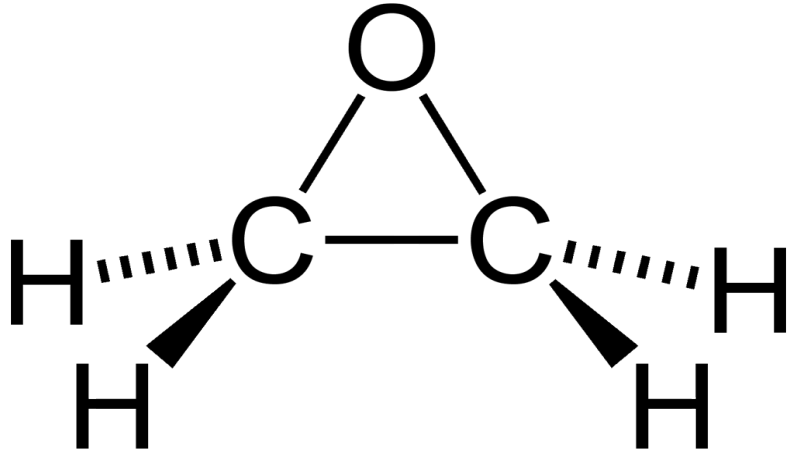


Ethylene glycol



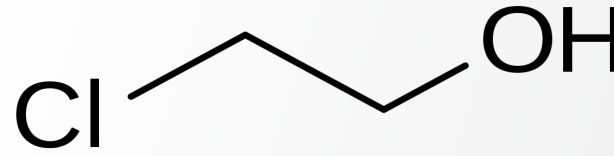
Ethylene oxide

EO and its degradation products



Ethylene oxide

+



2-chloroethanol

Ethylene oxide residue definition in the EU:

sum of ethylene oxide and 2-chloro-ethanol expressed as ethylene oxide

Reg. (EU) 2015/868



Challenges of the analysis

- Low detection limits required: The maximum residue level (MRL) depends on the commodity, and it ranges from 0.02 to 0.1 mg/kg
- EO is highly volatile:
 - Poorly retained chromatographically
 - Unstable and can be lost in vial via evaporation
- EO has a low molecular weight:
 - Difficult to determine selective SRMs
- Dry matrices:
 - Dirty extracts
 - Interferences can cause over estimation of results



Challenges



Ethylene oxide



GC MS/MS method

- **TRACE 1610** gas chromatograph,
- **TSQ 9610** GC triple quadrupole and a Thermo Scientific™
- **TriPlus™ RSH** autosampler
- TG-624SiIMS (30m x 0.25mm x 1.40um)
- GuardGOLD™ Capillary Columns (5m x 0.25mm)



Injector

Use this inlet
 Set default values

Temperature Settings
 Enable temperature control
 Temperature: 90 [0..450 °C]

Inlet Parameters
 Operating mode: Split
 Split flow control
 Split flow: 5.0 [5.0..1250.0 ml/min]
 Split ratio: 5
 Spillless time: [0.00..999.99 min]
 Purge flow control
 Purge flow: 5.000 [0.500..50.000 ml/min]
 Constant septum purge
 Stop purge for: [0.00..999.99 min]
 Surge pressure: [5.00..1000.00 kPa]
 Surge duration: [0.00..999.99 min]
 Vacuum compensation
 Enable gas saver mode
 Gas Saver Flow: 50.0 [5.0..500.0 ml/min]
 Gas saver time: 1.50 [0.00..999.99 min]
 Enable backflush
 Backflush Start Time: [0.00..999.99 min]
 Enable Custom Duration
 Custom Duration: [0.00..999.99 min]

PTV Ramp Settings
 Pressure [5..1000 kPa] Rate [0.1..14.5 °C/s] Temp [0..450 °C] Time [0..999.99 min] Flow [5..1250 ml/min] Back flush

Injection: 0.80 50.0
 Evap: [] [] [] []
 Transfer: 12.0 250 10.00
 Cleaning: [] [] [] []
 Enable evaporation phase
 Enable clean phase
 Enable pressure ramps
 Transfer delay time: 0.00 [0.00..999.99 min]
 Post cycle temperature: Maintain
 Display phase program plot

Utilities
 Vapour volume calculator
 Column flow calculator
 Retention time alignment tool

Oven program

No	Retention time [min]	Rate [°C/min]	Target value [°C]	Hold time [min]
1	0.000	Run		
2	2.000	0.00	45.0	2.00
3	4.100	50.00	150.0	0.00
4	16.000	100.00	300.0	10.40
5		New Row		
6	16.000	StopRun		

Transfer line 250°C

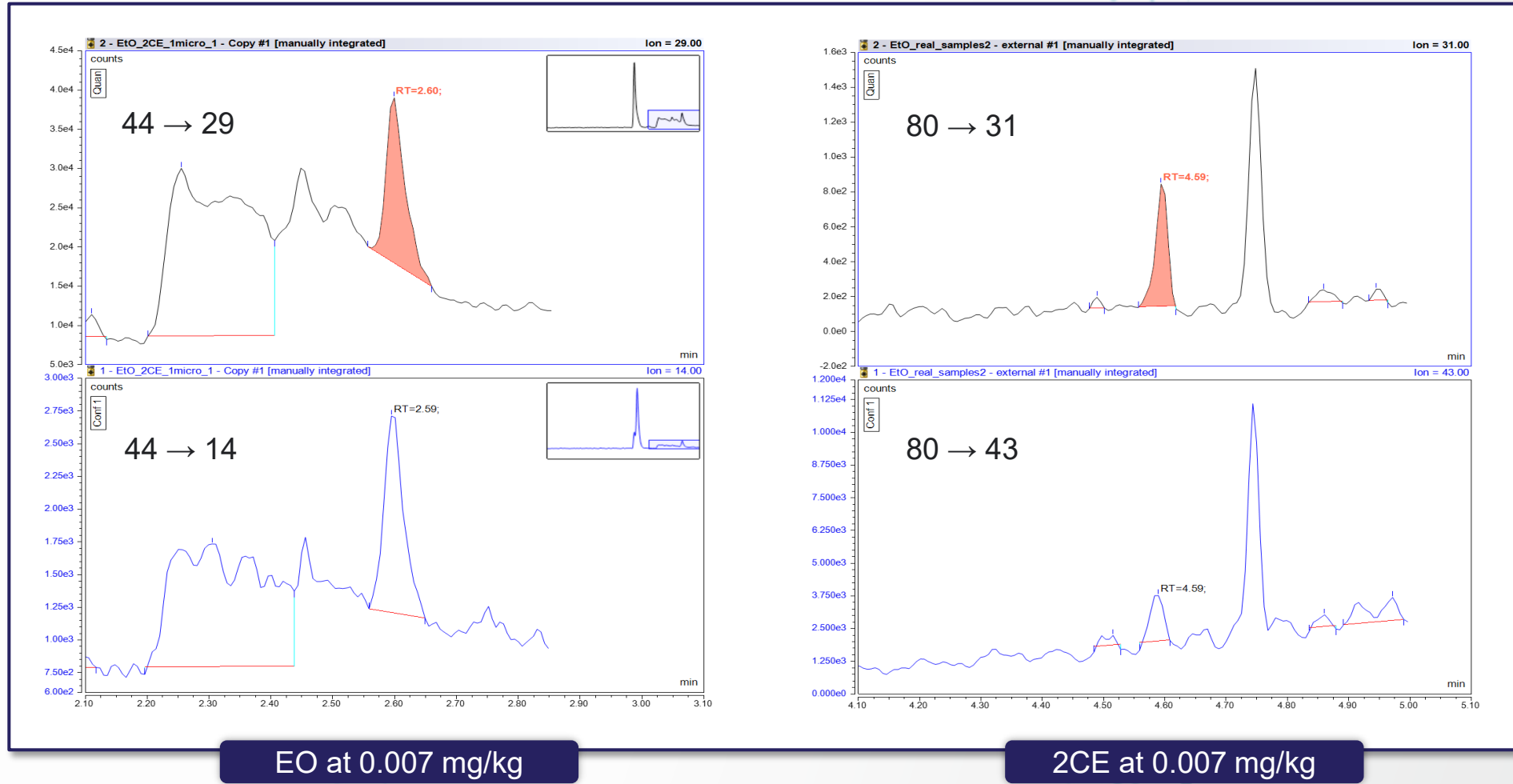
Ion source temperature 270 °C

Mass transitions

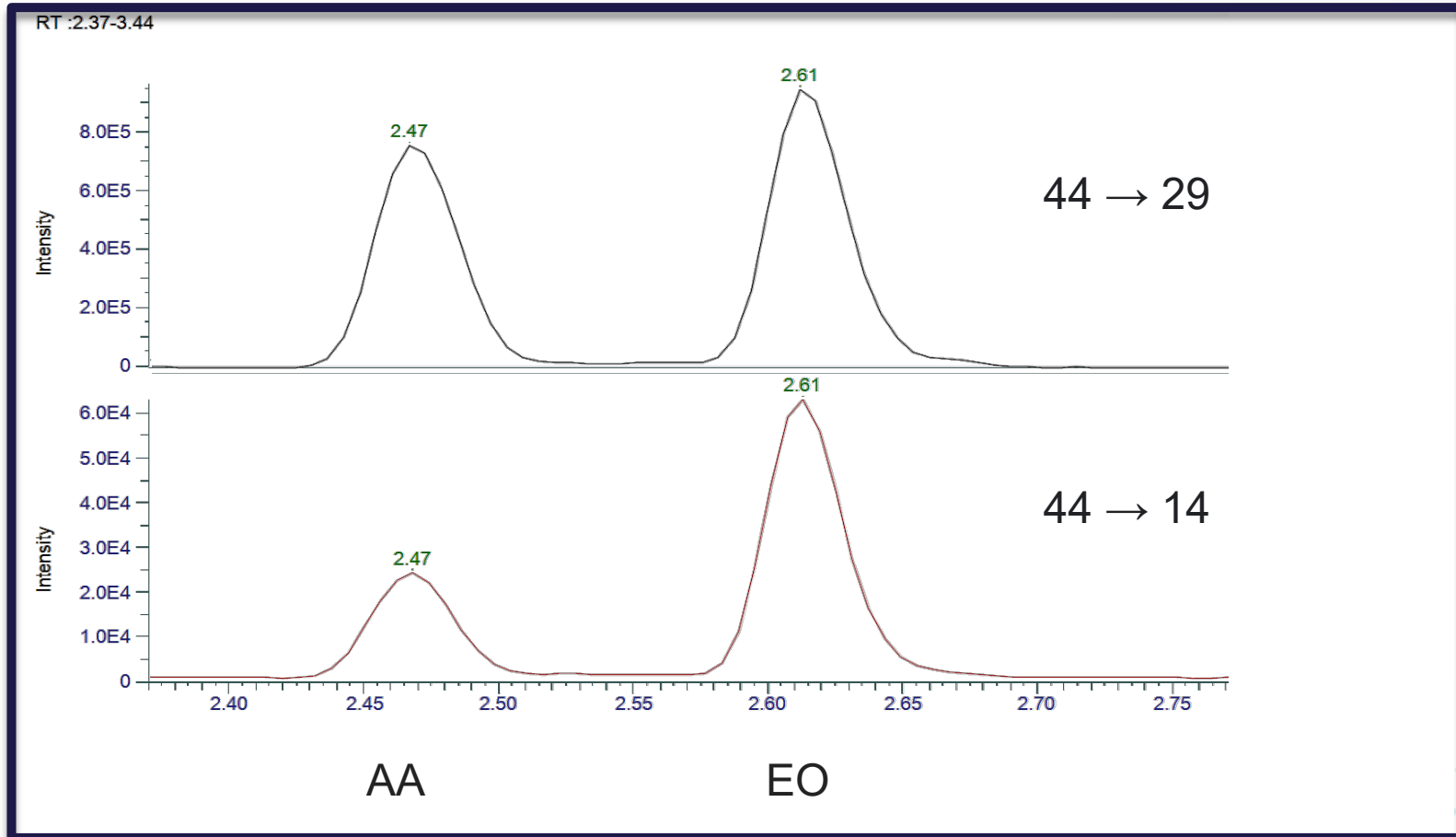
Compound	CE	Transition
EtO	20	44 -> 14
EtO	5	44 -> 29
2CE	5	80 -> 31
2CE	5	80 -> 43
2CE-d4	5	84 -> 33
2CE-d4	5	86 -> 33



Sensitivity of analysis



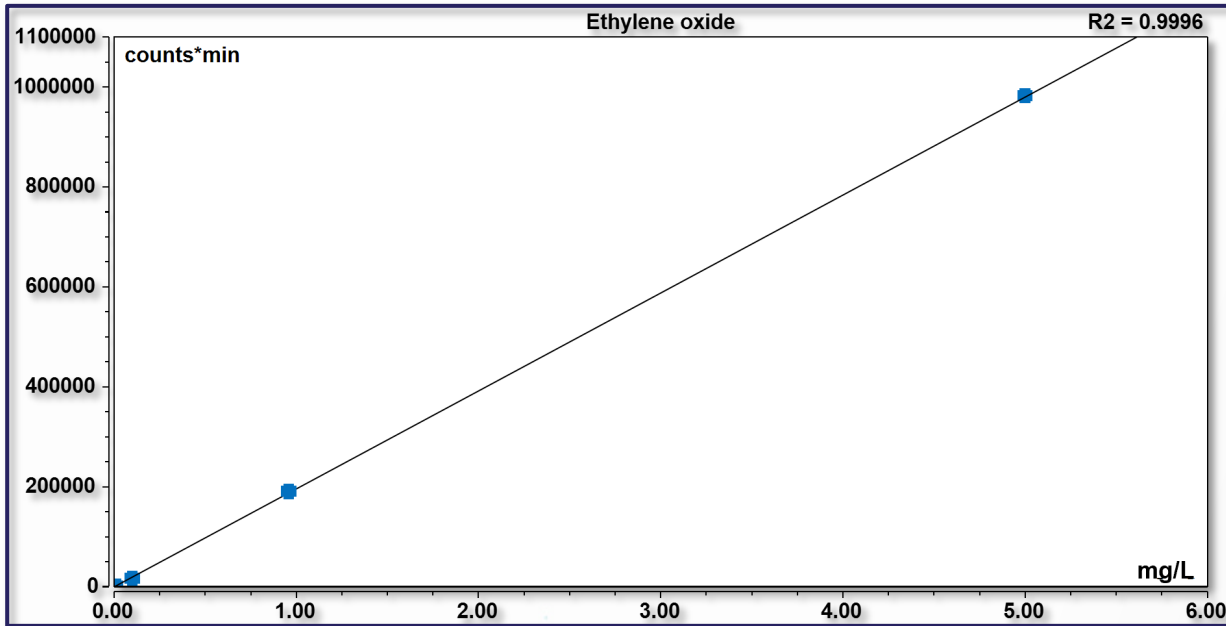
Selectivity in presence of interference



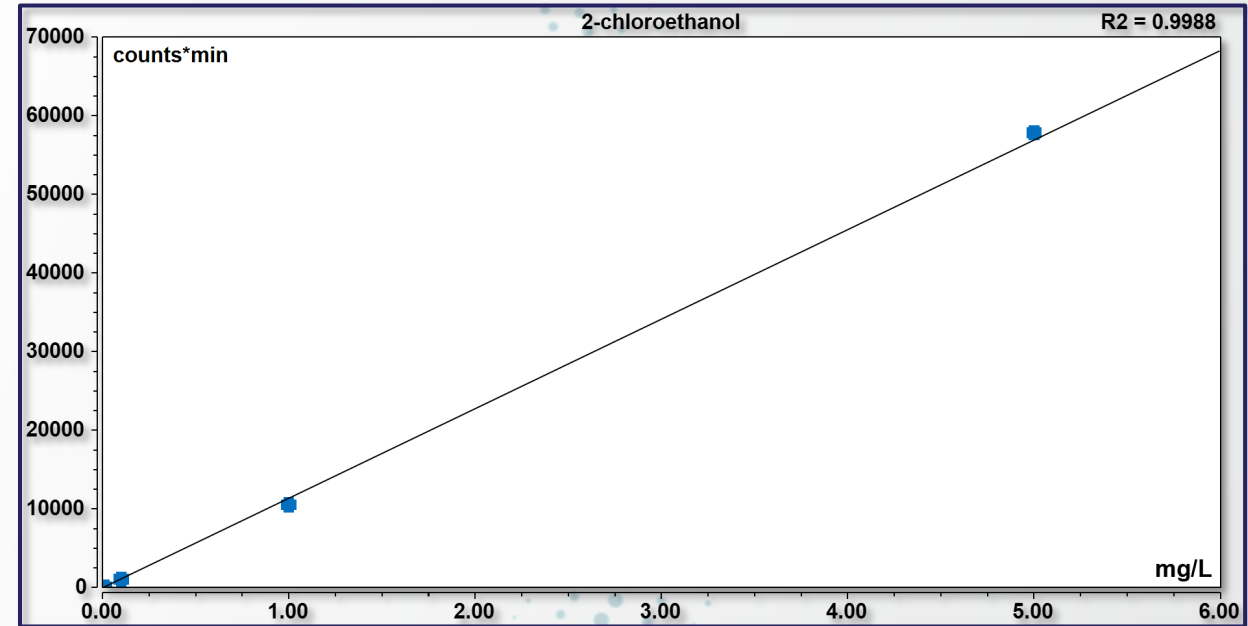
- Most common interfering compounds is acetaldehyde (AA)
- AA has the same transitions as EO
- If chromatographic separation must be achieved to prevent overestimation of the EO concentration



Linearity for the analysis



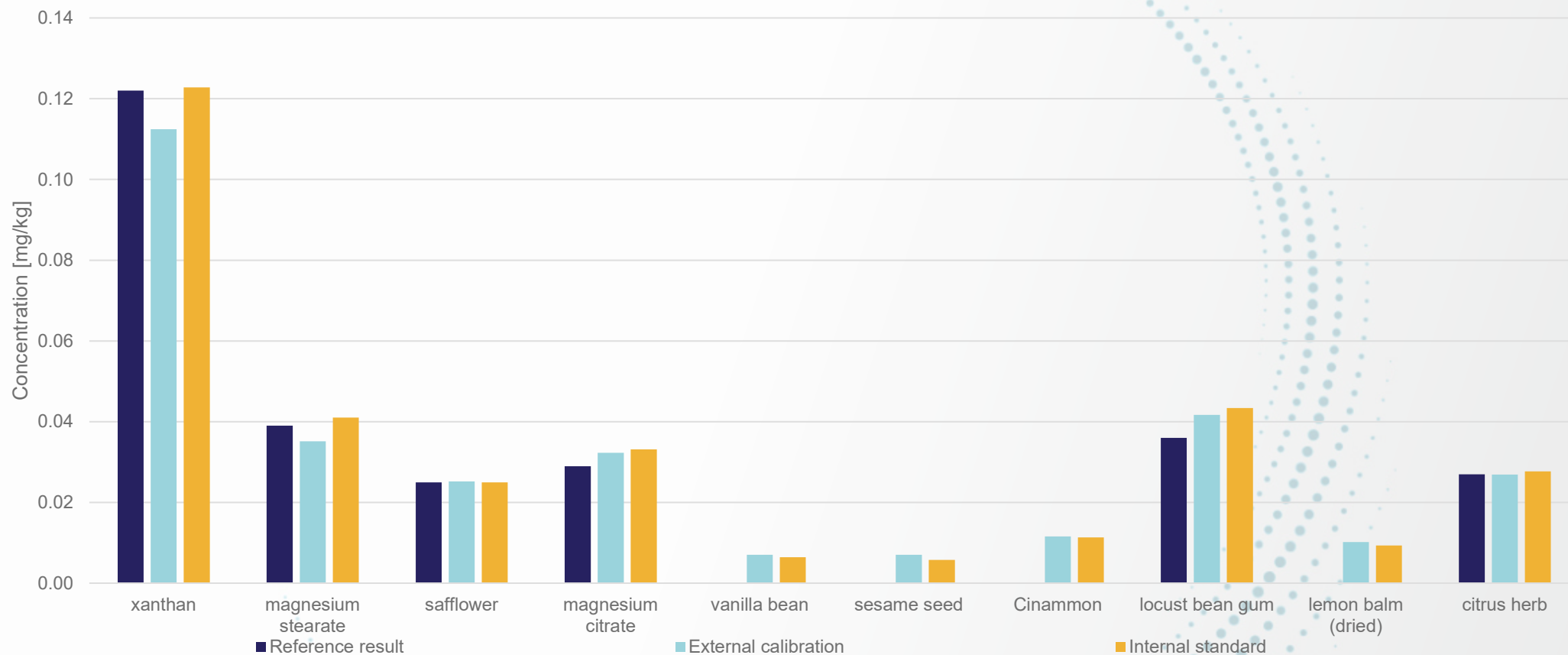
Calibration curve for EO between 0.007 mg/kg to 16.5 mg/kg



Calibration curve for 2CE between 0.007 mg/kg to 16.5 mg/kg



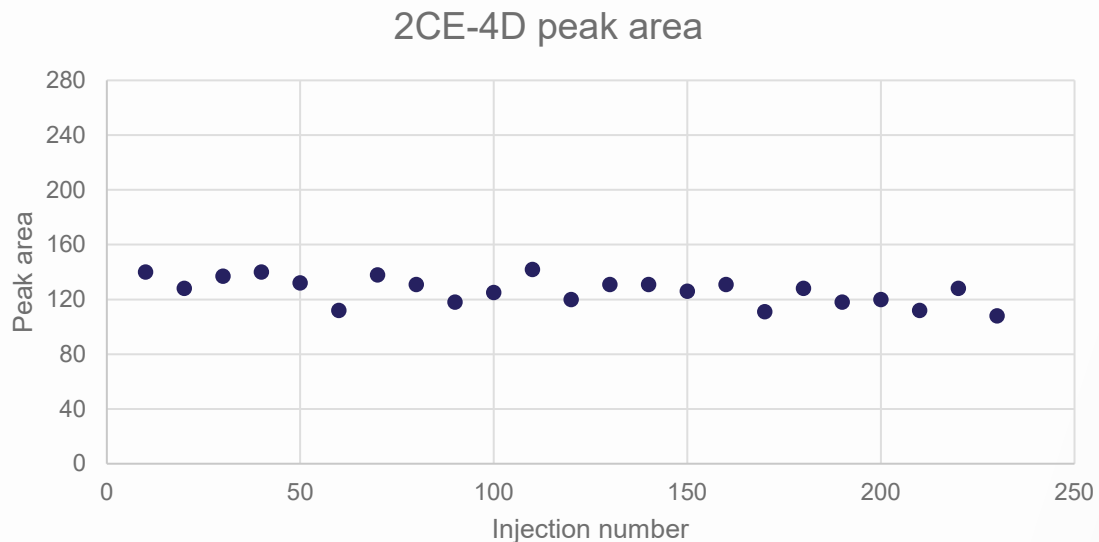
Quantification of samples for 2CE



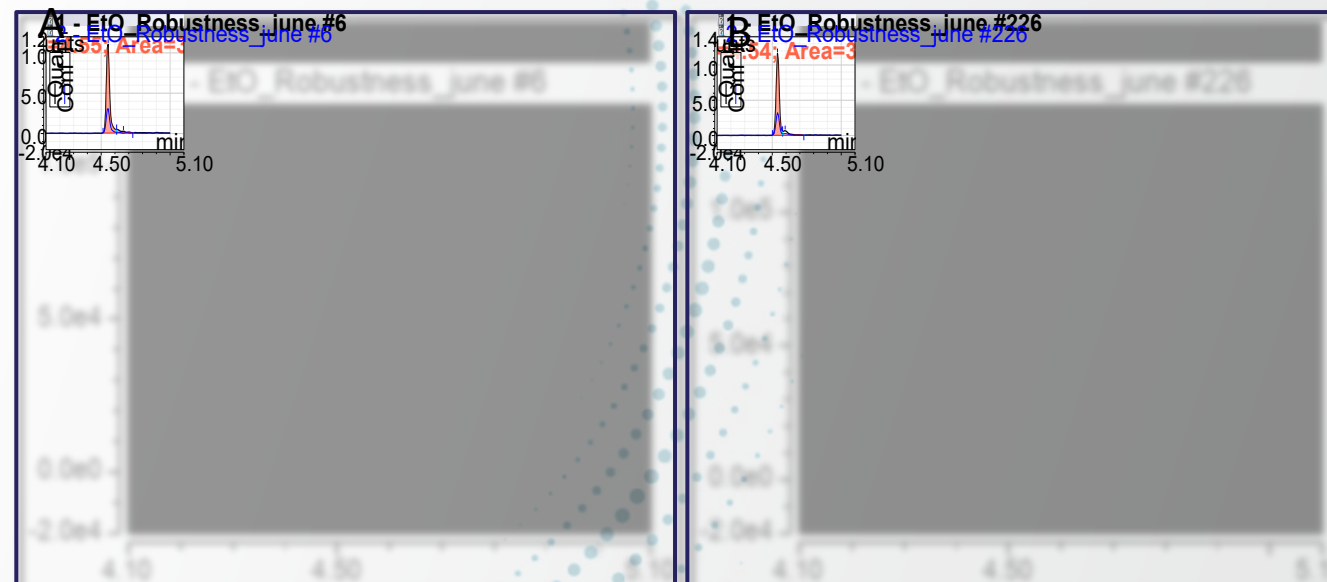
Real samples quantitation results. Since no ethylene oxide residue was found, the graphic contains only 2-chloroethanol results



Robustness of the analysis



Summary of the robustness test. Response of 2CE-4D standard in every 10th injection of the sequence (total number of injections: 230)



2CE-4D in sesame seed sample; A beginning of the sequence; B end of the sequence



Summary of results

- Chromatography: the chromatographic method provided a very good retention of the analytes and separation from the matrix interferences
- The quantitation at MRL was easily achieved, even with 1 μ L injection volume showing excellent sensitivity
- The XLXR detector facilitates quantitation in a broad range on concentration showing good linearity between 0.007 – 16.5 mg/kg in the samples
- Robustness: the system provided stable results during a 3-days long unattended sequence



TSQ 9610 GC-MS/MS summary



NeverVent technology

- Available with ExtractaBrite and AEI
- Increases instrument uptime

Off-axis ion guide pre-filter

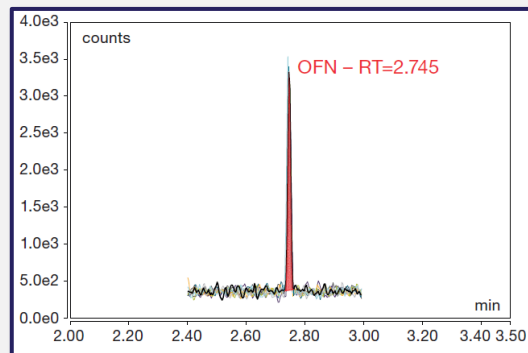
- Eliminates the neutral noise



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



XLXR detector as standard

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

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



Stay ahead with Thermo Scientific GC-MS

The TSQ 9610 offer **unstoppable confidence** and allow you to **stay ahead** by:



Increasing instrument uptime:

- With **NeverVent technology**, allowing maintenance to be performed without interrupting laboratory production:
 - Available with the AEI and ExtractaBrite on the TSQ 9610
- With inherent robustness, producing consistent results at low limits of detection and extended uptime.



Maximizing sample throughput:

- With the **XLXR detector**, allowing method consolidation and longer service intervals increasing throughput
 - Standard on all systems
- With inherent robustness, producing consistent results at low limits of detection and extended uptime.



Providing a rapid ROI:

- With innovative software solutions, including **instrument health**, **compliant SmartTune** and **ready-to-implement methods**, for quick system implementation for any laboratory in order to facilitate rapid revenue generation.



TSQ 9610 GC-MS/MS



Available collaterals

apps.lab.thermo.com

Mass Spectrometry

Stay ahead with unstoppable confidence

Thermo Scientific™ TSQ 9610* Triple Quadrupole GC-MS/MS System

TSQ 9610 Brochure

Mass Spectrometry

Stay ahead with unstoppable confidence

Thermo Scientific™ ISQ 7610* Single Quadrupole GC-MS System

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Gas Chromatography

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TRACE 1600 Series Gas Chromatograph
AJAS 1610 Liquid Autosampler

Trace 1610 Brochure

Environmental

Low-level consistent analysis of water and food matrices using purge and trap coupled to single quadrupole GC-MS

Authors: Terry Jeffers*, Adam Ladak*, and Amy Nutter*

Keywords: Polycyclic aromatic hydrocarbons (PAHs), food, environment, gas chromatography-mass spectrometry, GC-MS, purge and trap, single quadrupole mass spectrometry, headspace, advanced ion source (AIS), TRACE 1610 GC, programmable temperature injector system, PTV, AIA6 9510

Environmental analysis

Analysis of multiple matrices with curve for polycyclic aromatic hydrocarbons using the ISQ 7610 GC-MS system

Authors: Chaitan Chaturvedi, Brian Heier, Guilia Riccardoni*, Adam Ladak*, and Paul Skooba*

Keywords: Polycyclic aromatic hydrocarbons (PAHs), EPA Method 8210, ISQ 7610 mass spectrometry, established detection range, gas chromatography-mass spectrometry (GC-MS), Extractions, Chromatography, Environmental Analysis

Environmental analysis

Uninterrupted analysis of volatile organic compounds in drinking water

Authors: Adam Ladak*, Terry Jeffers*, and Amy Nutter*

Keywords: EPA, VOCs, phthalates, trace analysis, gas chromatography, single quadrupole mass spectrometry, selected ion monitoring, sensitivity, GPC, THM, environmental sample analysis, analytical testing laboratories

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Rapid quantification of 12 nitrosamines in metformin using triple quadrupole GC-MS/MS with Advanced Electron Ionization (AEI)

Authors: David Lee*, Aaron Lamb*, Andrea Romano*, and Guilia Riccardoni*

Keywords: Nitrosamines, pharmaceutical, N-nitrosodimethylamine (NDMA), N-nitrosodipropylamine (NDIPA), N-nitrosodipropylamine (NDIPA), GC-MS/MS, TSQ 9610 mass spectrometer

Food safety

Confident analysis of ultra-trace pesticide residues in baby food using triple quadrupole GC

Authors: Guilia Riccardoni*, Adam Ladak*, and Paul Skooba*

Keywords: Pesticides, baby food, gas chromatography-mass spectrometry, GC-MS, triple quadrupole, headspace, advanced ion source (AIS), Trace 1610 GC, programmable temperature injector system, PTV, AIA6 9510

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Analysis of volatile organic compounds in water using purge and trap coupled to single quadrupole GC-MS

Authors: Terry Jeffers*, Adam Ladak*, and Amy Nutter*

Keywords: ISQ 7610, TRACE 1610 GC, GC-MS, HJ 639, U.S. EPA 8260, VOCs, trace analysis, gas chromatography, single quadrupole mass spectrometry, selected ion monitoring, environmental laboratories, water analysis

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Analysis of volatile organic compounds in soil using purge and trap coupled to single quadrupole GC-MS

Authors: Terry Jeffers*, Adam Ladak*, and Amy Nutter*

Keywords: ISQ 7610 MS, TRACE 1610 GC, GC-MS, HJ 605, U.S. EPA 8260, VOCs, phthalates, trace analysis, gas chromatography, single quadrupole mass spectrometry, selected ion monitoring, sensitivity, GPC, THM, environmental sample analysis, analytical testing laboratories

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Phenolics using triple quadrupole

Authors: Terry Jeffers*, Adam Ladak*, and Amy Nutter*

Keywords: Phenolics, environmental, gas chromatography, single quadrupole mass spectrometry, selected ion monitoring, sensitivity, GPC, THM, environmental sample analysis, analytical testing laboratories



Questions?

