Implementing new GC-MS technology to stay ahead with your pesticides analysis

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The world leader in serving science

Overview

1. Introduction the new Thermo Fisher Scientific GCMS line up
2. Ehtylene oxide
3. Pesticides in baby food
4. Pesticides in black tea
5. Summary

New GCMS line up from Thermo Scientific

Thermo Fisher Scientific's GC and GC-MS Portfolio

- Thermo Scientific™ **Trace™ 1600/1610 GC**
  - A flexible, workhorse GC providing day-in, day-out performance
- Thermo Scientific™ **ISQ 7610™ – Single Quadrupole GC-MS**
  - Robust and reliable for routine mass spec analysis
- Thermo Scientific™ **TSQ 9610™ – Triple Quadrupole GC-MS/MS**
  - Sensitivity and selectivity for the most demanding research
- Thermo Scientific™ **Orbitrap™ Exploris™ GC**
  - High resolution, accurate mass for untargeted analysis and identification of unknowns

- **Autosamplers**
  - Thermo Scientific™ **AI/AS 1610 Liquid Autosampler** Cost effective and simple solution for liquid sample injections
  - Thermo Scientific™ **TriPlus™ RSH SMART** for enhanced sampling techniques capability and automation for sample preparation workflows

TRACE 1610

ISQ 7610

TSQ 9610

Orbitrap Exploris GC

TRACE 1610 GC

Enhanced interaction

- Easy navigation through intuitive multi-function touchscreen interface
- Multi-language
- Instrument health icon always visible for status notification
- Consumables usage counters
- Automatic leak check
- Diagnostic information
- USB port for video uploads and software updates

TRACE 1610 GC

Simplified operations

- How-to videos instructions
- Tool-free iConnect Column Lock
- Illuminated GC oven
- Tubing-free inlet design
- Integrated backflush in the SSL and PTV injector for simplified pre-, mid-, post-column operation

AI/AS 1610 Liquid Autosampler

Simplified operations

- Illuminated syringe holder and magnifier lens
- Single cable connection with the AI/AS 1610
- Simplified dual-tower Gemini control and method setup
- Easy slide-in to quickly access to the inlet
- Color-coded status indicator on top of the tower
- Removable vial tray
- AI/AS 1610 control through the GC touchscreen

Introducing the new TSQ 9610 GC-MS/MS

The TSQ 9610 GC-MS/MS offer **unstoppable confidence** and allow your customer to **stay ahead** by:

- **Increasing instrument uptime**
- **Maximizing sample throughput**
- **Providing a rapid ROI**

TSQ 9610 GC-MS/MS

New Features

Hardware	AEI + VPI + Filament (NeverVent AEI)	• Eliminate the need to vent the instrument for routine maintenance including source cleaning, column changing and filament replacement
	Next Generation Detector	• Extended linear dynamic range • Extended lifetime (~8x more)
Software	Native Chromeleon Driver	• Regulatory Compliance • In-sequence tuning • Language localization
	Instrument Health	• Improve maintenance records • Make informed decisions to prevent unnecessary downtime

Increasing instrument uptime

NeverVent Technology

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

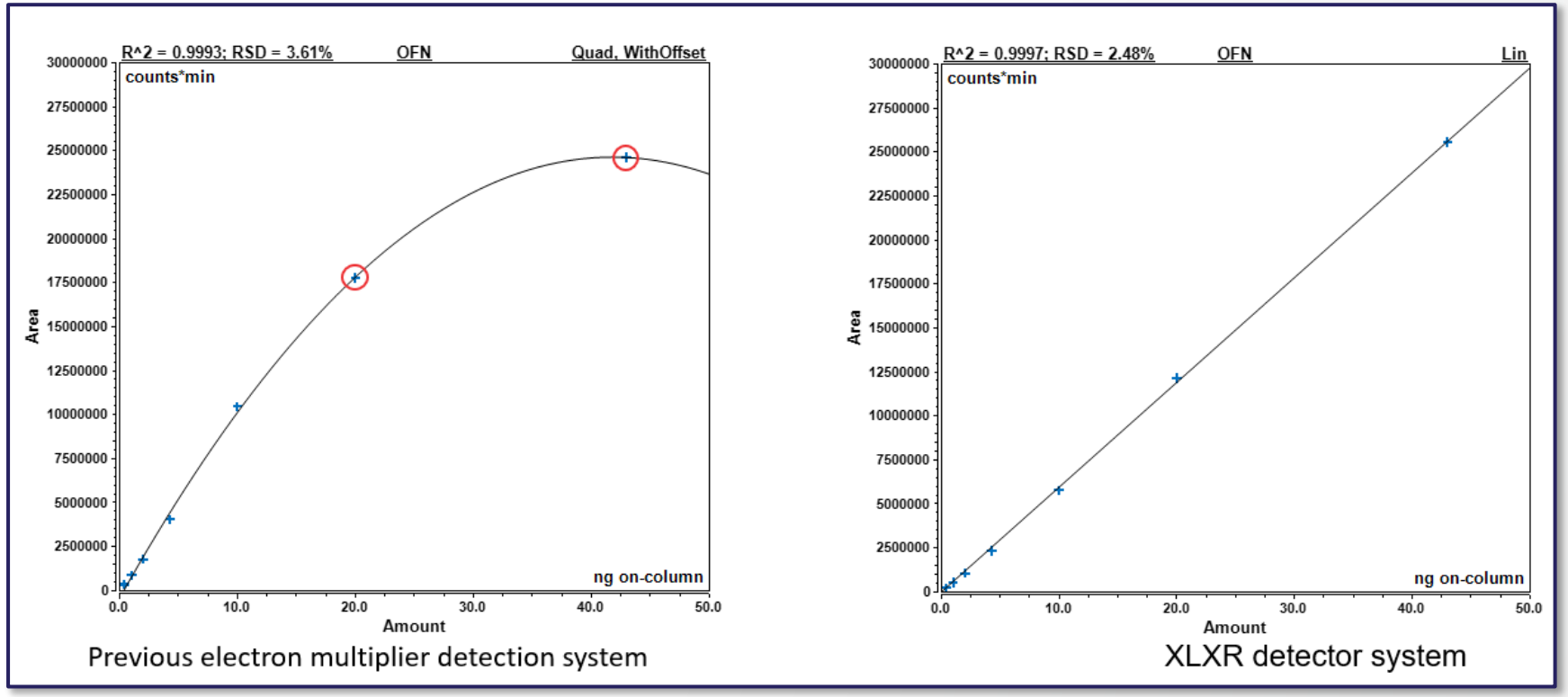
Available on the TSQ 9610 with the Thermo Scientific™ ExtractaBrite™ and Advanced Electron Ionization (AEI) source

		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%

Maximizing sample throughput

Extended dynamic range detector

The XLXR detector provides extended dynamic range allowing extended calibration ranges



XLXR detector is not saturated at high concentrations

TSQ 9610 GC-MS/MS summary

NeverVent technology

- Available with ExtractaBrite and AEI
- Increases instrument uptime

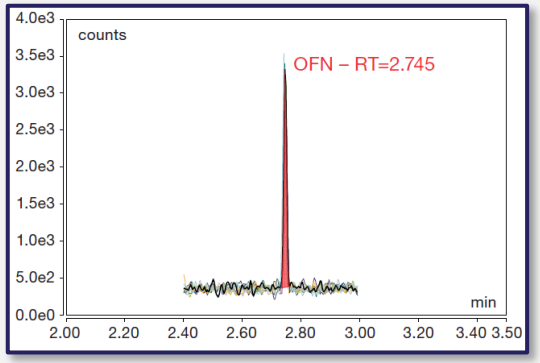
Off -axis ion guide pre-filter

- Eliminates the neutral noise

Evo collision cell

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

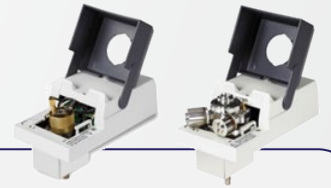
Class-leading sensitivity



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

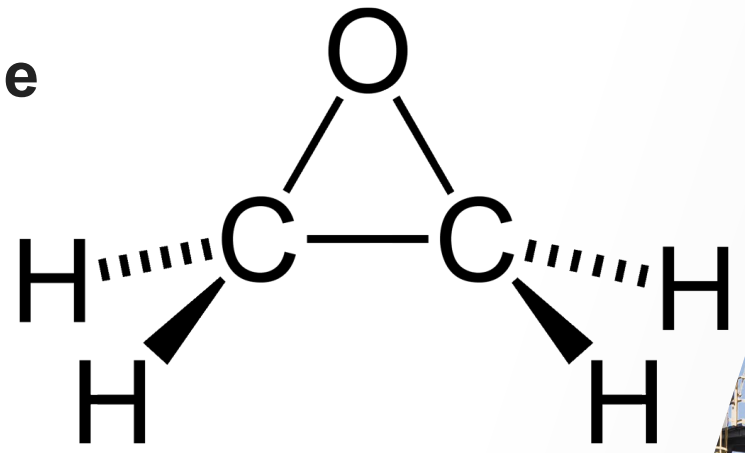
- Unique modular injector and detector design
- Easy-to-use touchscreen with real-time instrument monitoring and video guides

Software productivity tools

- Compliant-ready software
- Instrument health

Ethylene oxide

Uses of ethylene oxide

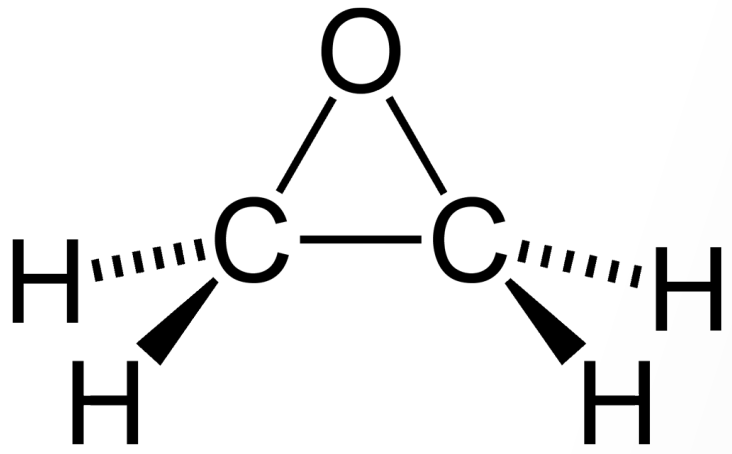


- Synthesis of polymers
- Synthesis of solvents
- Synthesis of adhesives
- Synthesis of detergents
- Synthesis of modified polysaccharides
- Sterilization of medical equipment
- Fumigation of dry food commodities

Ethylene oxide

Typical commodities fumigated with EO

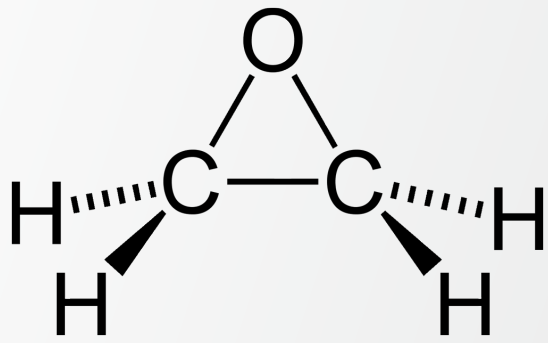
- Herbs
- Spices
- Nuts
- Dates
- Raisins
- Oily seeds
- Milled cereals
- Feed
- Milk powder



Ethylene oxide

107 RASFF notifications from 01.01.2022 to 15.06.2022

- Food supplements
- Crushed chilli
- Sesame seeds
- Animal feed
- Spice blends
- Ice cream
- Instant noodle
- Xanthan gum
- Locust bean gum
- Wheat protein
- Spice mix

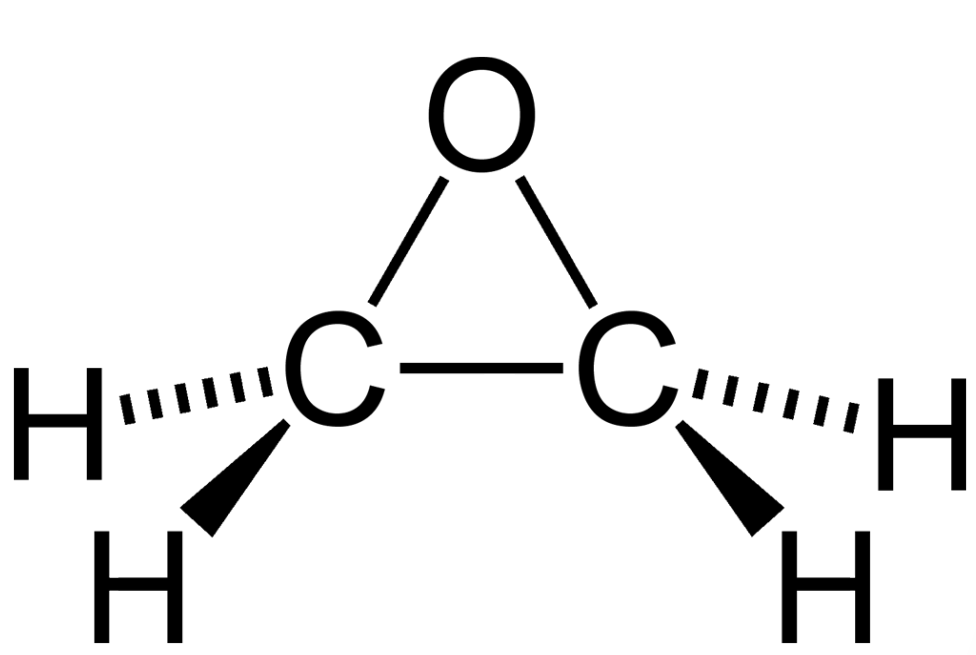


RASFF

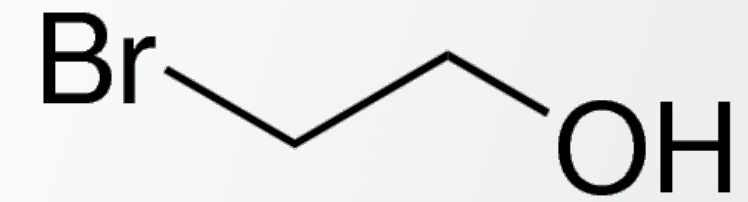
Rapid Alert System for Food and Feed

Ethylene oxide

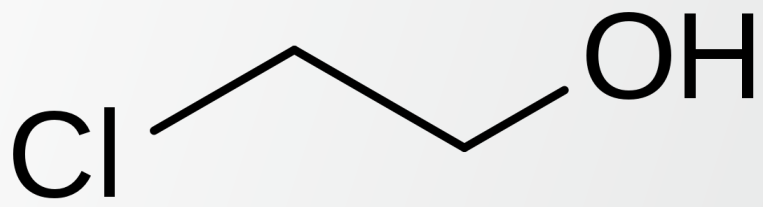
EO and its degradation products



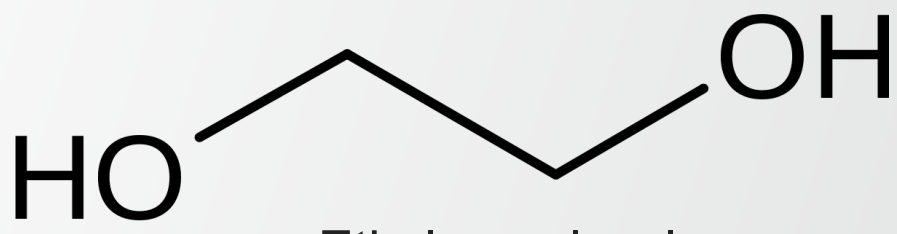
Ethylene oxide



2-bromoethanol



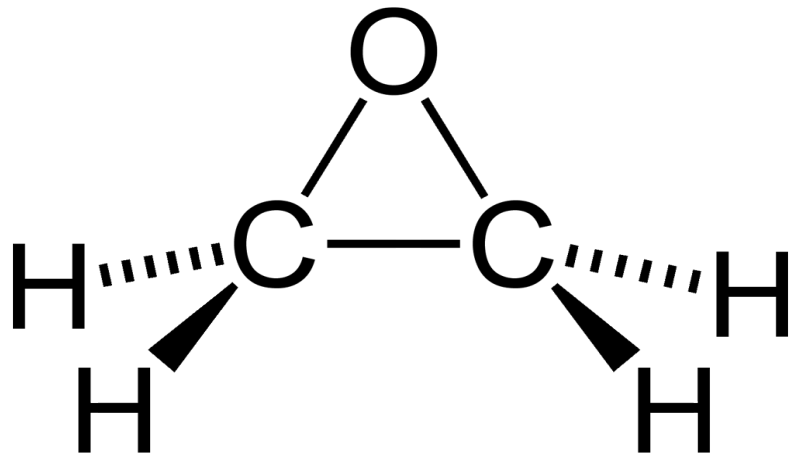
2-chloroethanol



Ethylene glycol

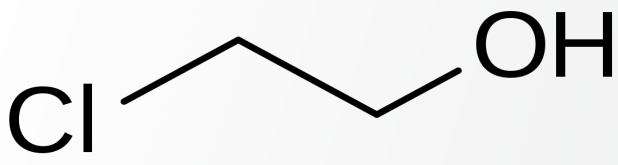
Ethylene oxide

EO and its degradation products



Ethylene oxide

+



2-chloroethanol

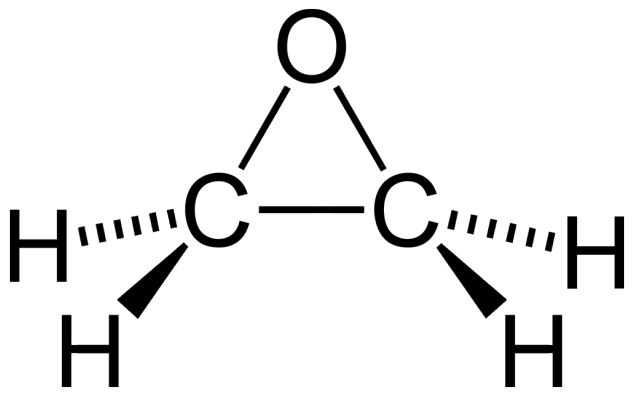
Ethylene oxide residue definition in the EU:

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

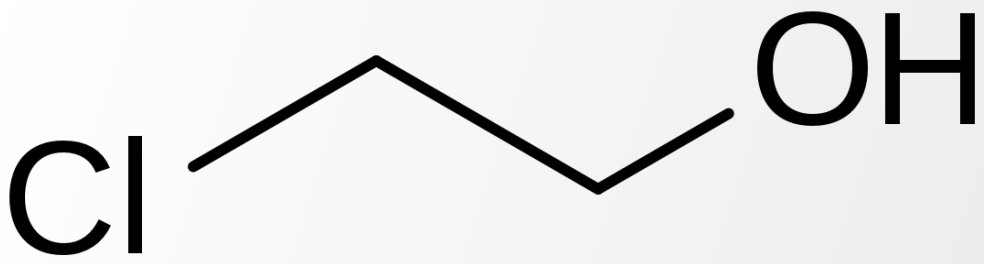
Reg. (EU) 2015/868

Ethylene oxide

Physicochemical properties



Formula C_2H_4O
Boiling point 10.4 °C
Vapor pressure 146 atm (20 °C)
Molecular mass 44 Da

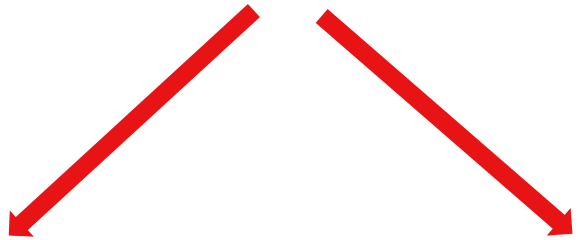


Formula C_2H_5ClO
Boiling point 130 °C
Vapor pressure 0.007 Pa (20 °C)
Molecular mass 80 Da

Ethylene oxide

Analytical challenges

Low boiling point



Losses in the extraction

Poor retention in the chromatographic column

Low molecular mass

Non-selective transitions

Dry matrices

Dirty extracts

Interreferences

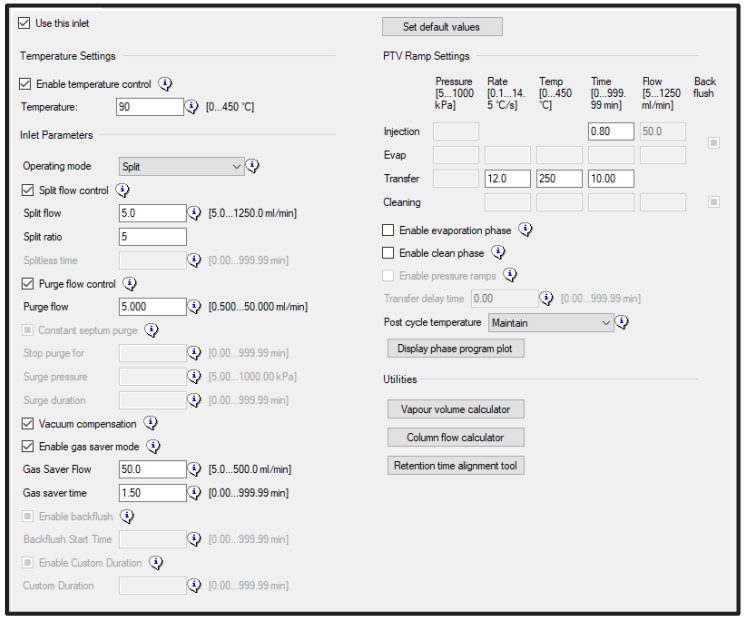
Robustness problems

Ethylene oxide

GC MS/MS method

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

Injector



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

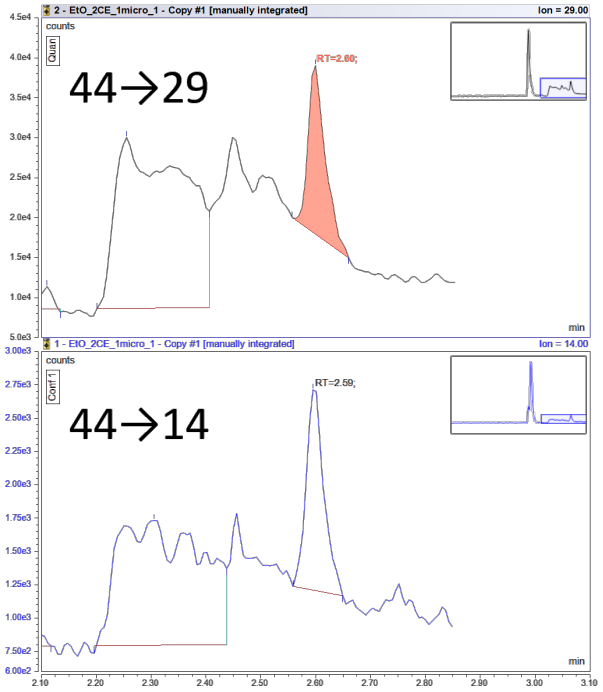
Compound	CE	Transition
EtO	20	44 -> 14
EtO	5	44 -> 29
2CE	5	80 -> 31
2CE	5	80 -> 43
2CE-d4	5	84 -> 33
2CE-d4	5	86 -> 33

Ethylene oxide

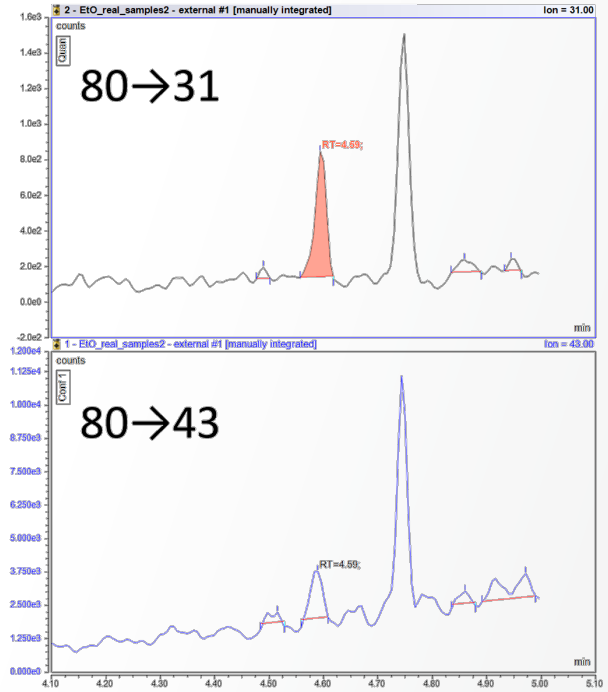
Sensitivity

Concentration: 2 mg/L

Injection volume: 1 µL



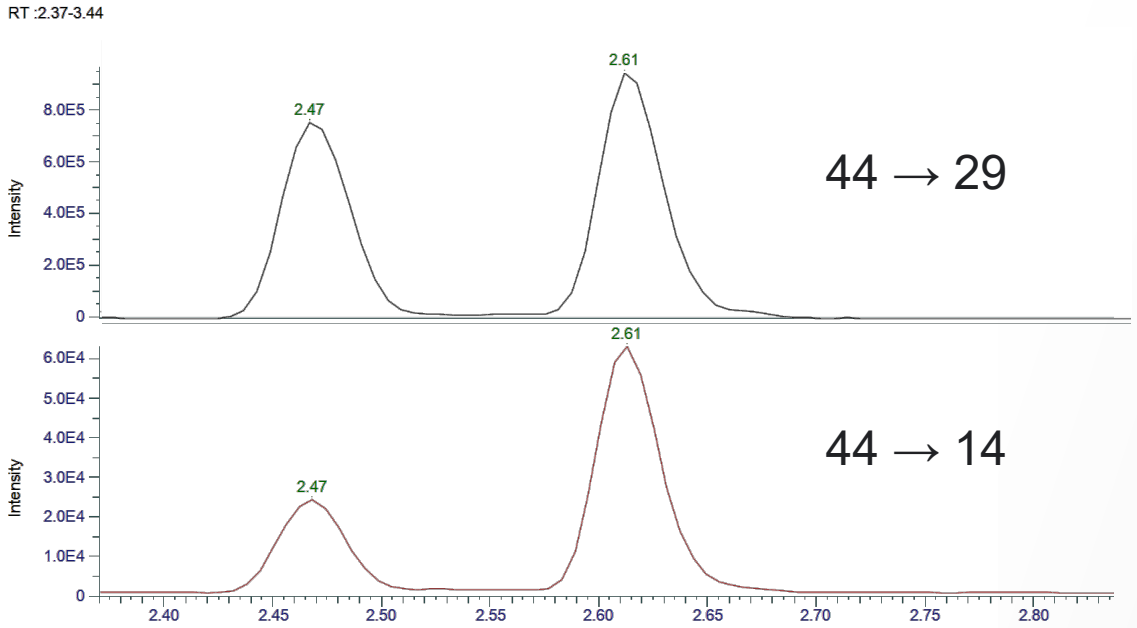
Ethylene oxide



2-chloroethanol

Ethylene oxide

Selectivity- separation from acetaldehyde

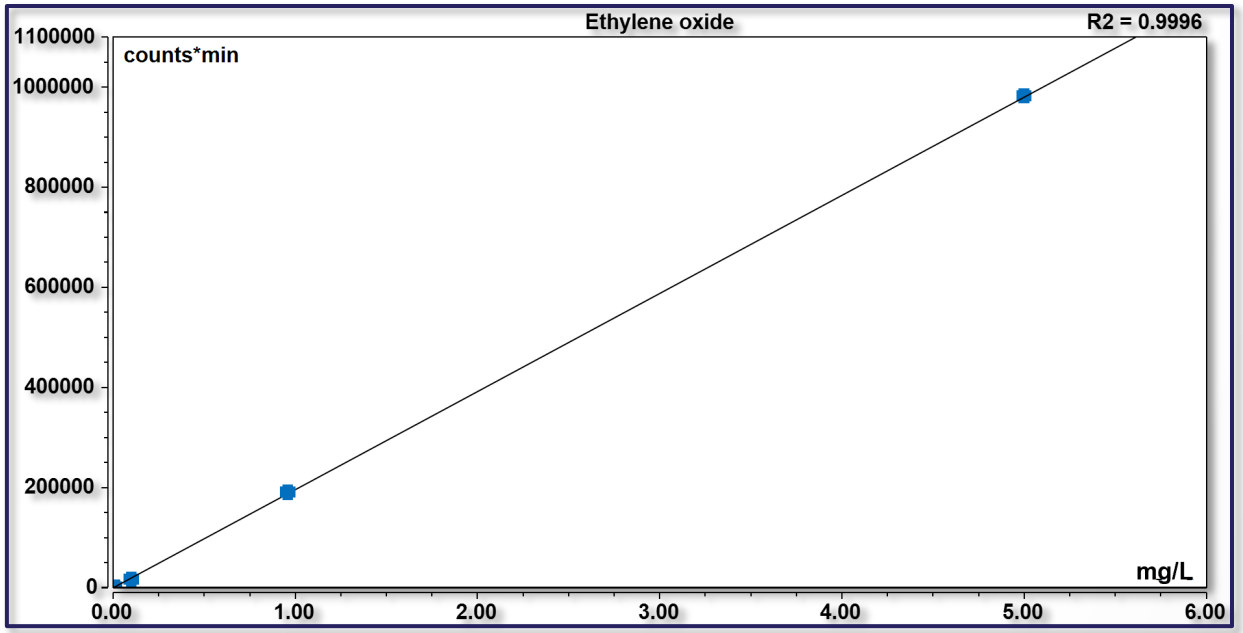


Acetaldehyde

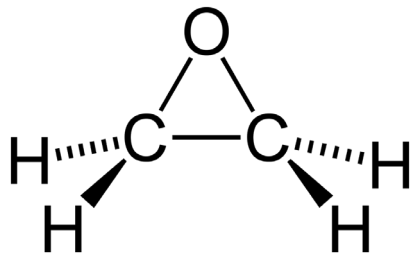
Ethylene oxide

Ethylene oxide

Linearity

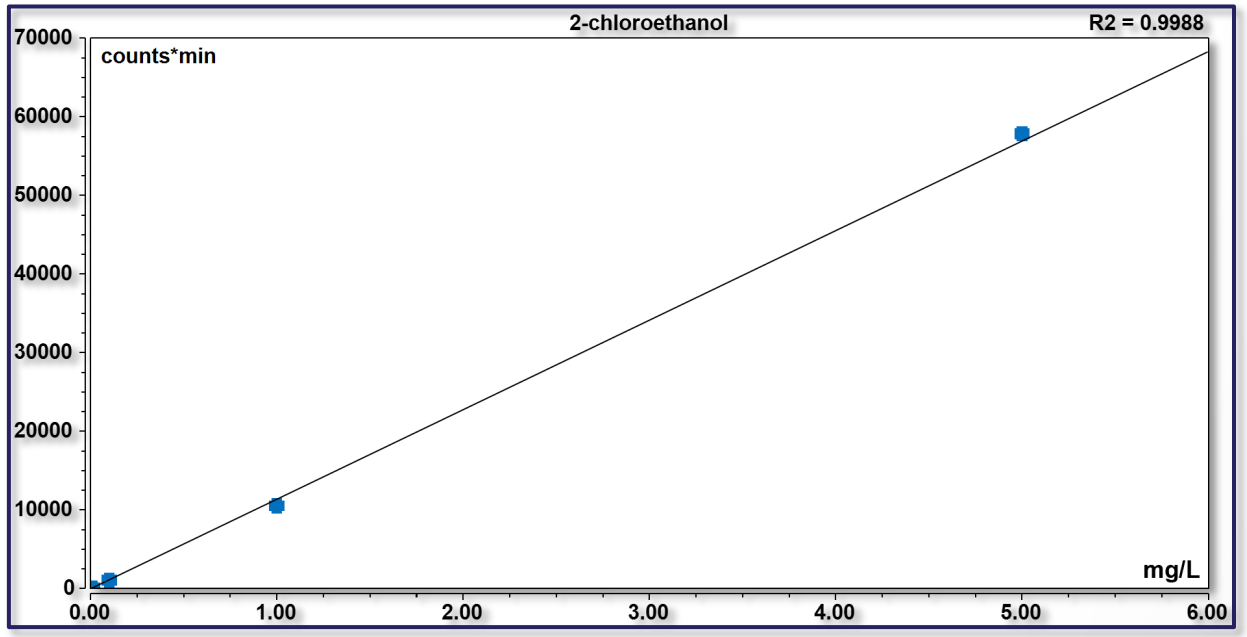


Theoretical concentration	Peak area	Calculated concentration	Deviation of back calculated concentration	Ion ratio
[mg/L]	[counts · min]	[mg/L]	[%]	[%]
0.002	249	0.002	18	7.52
0.005	831	0.005	7	6.86
0.010	1499	0.009	-13	7.50
0.100	16883	0.087	-13	7.17
1.000	199845	1.025	0	6.78
5.000	982577	5.013	0	6.53

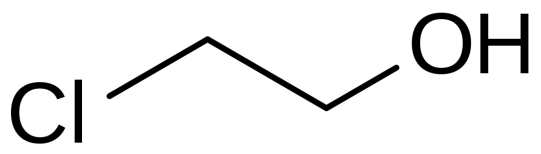


Ethylene oxide

Linearity

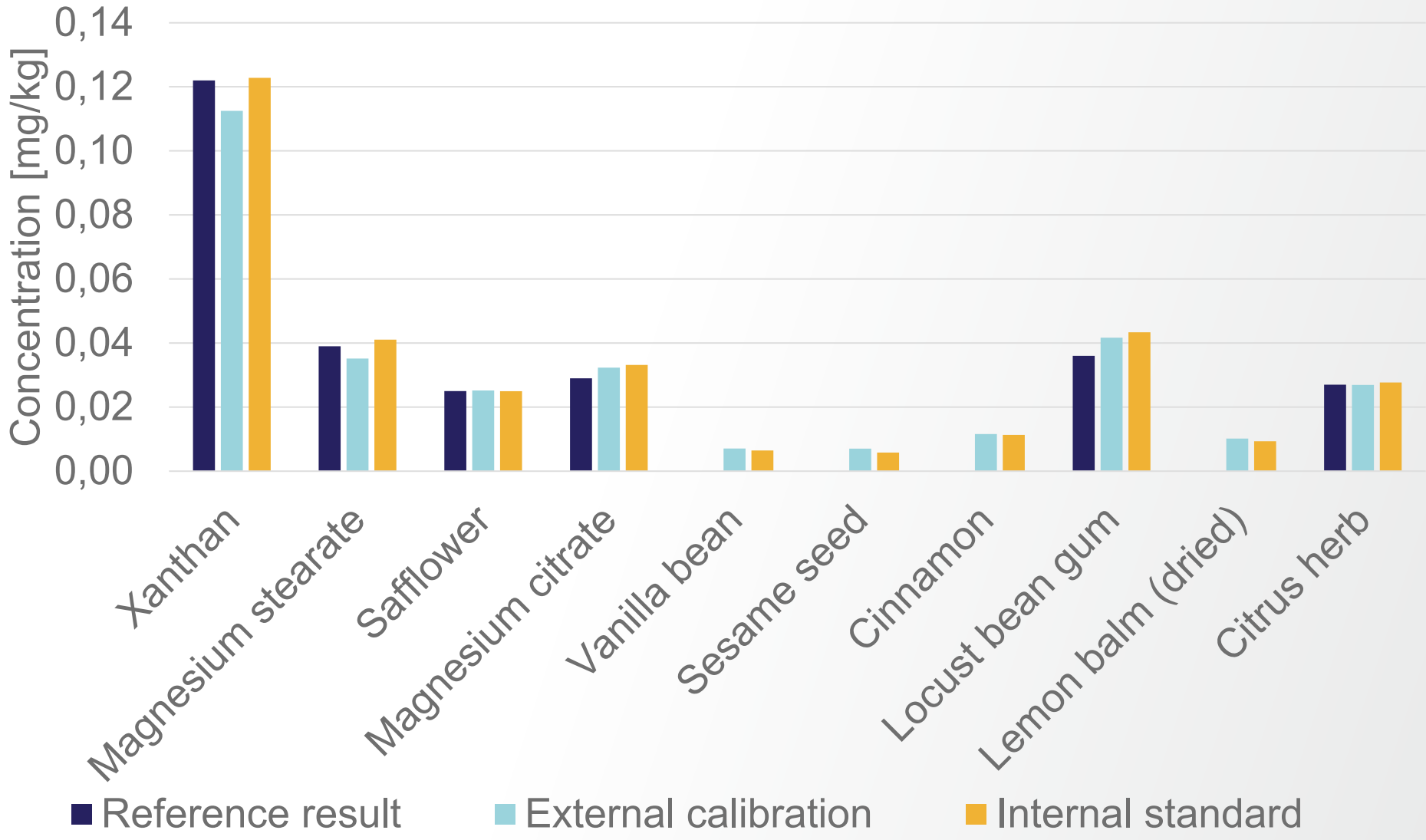


Theoretical concentration	Peak area	Calculated concentration	Deviation of back calculated concentration	Ion ratio
[mg/L]	[counts · min]	[mg/L]	[%]	[%]
0.002	16	0.002	7	111
0.005	56	0.006	13	117
0.010	98	0.009	-7	91
0.100	1049	0.093	-7	106
1.000	10531	0.926	-7	105
5.000	57839	5.081	2	98

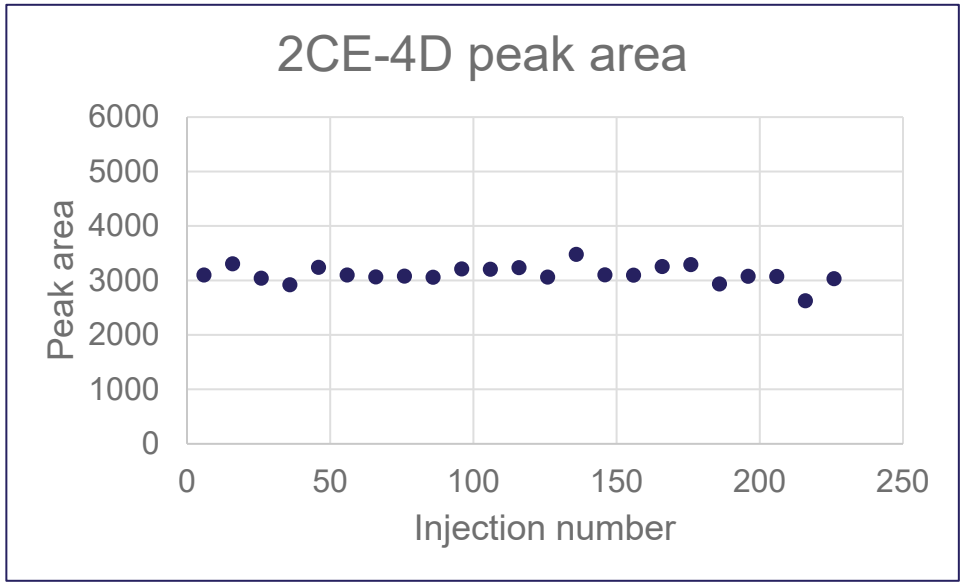


Ethylene oxide

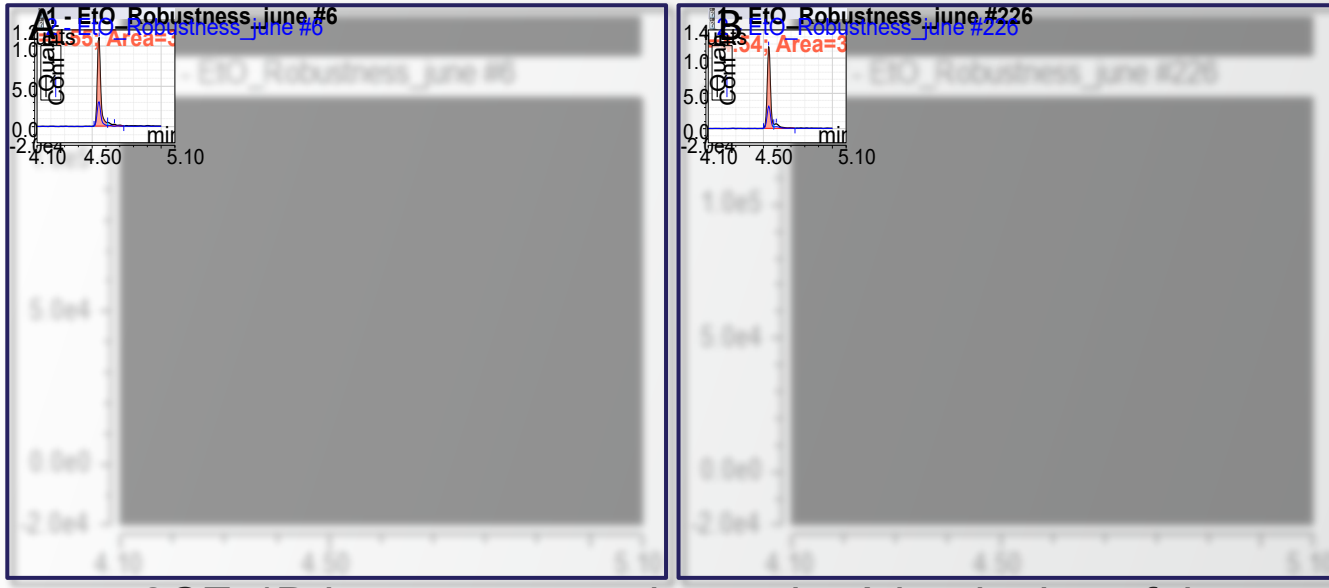
Real samples



Robustness of the analysis



The system was stable during a three-day long sequence (figure shows every 10th injection)

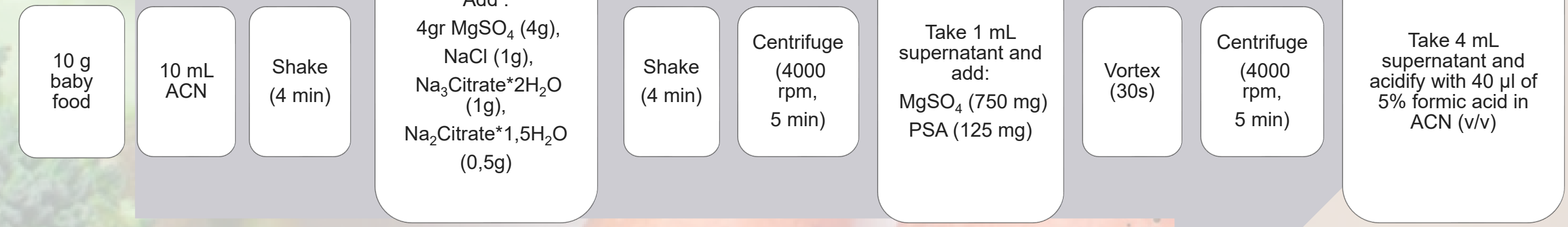


2CE-4D in sesame seed sample; A beginning of the sequence; B end of the sequence

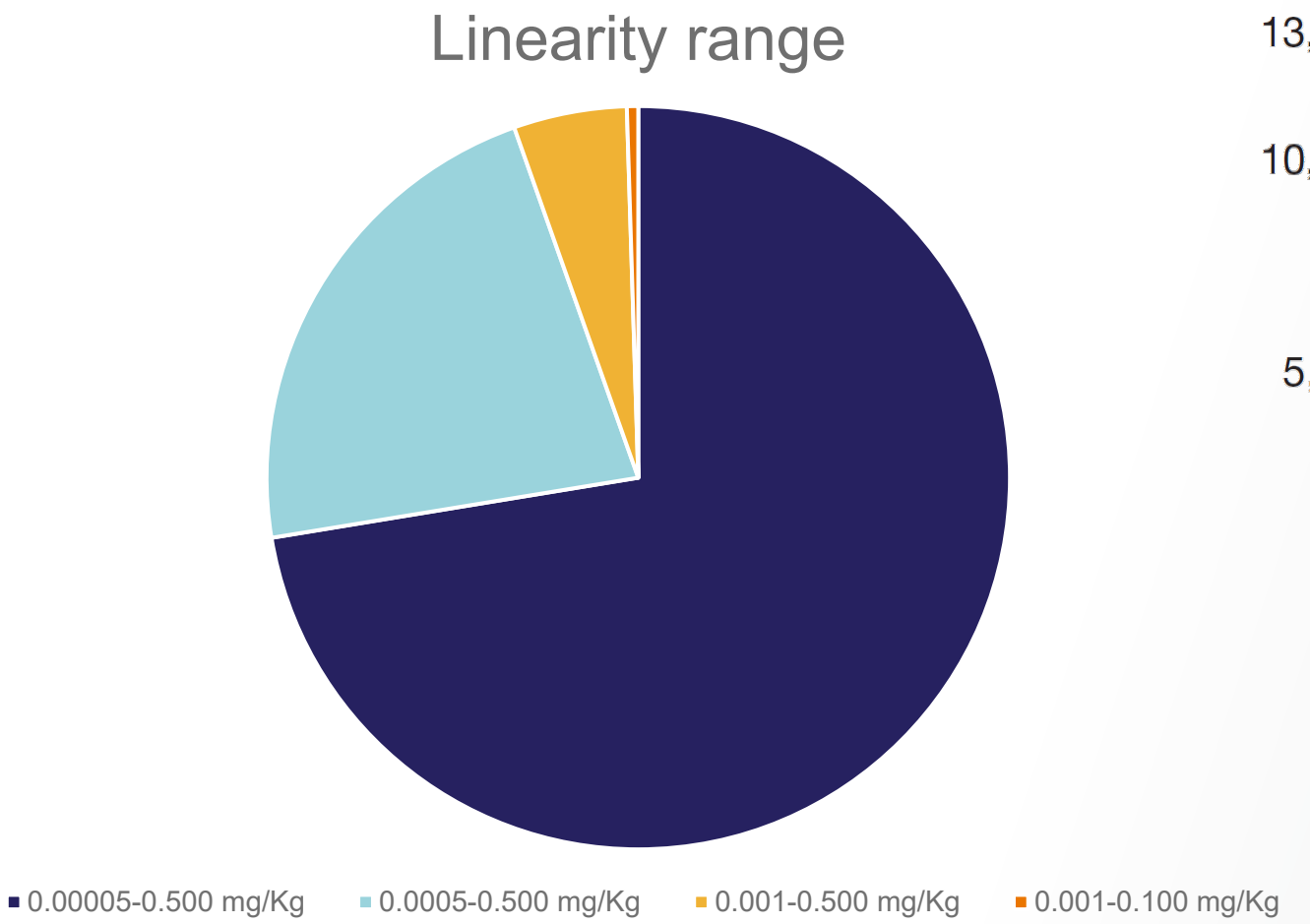
Summary of results

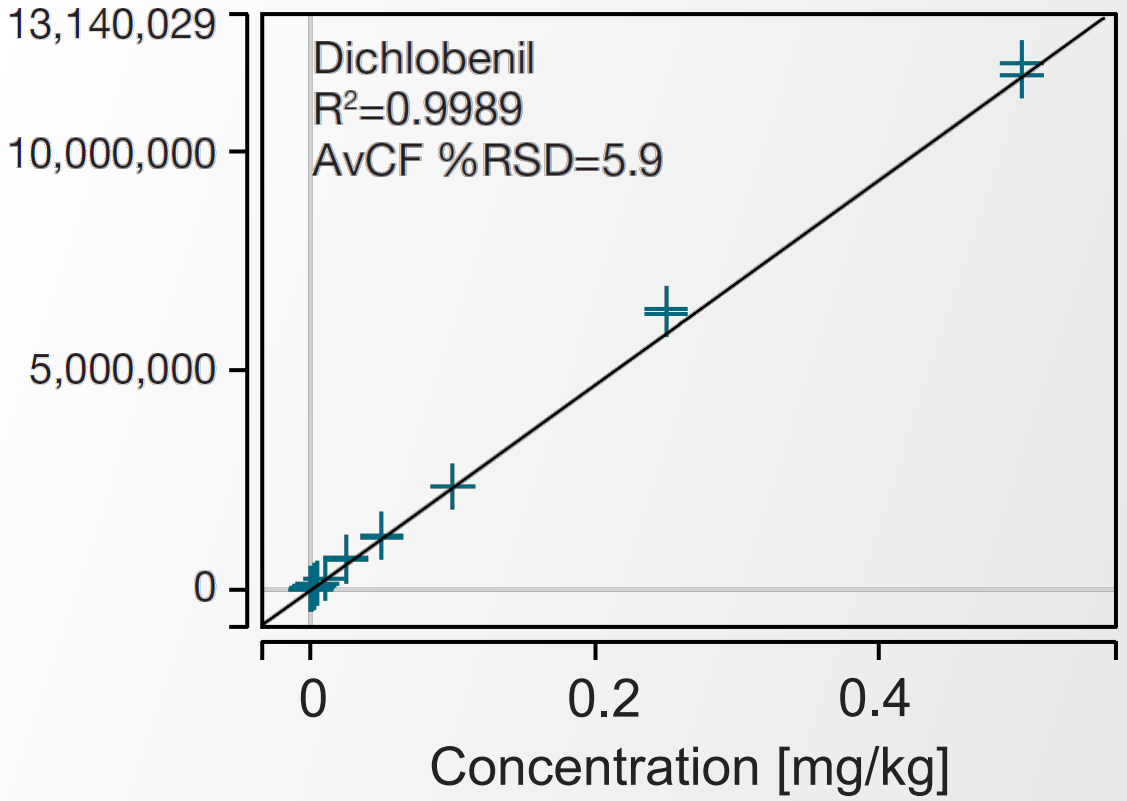
- Chromatography: the chromatographic method provided a very good retention of the analytes and separation from the matrix interferences
- The quantitation at MRL was easily achieved, even with 1 µL injection volume showing excellent sensitivity
- The XLXR detector facilitates quantitation in a broad 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

Sample preparation with QuEChERs



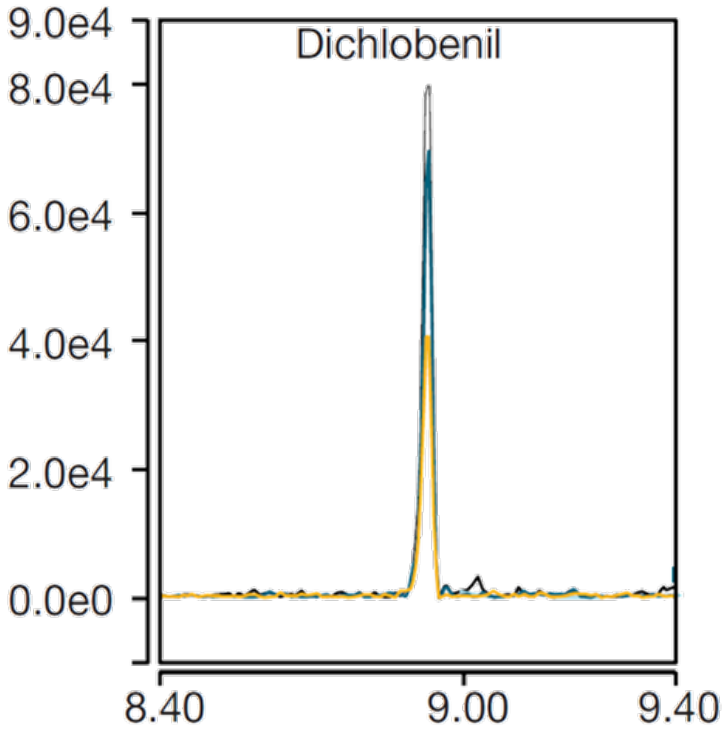
Linearity

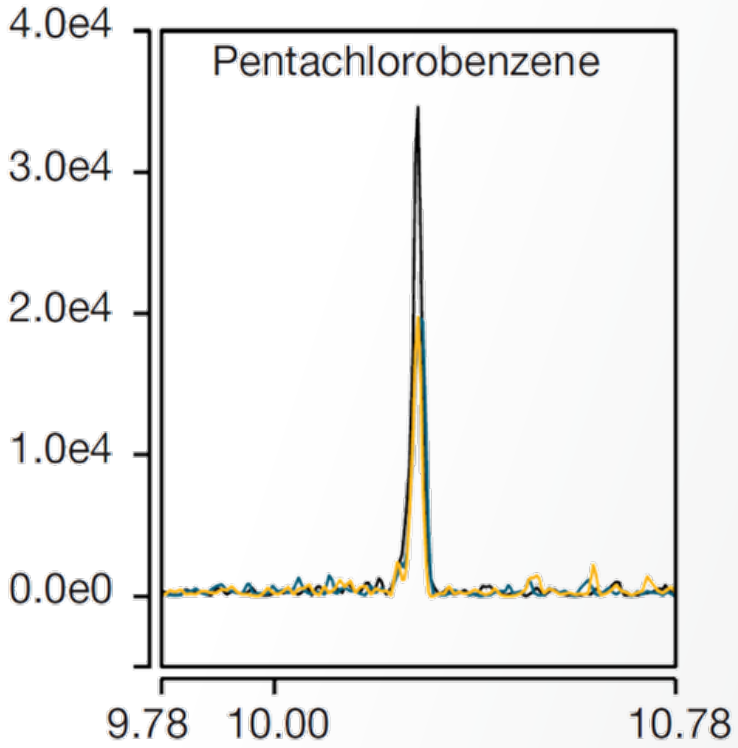

Linearity range
0.00005-0.500 mg/Kg
0.0005-0.500 mg/Kg
0.001-0.500 mg/Kg
0.001-0.100 mg/Kg

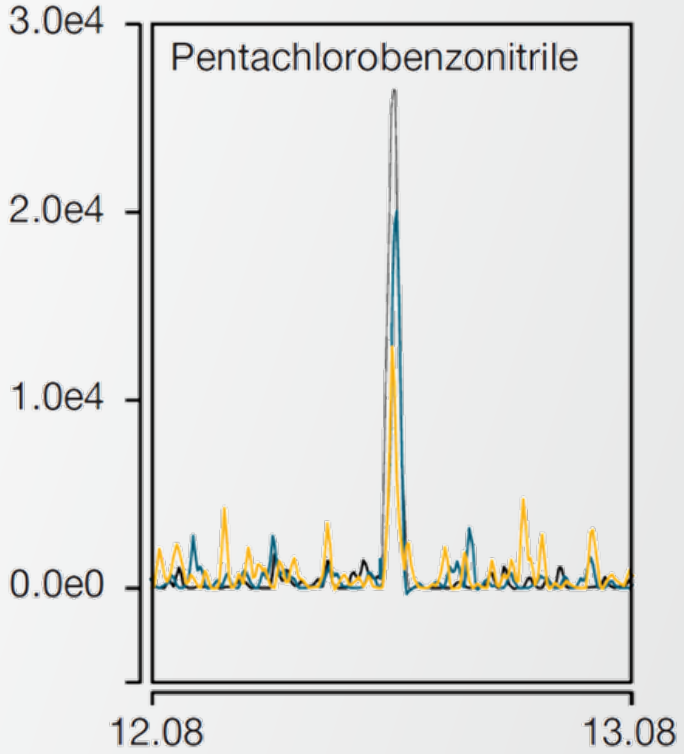

13,140,029
10,000,000
5,000,000
0
Dichlobenil
R²=0.9989
AvCF %RSD=5.9
0
0.2
0.4
Concentration [mg/kg]

Sensitivity

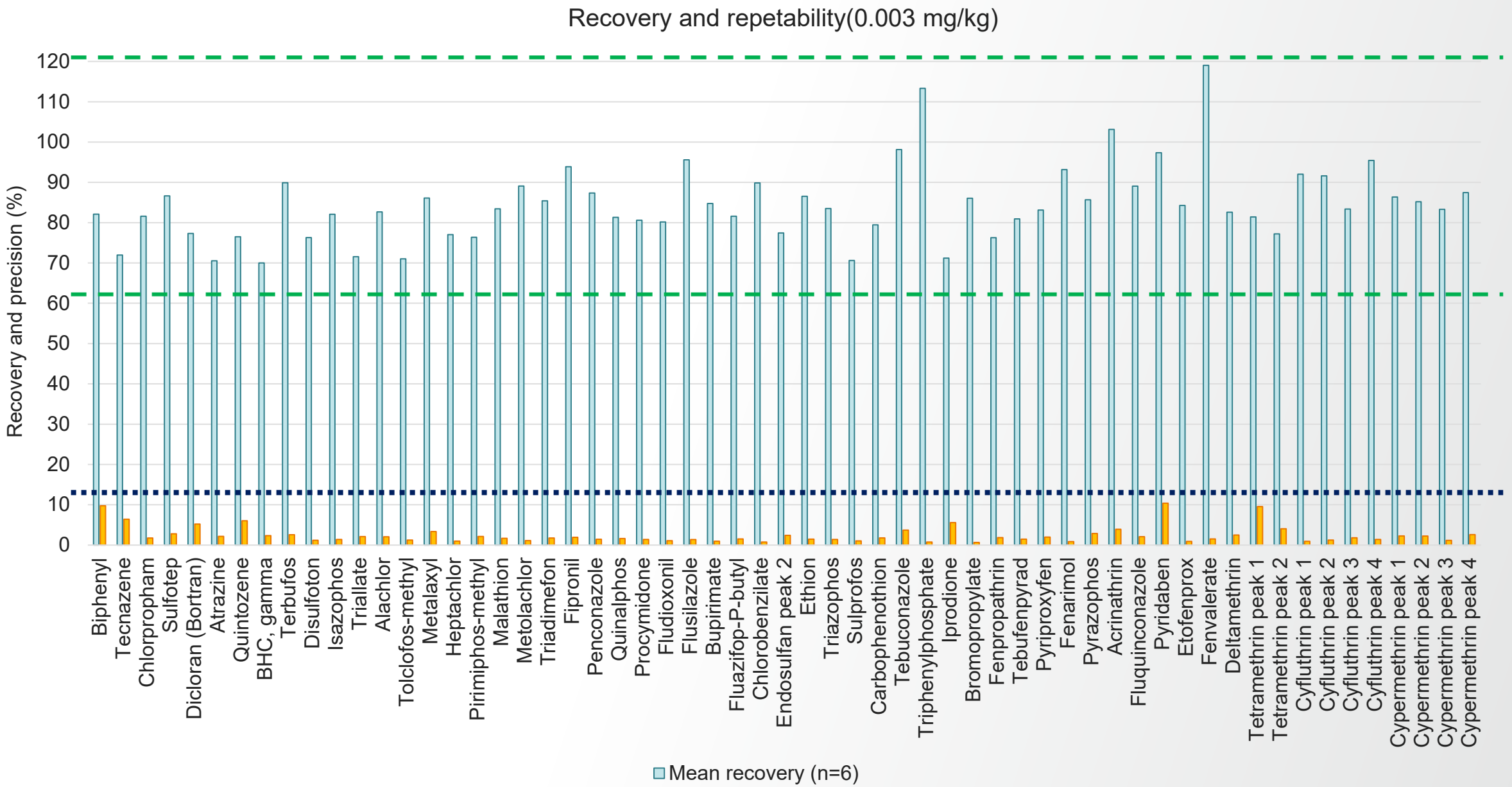
Pesticides at 0.00005 mg/kg (0.05 ppb)





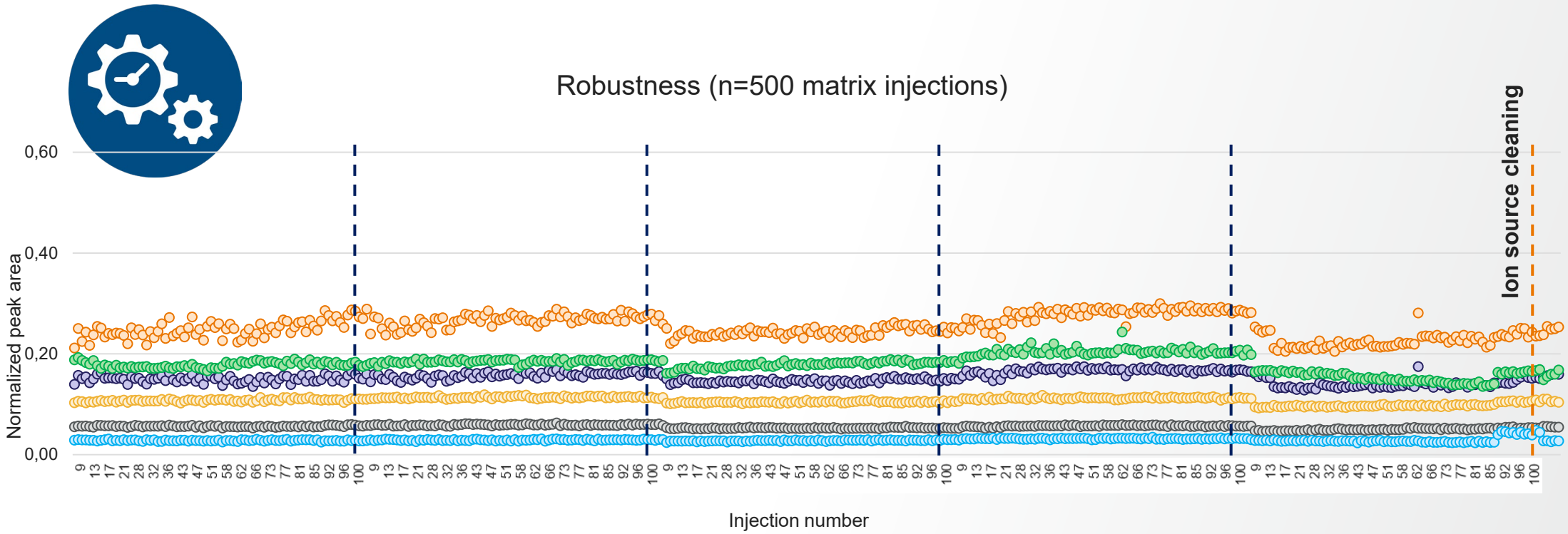


Recovery and precision in baby food



Increasing instrument uptime: Assessment of robustness

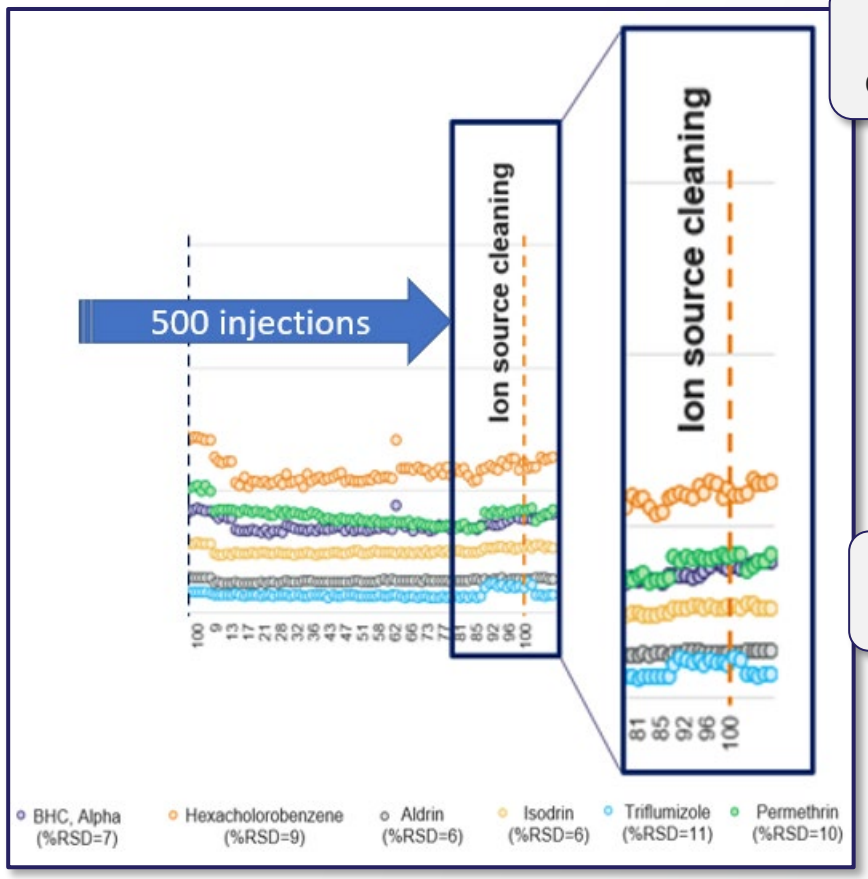
Consistent results at low levels



Increasing instrument uptime

Consistent results and NeverVent Technology

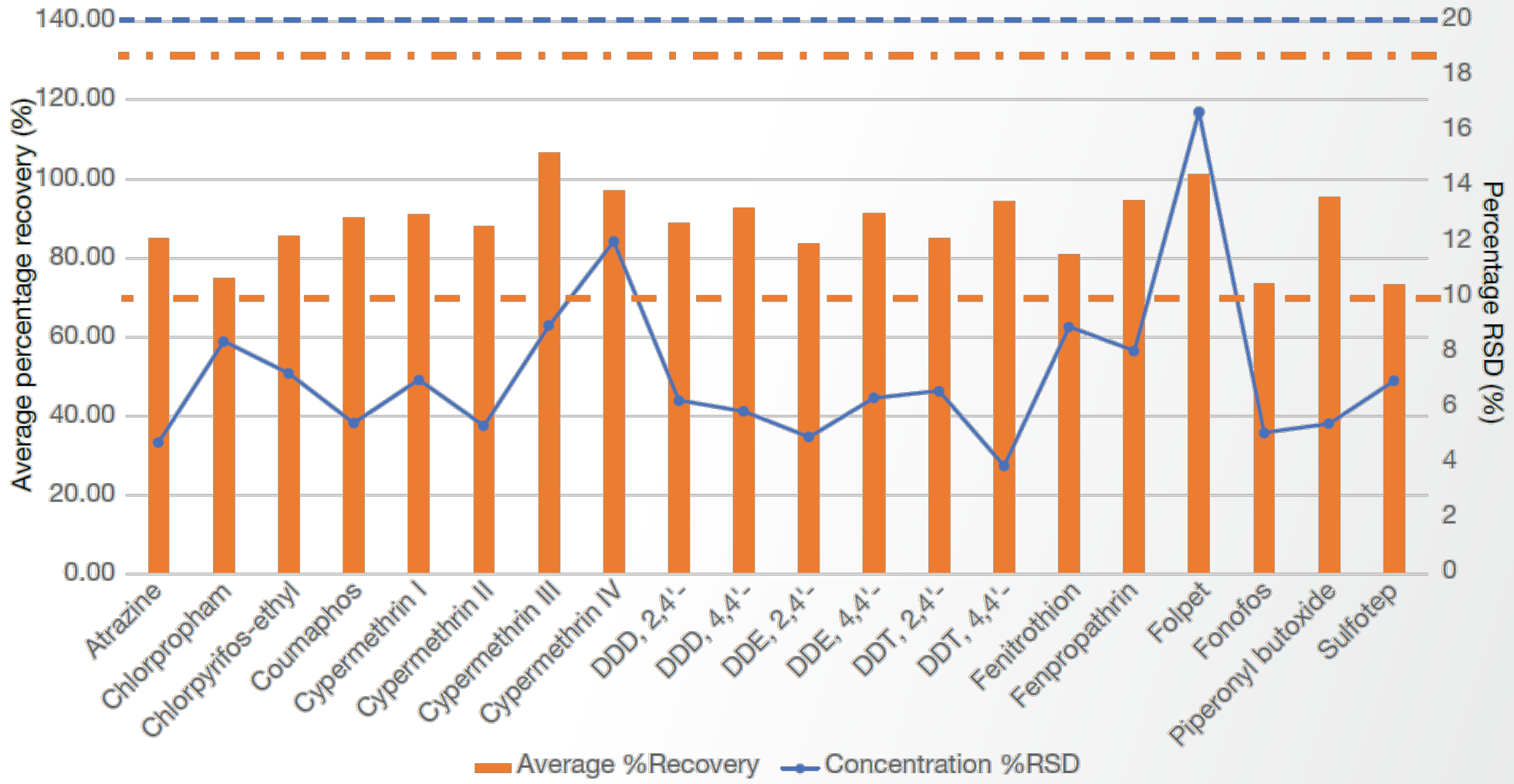
Even when maintenance is performed on the ionization source, the instrument produces consistent results at low levels



Maintenance performed to demonstrated stability after source clean

Instrument delivering consistent results again in under 2 hours

Recovery and precision in black tea

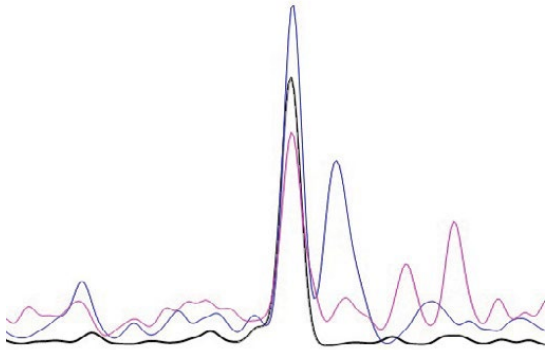


Recovery and precision in black tea

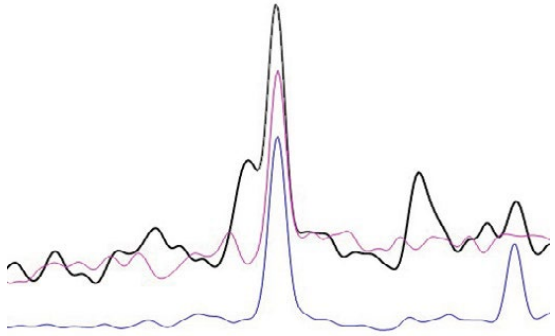
Compound	RSD [%]			Recover [%]		
	0.01 mg/kg (n=6)	0.25 mg/kg (n=6)	0.050 mg/kg (n=6)	0.01 mg/kg (n=6)	0.25 mg/kg (n=6)	0.050 mg/kg (n=6)
Atrazine	3.4	4.1	5.5	83.3	84.5	85.5
Chlorpropham	7.8	7.0	2.5	77.7	78.7	74.3
Chlorpyrifos-ethyl	4.7	6.0	3.5	84.0	78.9	81.5
Coumaphos	6.1	6.5	5.5	91.3	92.0	91.1
Cypermethrin I	8.0	3.4	4.1	92.9	91.5	91.3
Cypermethrin I	5.0	3.4	3.7	88.3	896	89.2
Cypermethrin I	9.7	4.1	3.6	101.2	91.6	90.7
Cypermethrin I	7.7	5.9	6.2	88.9	87.9	90.1
DDD, 2,4'-	3.4	5.0	2.2	93.3	91.8	91.3
DDD, 4,4'-	3.1	5.7	2.6	97.0	95.3	93.6
DDE, 2,4'-	3.8	4.7	2.2	86.1	83.4	81.6
DDE, 4,4'-	5.8	4.2	3.5	94.5	88.4	85.6
DDT, 2,4'-	3.8	4.4	3.8	89.6	90.2	87.6
DDT, 4,4'-	3.6	3.0	4.2	96.9	92.7	89.3
Fenitrothion	9.8	7.7	3.8	83.2	93.0	90.9
Fenpropathrin	6.0	7.5	5.0	99.1	92.2	92.6
Folpet	20.6	10.3	6.6	107.6	86.2	61.1
Fonofos	4.4	3.8	6.1	76.0	73.2	72.6
Piperonyl butoxide	4.8	3.6	4.3	98.5	95.7	95.0

Pesticides in black tea

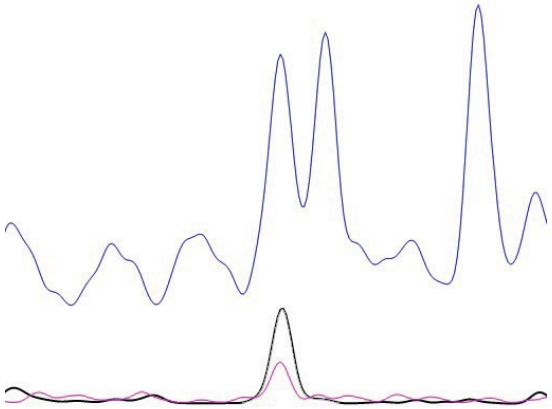
Chromatograms at 0.0005 mg/L (0.5 ppb)



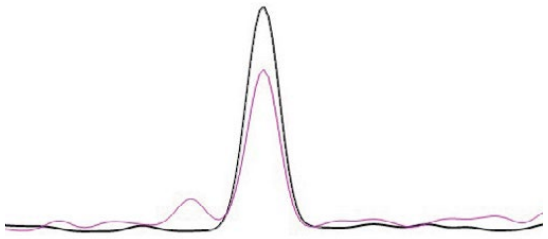
Atrazine



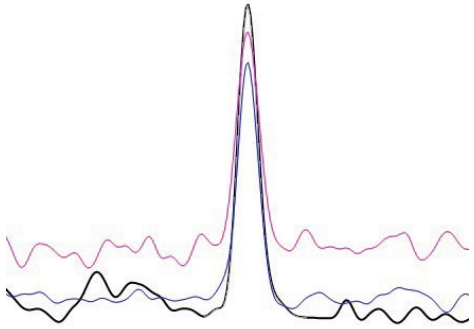
Chlorpopham



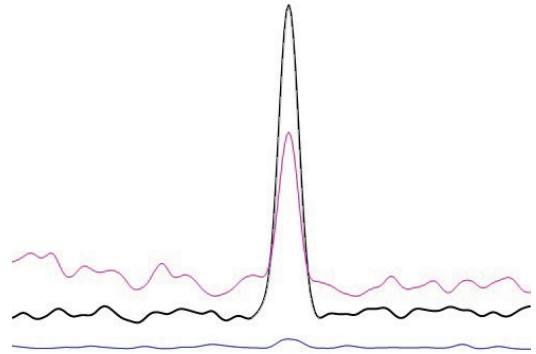
Chlorpyrifos-ethyl



Fonofos

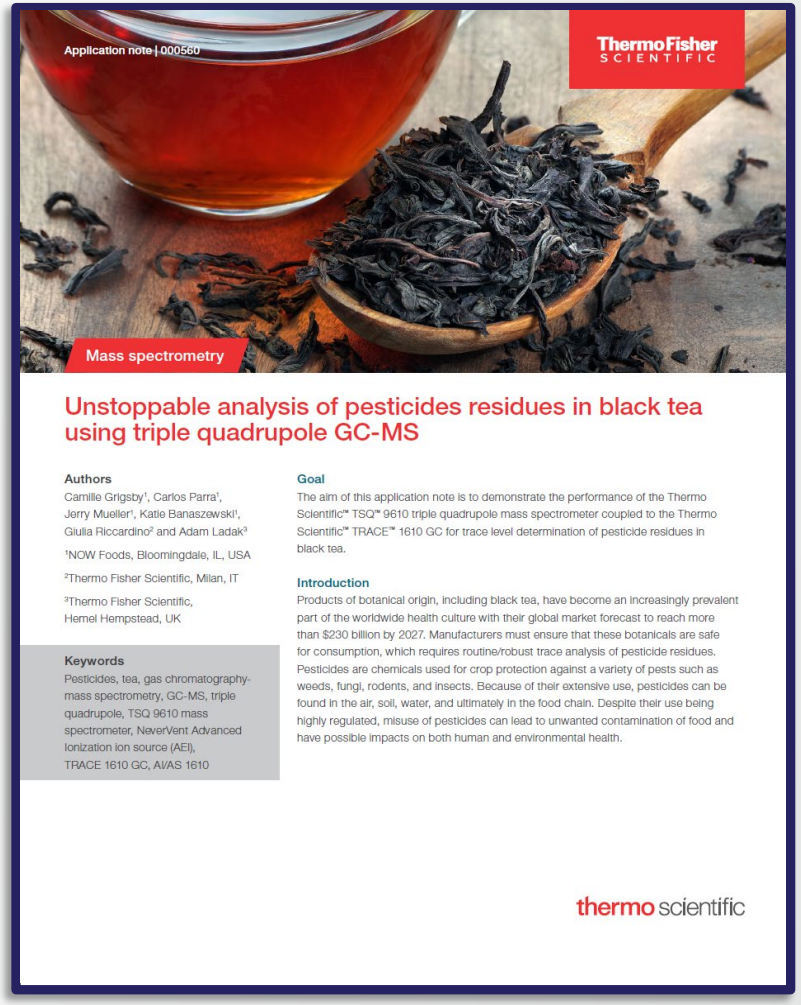


Piperonyl butoxide



DDT, 4,4’

Further information



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Thank you