
ThermoFisher SCIENTIFIC

# GC and GC/MS Q Exactive and applications

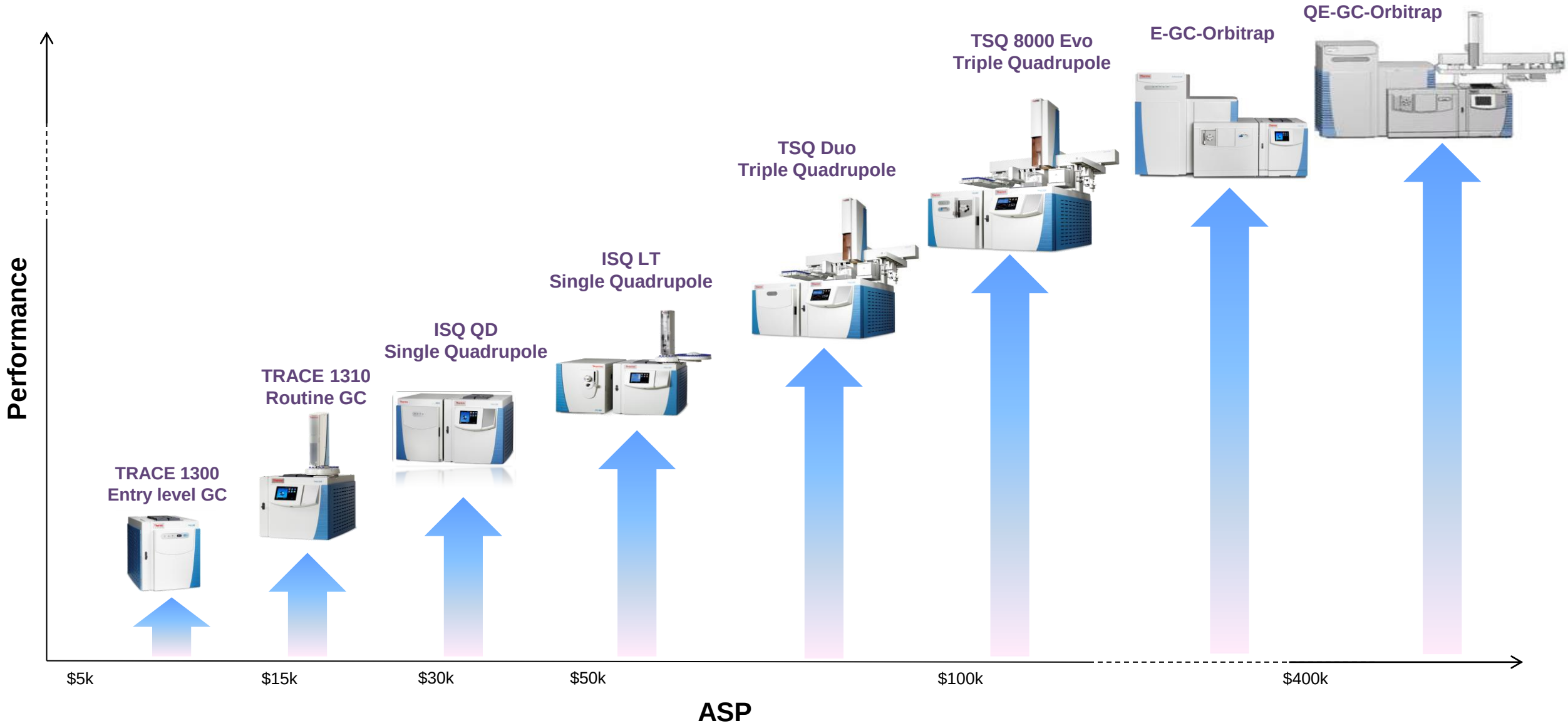
**Miloš Korman**
EMEA Sales Manager GC/GCMS

Sofia, October 22nd, 2016

# Agenda

- **GC&GCMS portfolio 2016**
  - Expanded GC/GCMS product offering
- **GC news for 2016**
  - Injectors & Detectors
- **GCMS ISQ news for 2016**
  - GC/GCMS Product Portfolio and Application
- **GCMSMS TSQ news for 2016**
  - Application in Tox & Forensic
- **QEGC Update**
- **Conclusion**

# GC & GC-MS Products portfolio






ThermoFisher SCIENTIFIC


ThermoFisher
SCIENTIFIC

# GC news for 2016

# TRACE 1300 Series GC – Two Models Available

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


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


**Modules available:**

**Injectors**: SSL - SSL backflush - PTV - PTV backflush - **TSI** - **OCI** - **Helium Saver SSL**[+]

**Detectors:** FID - TCD - ECD - NPD – **FPD** - **PDID** - MS*

**Other Options**: **MS NoVent, Auxiliary Oven,** Inj/Oven Cryo, Aux carrier

**Software drivers**: Chromeleon **6.8**, 7.1 and **7.2** CDS, Xcalibur, ChromQuest, ChromCard

Agilent™ **OpenLAB**™ EZChrom ed. CDS, Agilent **EZChrom**™ *(Agilent is a trademark of Agilent Corporation)*

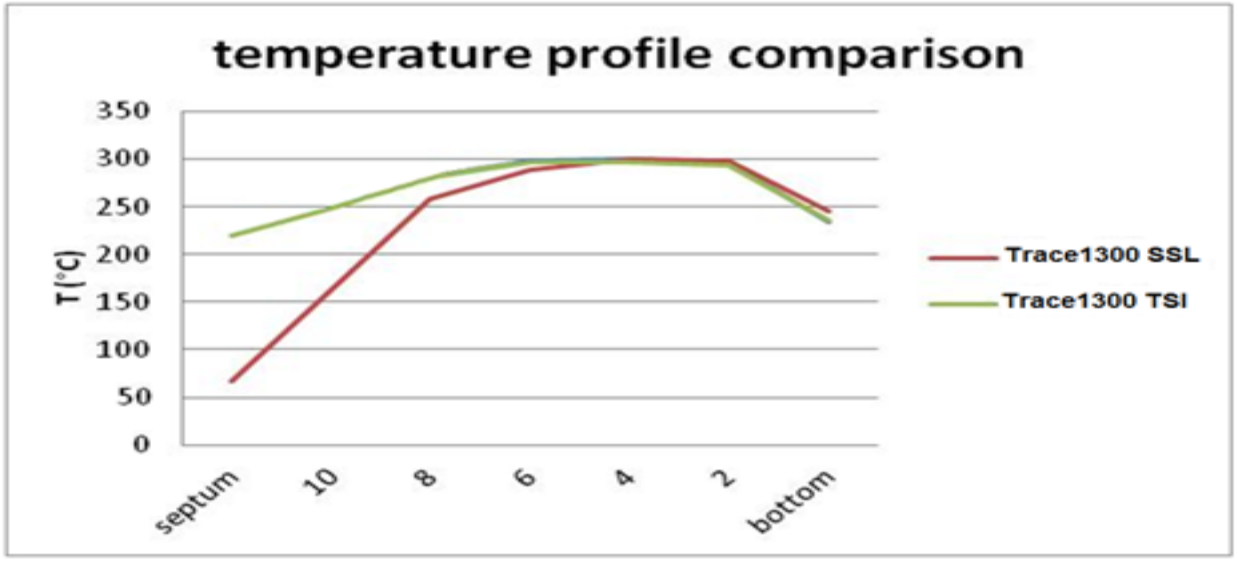
[+] **Newly Released Modules and Options**

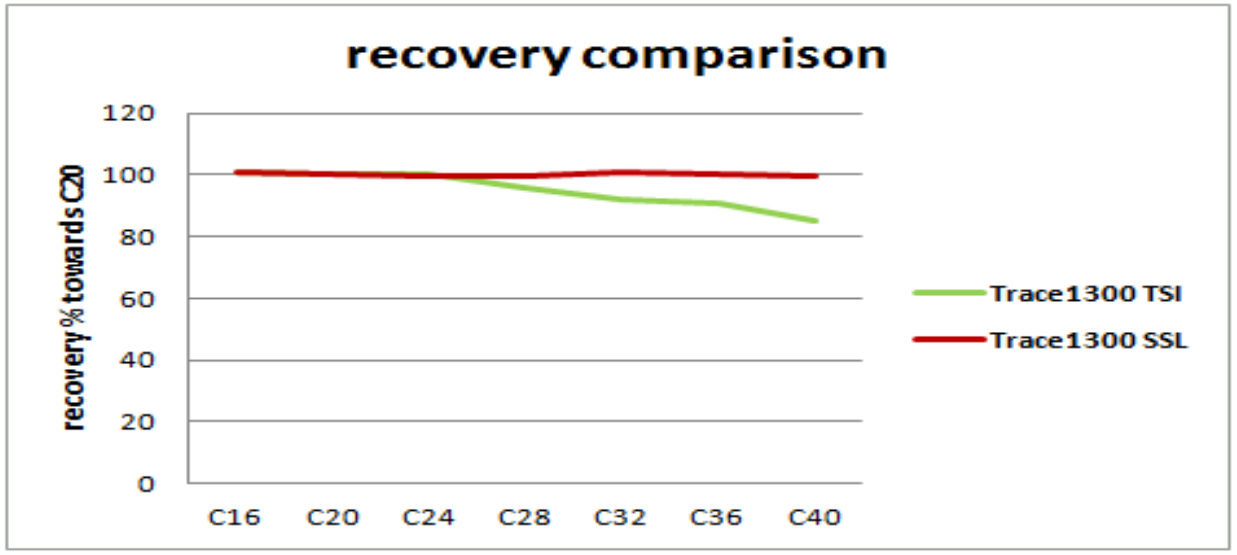
*Supported Thermo Scientific MS: ISQ ™ Series GC-MS; ITQ™GC-MS; TSQ Quantum XLS GC-MS/MS; DFS; Delta V


ThermoFisher
SCIENTIFIC

# Injectors update for 2016

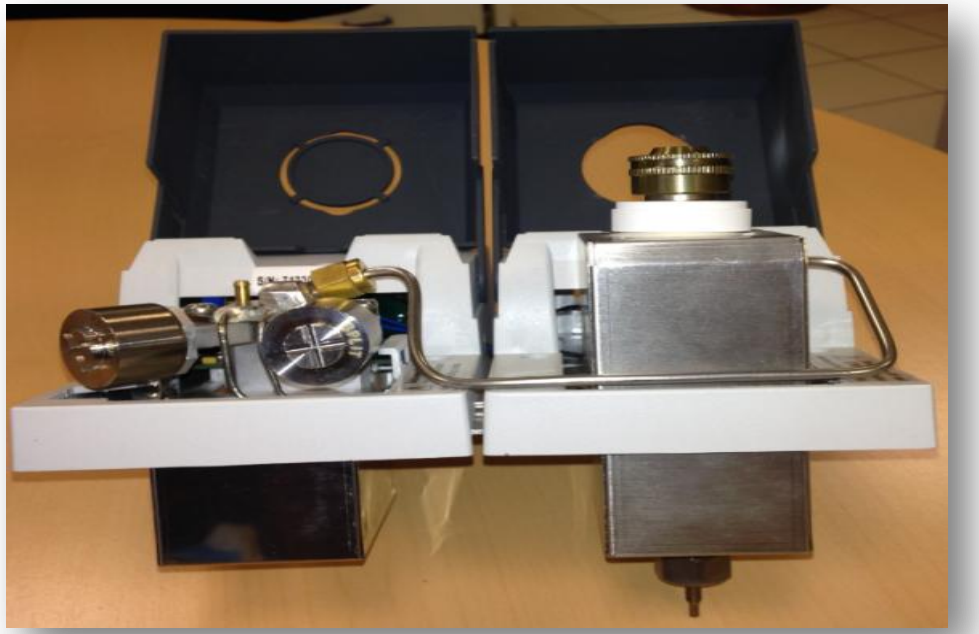
# What is iC-TSI= Instant Connect ThermoSpray Injector




| TRACE1300 SSL | TRACE1300 TSI |
|---|---|
| Cold head | Hot head |
| Liquid band injection | Thermospray injection |
| Needs fast injection | Suitable for “Hot Needle Injection” technique |
| Simple and easy to set up | Method transfer from TRACE Ultra GC |
| Not optimized for manual injection | Well performing with manual injection |
| Liner with glass wool required | Empty liner is used |
| Agilent like SSL injector | Required for specific applications |

# i-TSI module



**p/n 19070016** TRACE 1300/1310 TSI MODULE

It occupies two injector slots onto the Trace1300 GC Series

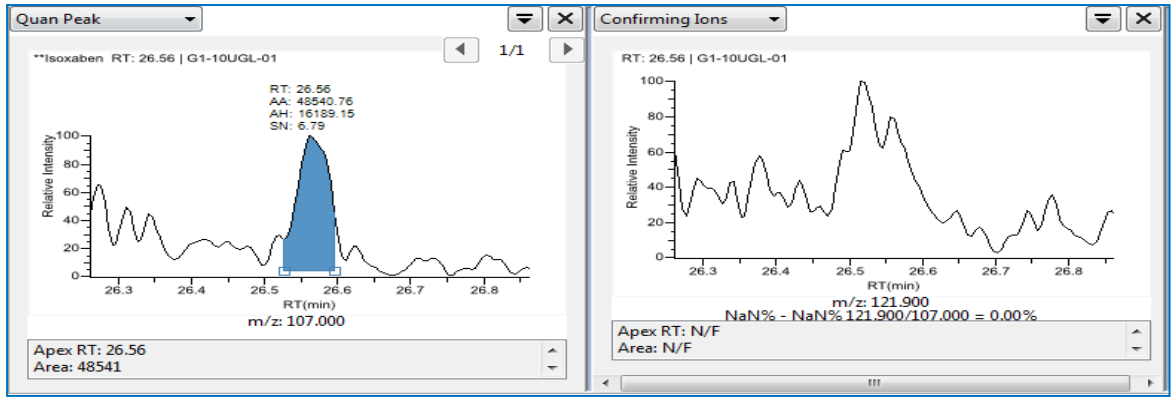
# Some of the challenging pesticides…

- ✓ Azole family (aim to tail in injector/T-line)
  - Azaconazole
  - Bitertanol
  - Bromuconazole
- ✓ Pyrethrinoids (always difficult)
  - Deltamethrine
  - Cyhalothrines
- ✓ OrganoChlorine compounds
  - Endosulfan sulfate
- ✓ Uracyl herbicide
  - Bromacil (difficult detection)
- ✓ Organophosphorus compounds (sensitive to injector activity)
  - Dichlorvos
  - Vamidothion
  - Demethon S methyl Sulfone
  - Dimethoate
- ✓ Phenyl sulfamide insecticides
  - Tolyfluanide
- ✓ Benzamide herbicides family
  - Isoxaben (sensitive to column, T-line…)

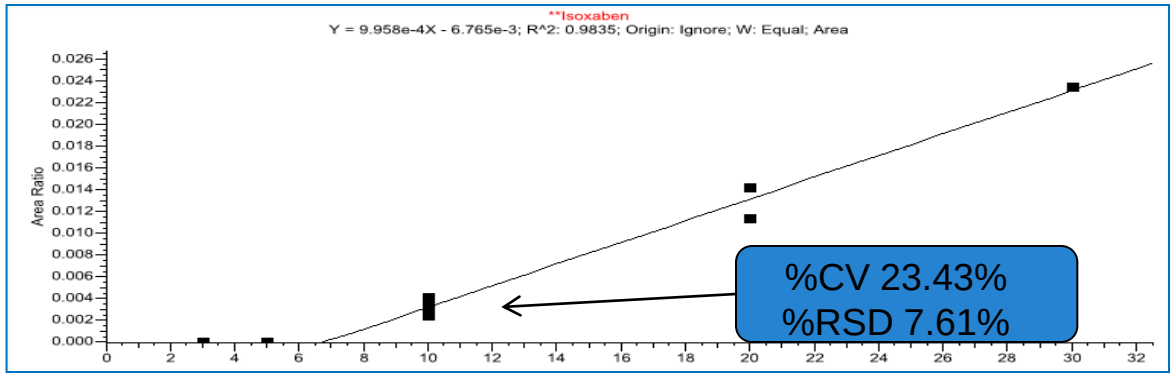
# Isoxaben

## i-SSL

Signal @**10**µg/L



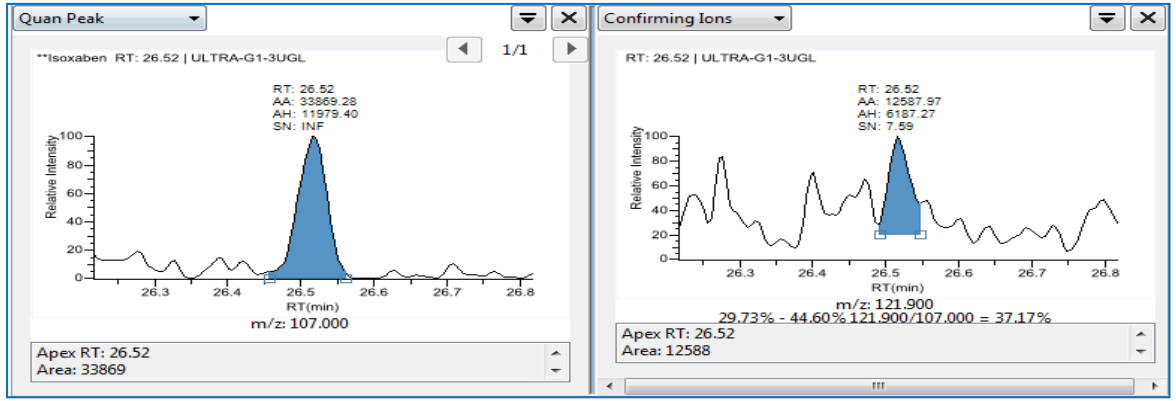

Linearity from 10pg to 30pg



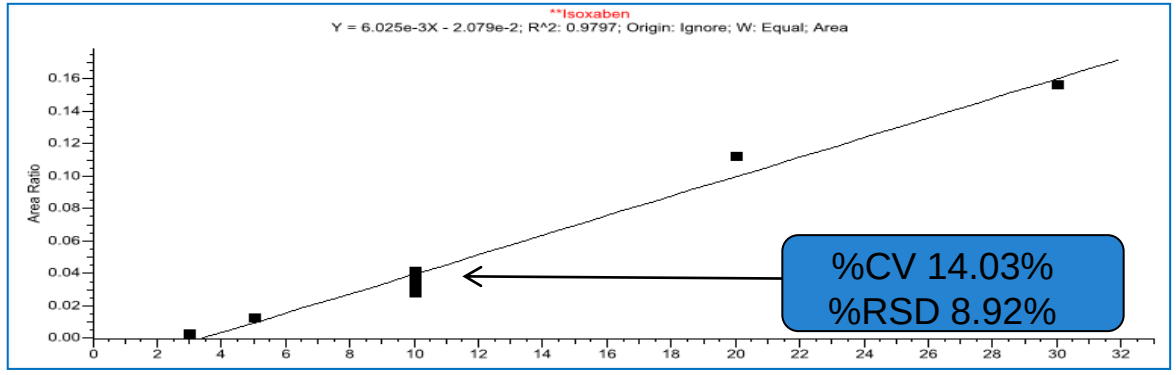

5 replicates @10µg/L

## i-TSI

Signal @**3**µg/L




Linearity from 3pg to 30pg




5 replicates @10µg/L

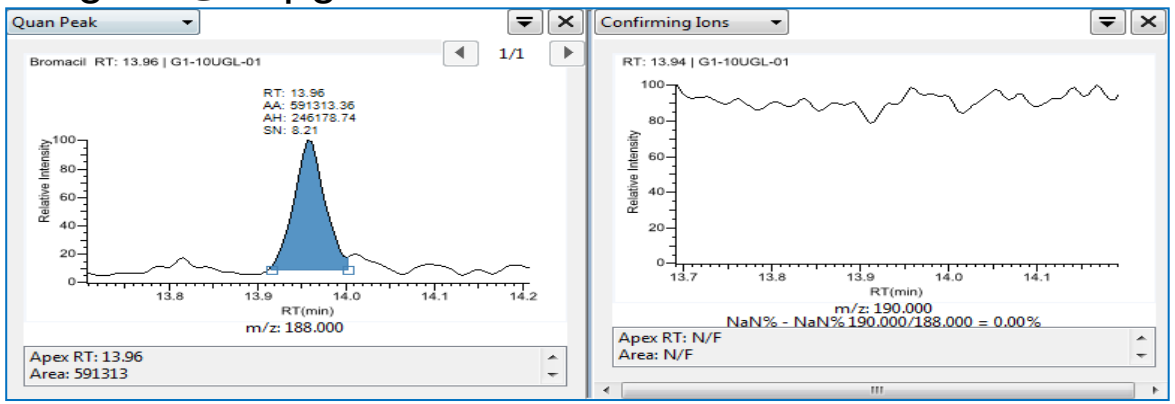


ThermoFisher SCIENTIFIC

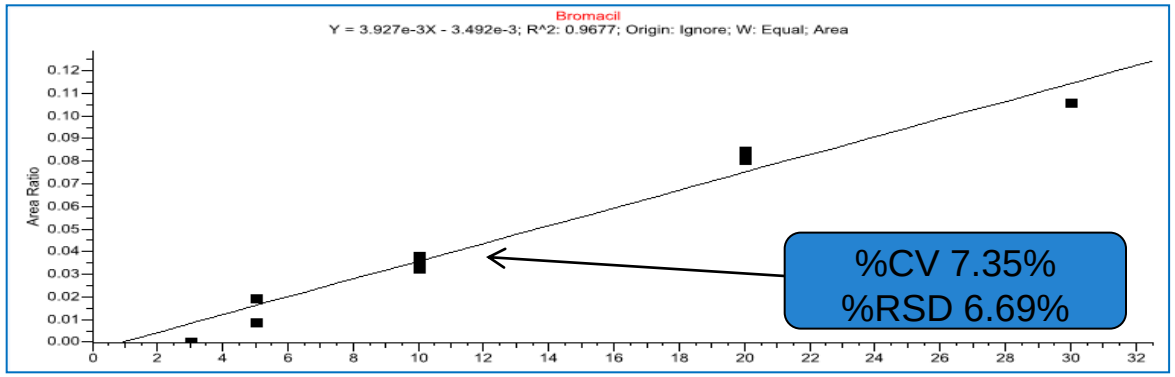
# Bromacil

i-SSL

Signal @10µg/L



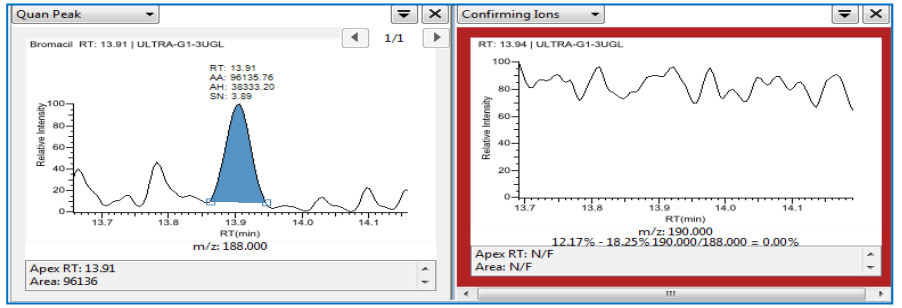

Linearity from 3pg to 30pg



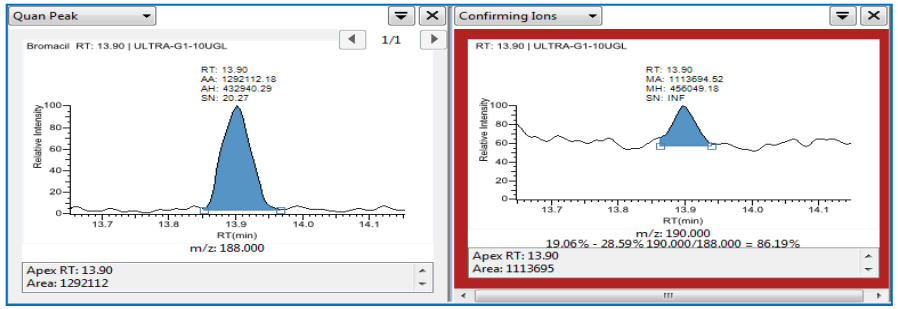

5 replicates @10µg/L

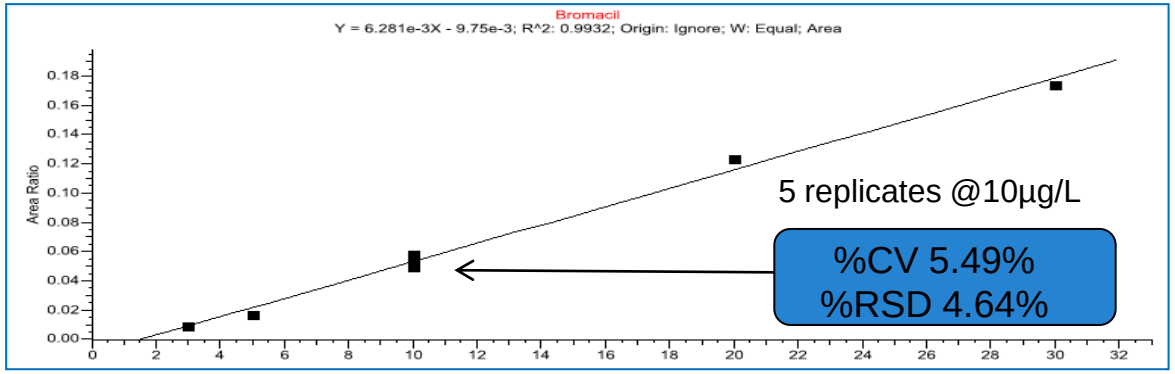
i-TSI

Signal @3µg/L




Signal @10µg/L



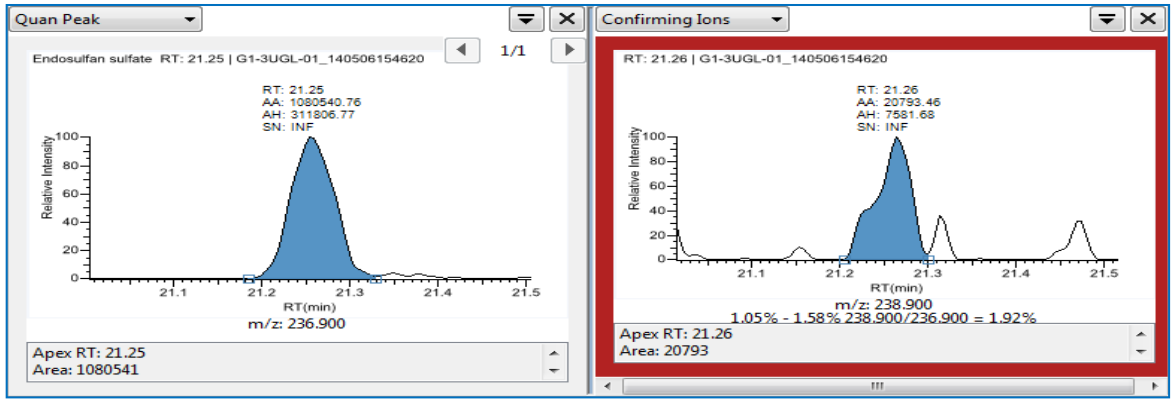



ThermoFisher SCIENTIFIC

# Endosulfan sulfate

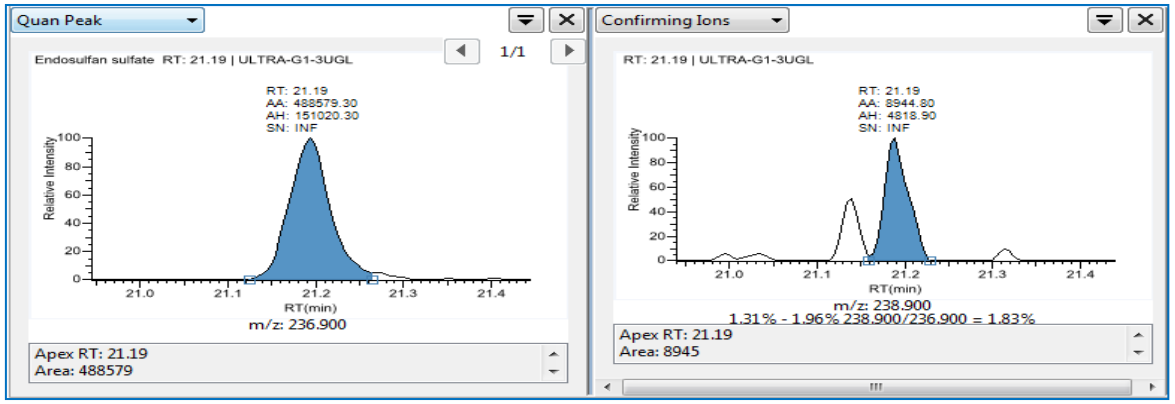
i-SSL

Signal @3µg/L

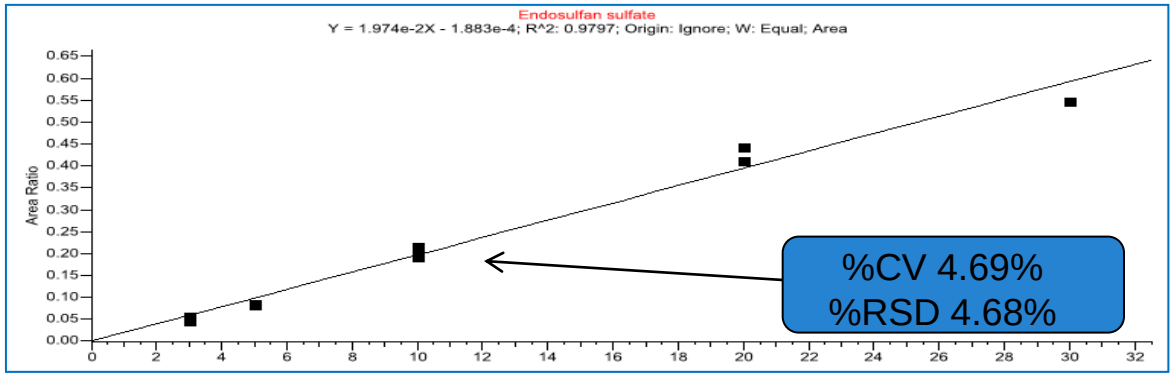



i-TSI

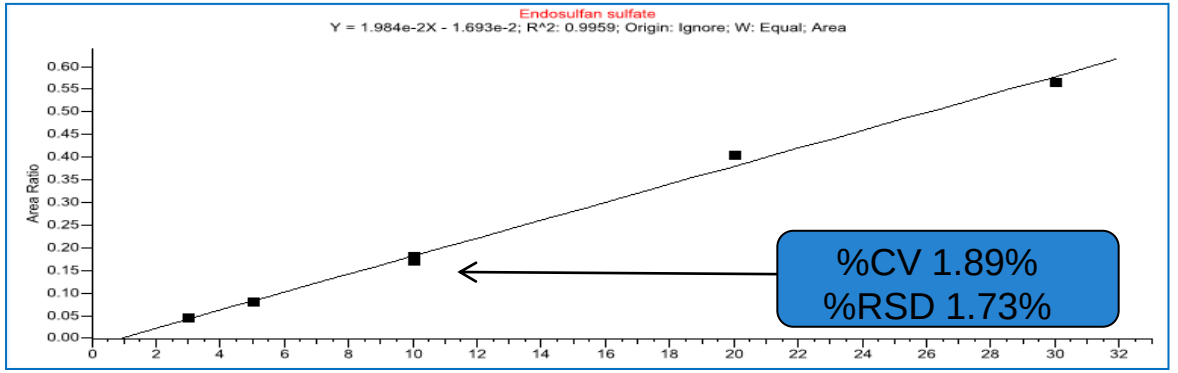
Signal @3µg/L




Linearity from 3pg to 30pg




5 replicates @10µg/L




5 replicates @10µg/L



ThermoFisher SCIENTIFIC

# When  i-TSI is the right solution?

Looking at limit of detection, SN, area, %CV at 10pg and linearity we can observe that :

- ✓i-TIS is a clearly better with improved limit of detection
  - ✓Isoxaben
  - ✓Vamidothion
  - ✓Bromacil

- ✓i-TIS is slightly better with higher SN
  - ✓Endosulfan sulfate
  - ✓Bitertanol
  - ✓Cyfluthrines
  - ✓Deltamethrines
  - ✓tolyfluanid
- ✓i-SSL and i-TIS are as excellent in matter of other Pesticides, detection, linearity and repeatability
- ✓Thermospray injection can be advantageous with some critical compounds particularly prone to thermal degradation

# iC-OCI: Instant Connect On-column Injector module

iC-OCI inlet

- ✓ Based on the Carlo Erba cold on-column injector
- ✓ Merlin Microseal septum for low maintenance
- ✓ Continuous cooling of the injector body thanks to the integrated fan
- ✓ Pre-column secondary cooling
- ✓ Compatible with manual injection and Triplus RSH autosampler
- ✓ Two OCI modules can be mounted by using 1 set of Aux Modules

# iC-OCI: Instant Connect On-column Injector module

## How to order:

Auxiliary Gas Module

Aux Temperature/Cryo Module


| | | |
|---|---|---|
| **p/n 19071065** | **iC-OCI Module kit** | *Includes the Merlin Microseal 26s, the solenoid valve for secondary cooling with mounting bracket, tubing* |
| **p/n 19070080** | **Aux Carrier Gas Module** | *For Carrier Gas supply and control* |
| **p/n 19070070** | **Aux Temp Module** | *For the timed actuating of the secondary cooling* |

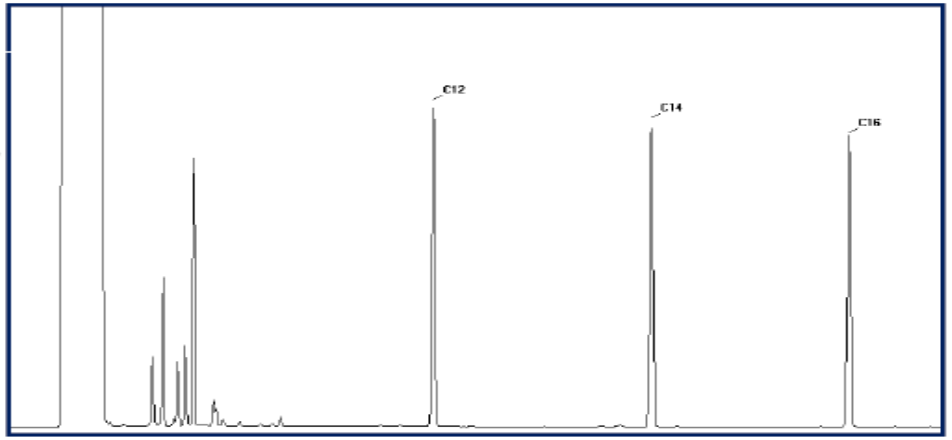
# iC-OCI: the right solution

- ✓ Thermolabile compounds → PBDE 209
- ✓ Very high boilers → triglycerides, HT SimDist
- ✓ Wide boiling point range
- ✓ When an alternative to the PTV injector is required
- ✓ When sample does not include no-elutable by-products (clean sample extract)

| Inj. | C12 | C14 | C16 |
|---|---|---|---|
| 1 | 1729812 | 1718526 | 1700241 |
| 2 | 1736398 | 1721253 | 1703718 |
| 3 | 1730131 | 1717829 | 1699899 |
| 4 | 1741246 | 1726306 | 1708989 |
| 5 | 1744551 | 1728775 | 1710122 |
| 6 | 1746308 | 1731325 | 1713732 |
| 7 | 1751230 | 1731861 | 1717433 |
| 8 | 1740056 | 1725927 | 1707828 |
| 9 | 1750468 | 1735191 | 1717330 |
| 10 | 1744906 | 1729495 | 1709880 |
| | | | |
| Average | 1741510 | 1726649 | 1708917 |
| Stdev | 7551 | 5851 | 6269 |
| RSD % | 0,43% | 0,34% | 0,37% |

## Benefits

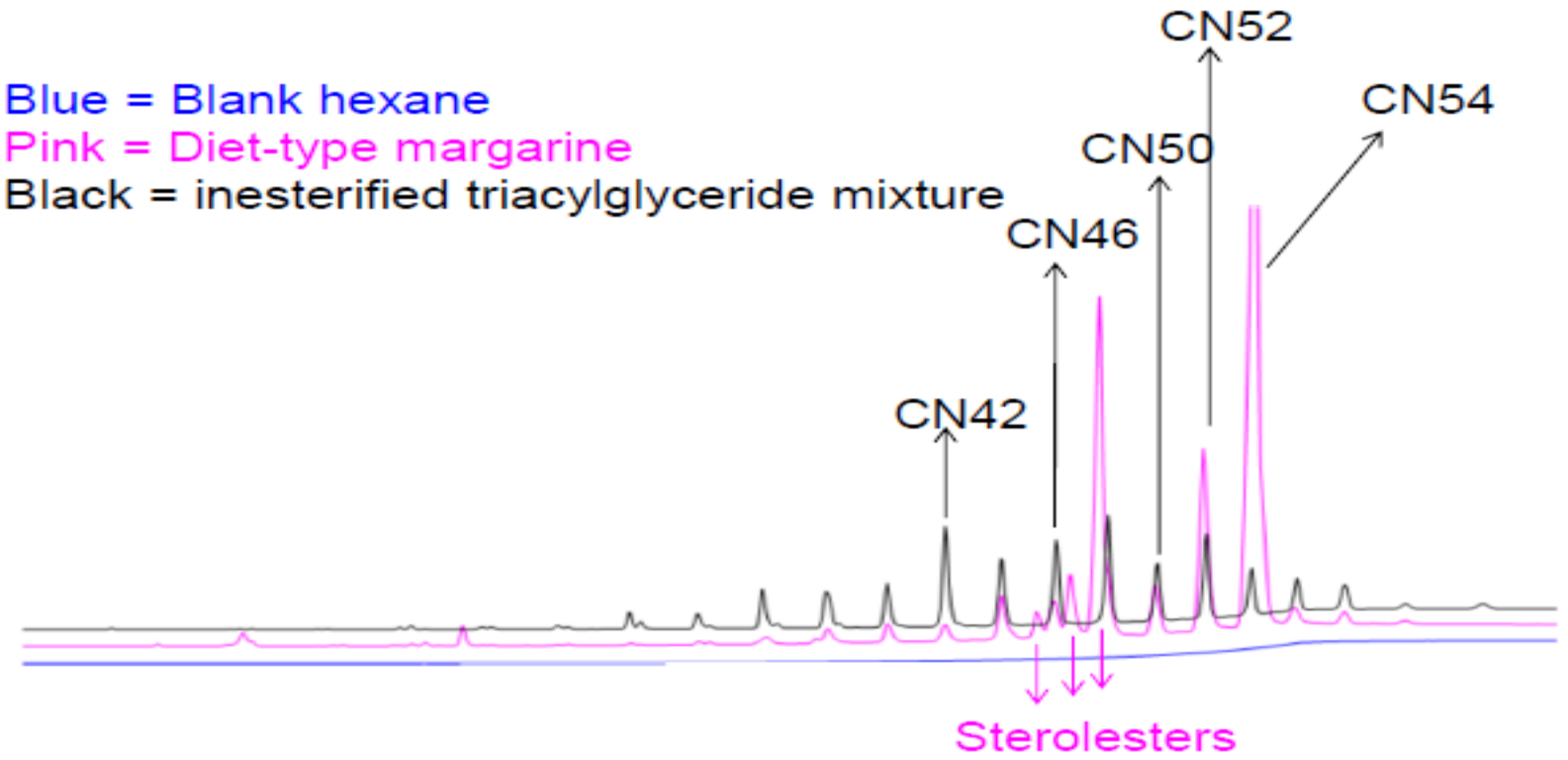
- ✓ True cold injection → no thermal breakdown
- ✓ Direct injection into the column → no discrimination
- ✓ Sensitivity → splitless and LV injection
- ✓ Excellent injection repeatability < 0.5% RSD






ThermoFisher SCIENTIFIC

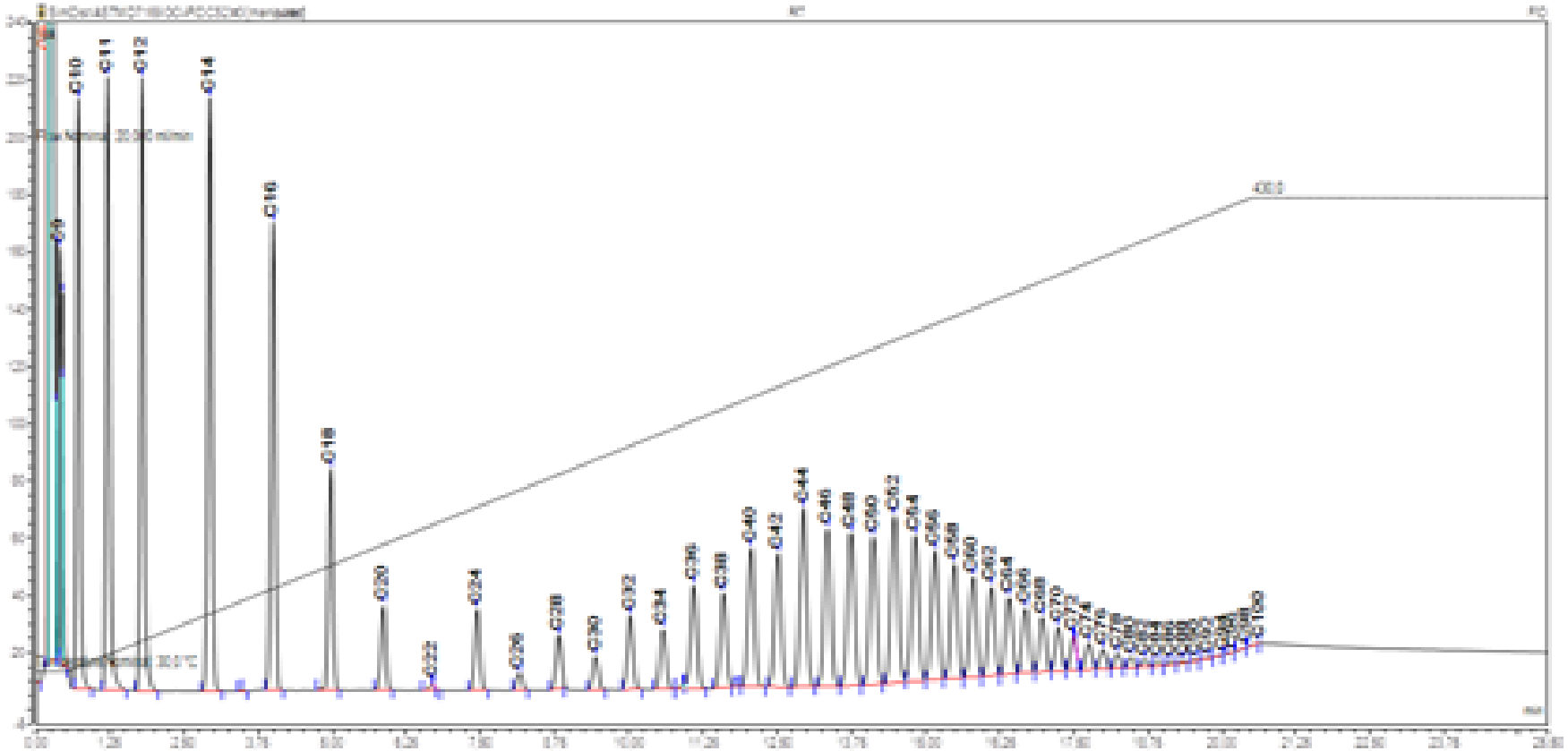
## Triglycerides




*CN54 = Tri-C18, glycerol backbone with three C18 fatty acids attached.*

# iC-OCI: the right solution

## HT SimDist





ThermoFisher SCIENTIFIC


ThermoFisher
SCIENTIFIC

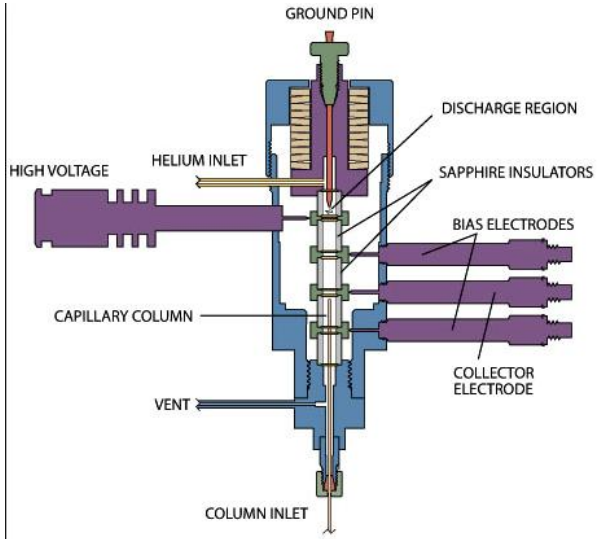
# Detectors update for 2016

# Instant Connect FPD detector

- Available as Instant Connect module, can be mounted on any existing TRACE 1300 Series GC
- Highest sensitivity for the determination of Sulfur, Phosphorous and Tin containing species
- Acquisition rate up to 300 Hz
- Available, as option, as dual wavelength option with two FPD independent Instant Connect modules

# iC-PDD Pulse discharge detector

- Alternative to universal detector for ppb concentration range
- Engineered solutions (eg. specialty gases)
- Alternative for ECD if radioactive source is not suitable
- Replacement for FID, PID specifically required for the low detectability range



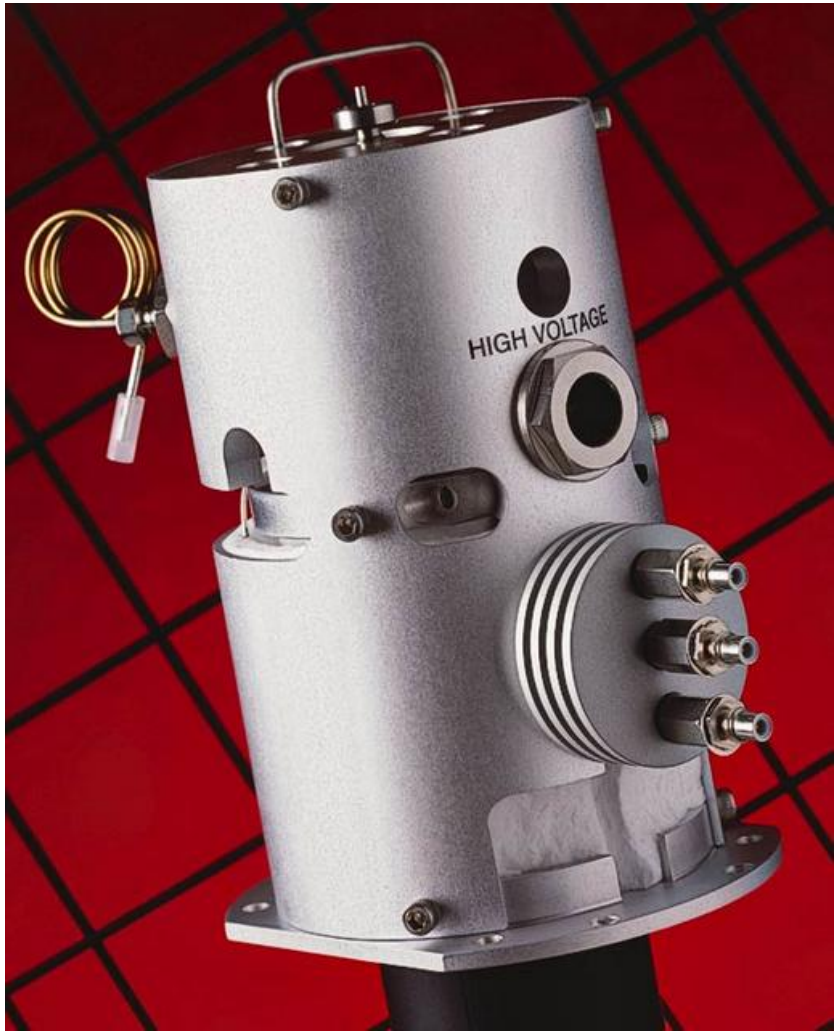

Instant Connect Pulsed Discharge Detector (PDD) for TRACE™ 1300 GC Series



ThermoFisher SCIENTIFIC

# PDD minimum detectable amounts

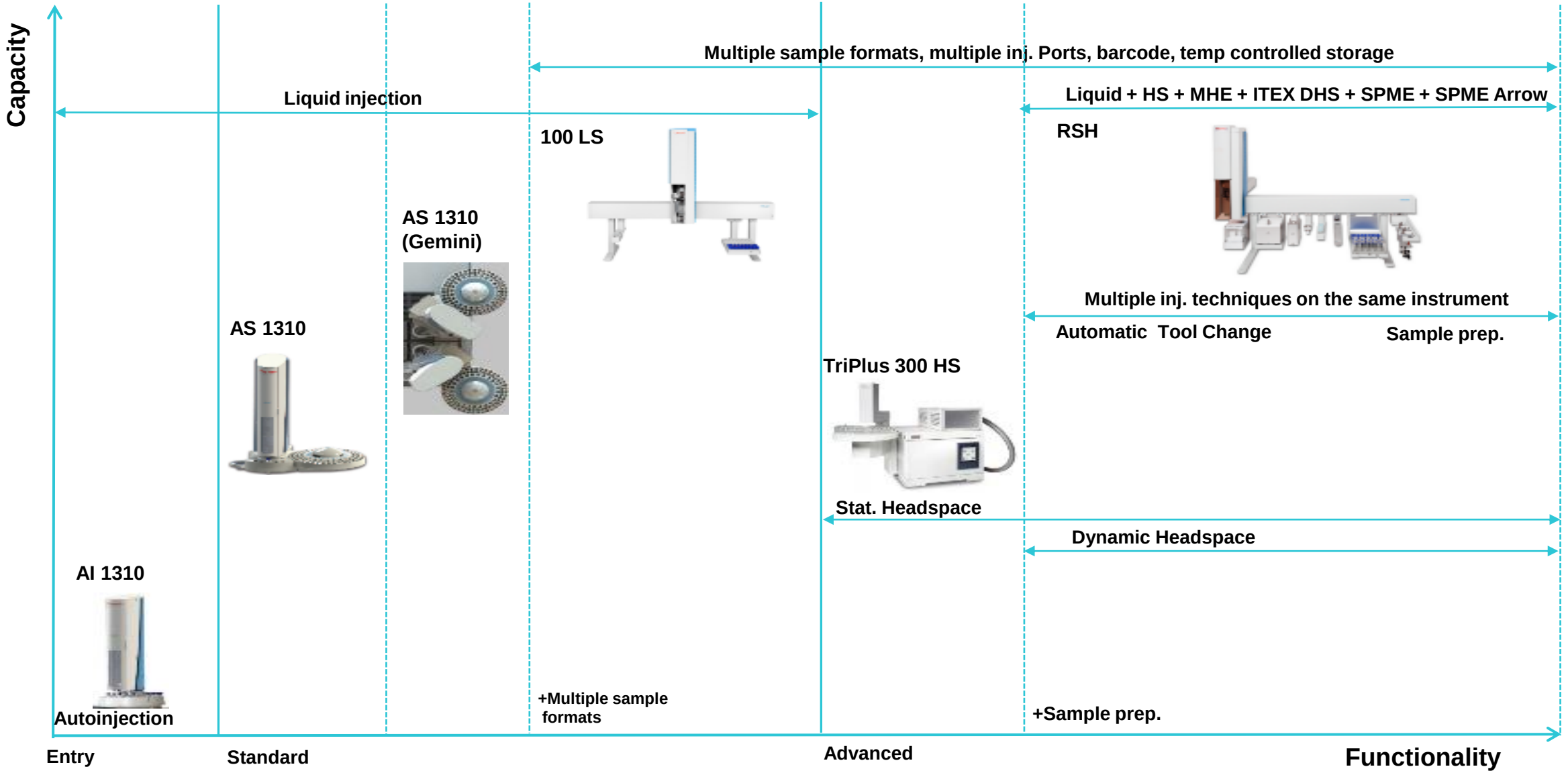
| MDQ S/N=3<br>*Sample injected 250uL, 1/10 split ratio* | | |
|---|---|---|
| ***compound*** | ***pg*** | ***ppb (v/v)*** |
| Carbon dioxide | 0,9 | 30 |
| Carbon monoxide | 4 | 150 |
| Nitrous oxide | 0,9 | 30 |
| Methane | 0,6 | 20 |
| Acethylene | 1 | 40 |
| Ethylene | 0,7 | 25 |
| Ethane | 0,7 | 25 |




ThermoFisher
SCIENTIFIC

# Autosamplers update for 2016

# Thermo GC Autosamplers Lineup






ThermoFisher SCIENTIFIC

# Solvent-free extraction of volatiles

*No enrichment of volatiles*

- Static Headspace Sampling (SHS)

*With enrichment of volatiles on adsorbent material*

- Purge&Trap (P&T)
- Solid Phase Micro Extraction (SPME, MEPS)
- Stir Bar Sorptive Extraction (SBSE)
- Headspace Sorptive Extraction (HSSE)
- Dynamic Headspace Sampling (DHS, ITEX)
- Thermal Desorber (TD)

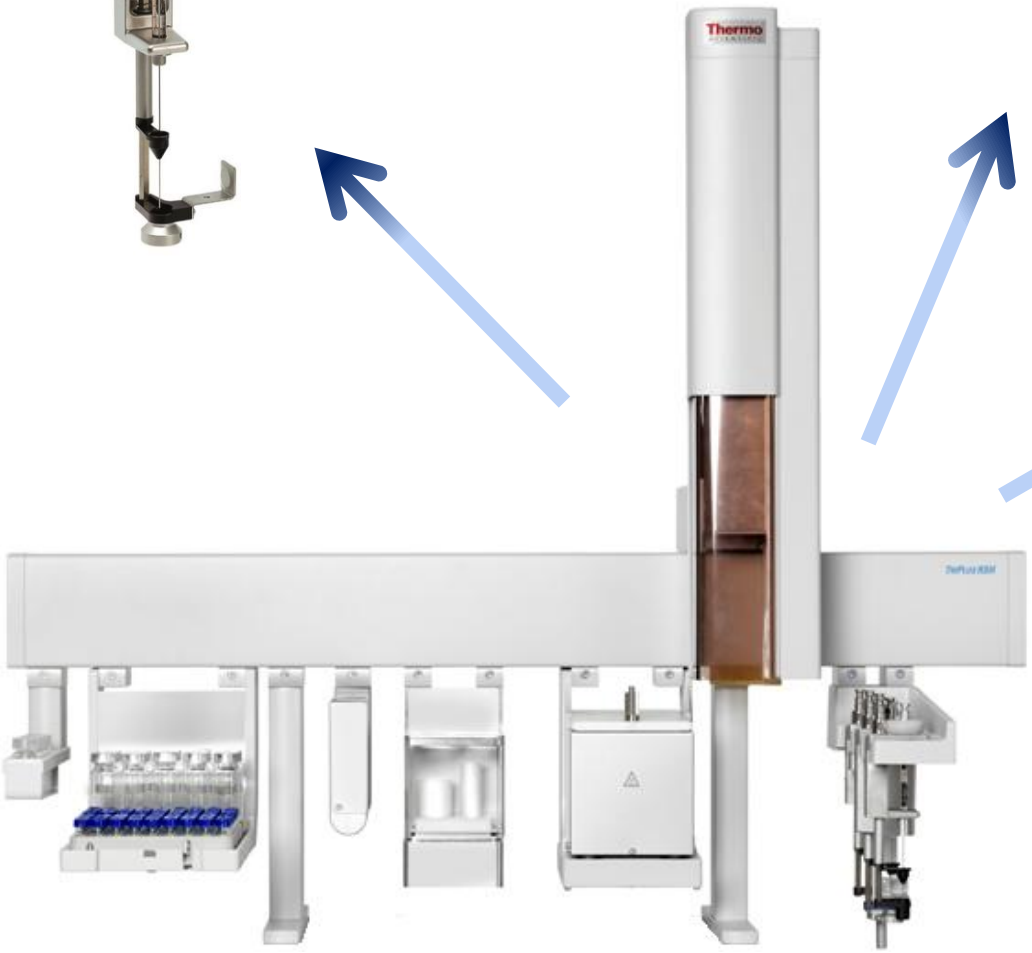
# Triplus RSH expanded options for VOC and SVOC market

Liquid

Static Headspace

ITEX- Dynamic Headspace

SPME

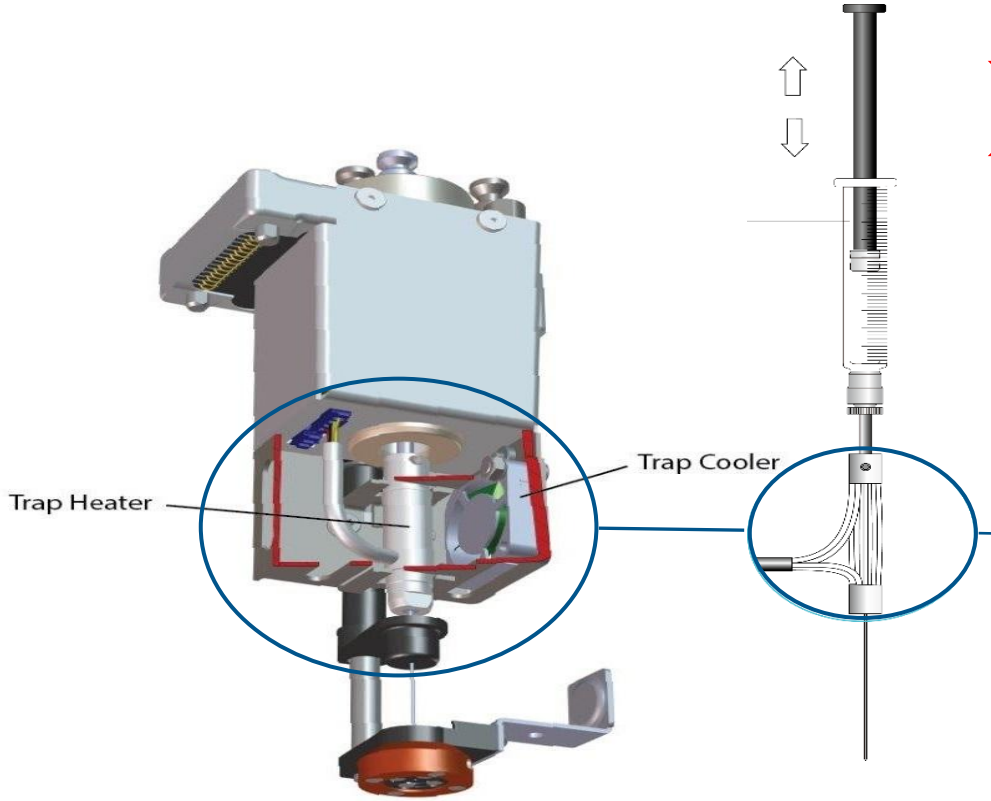





ThermoFisher SCIENTIFIC

# ITEX Dynamic Headspace

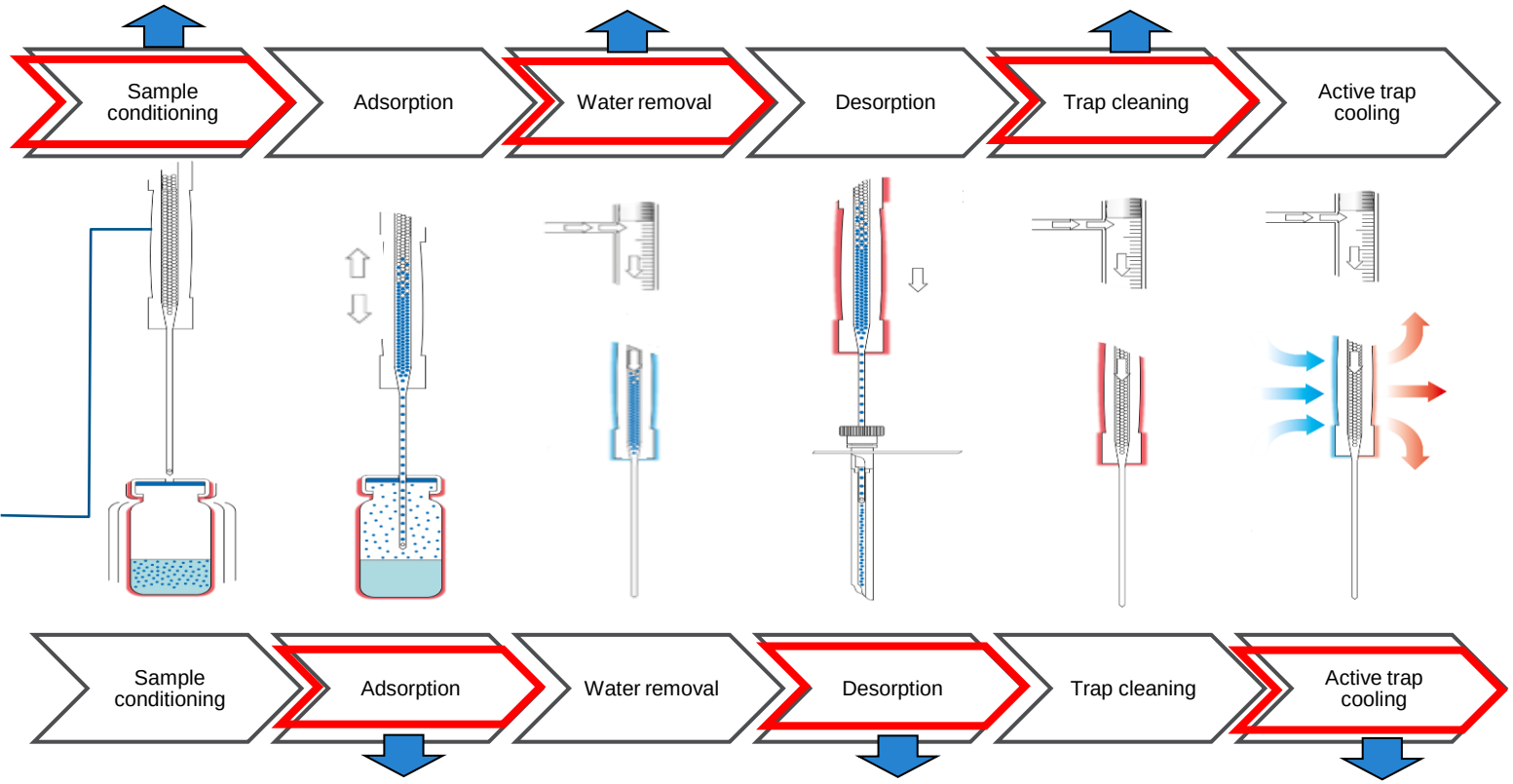
- ITEX Workflow




Sample is heated and / or agitated in a sealed sample vial

An optional step of water removal is achieved by flushing the trap with inert gas at low temperature

After thermal desorption the hot ITEX Trap is cleaned with inert flush gas




The ITEX Trap needle pierces the sealed sample vial and the heated gas tight syringe pumps with repeated strokes the gas phase through the ITEX Trap

The loaded ITEX Trap is flash heated up to 350°C and desorbed into the hot GC Injector

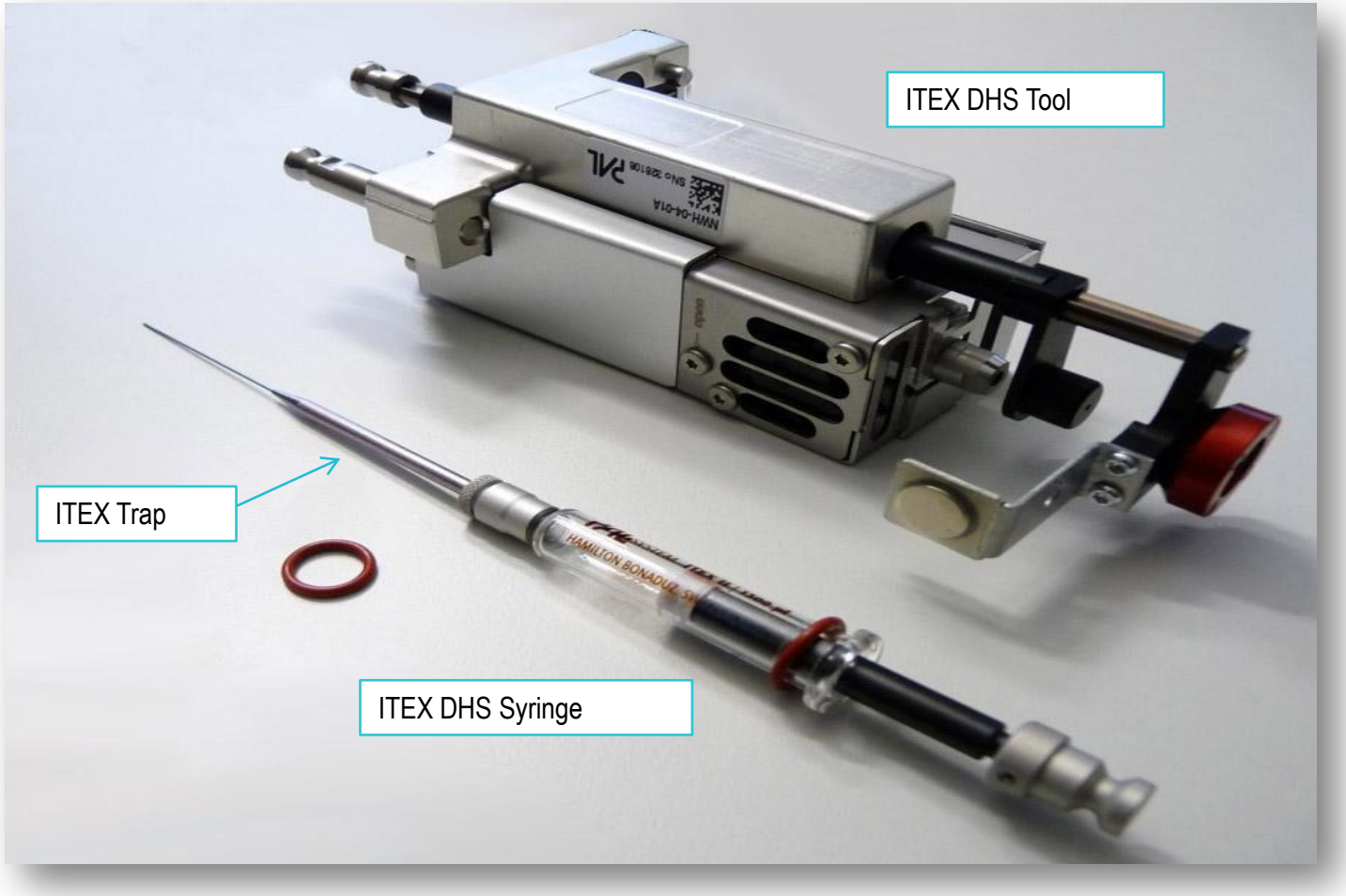
Active cooling allows short cycle times



ThermoFisher SCIENTIFIC

# ITEX Dynamic Headspace

## *.....Simplicity and handiness*



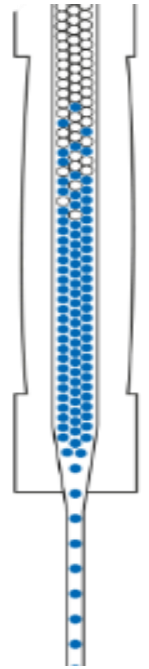

- Easy sample handling
- No loop, transfer line, or switching valve
- Easy access to the trap and syringe
- Straightforward troubleshooting and maintenance
- Minimum instrument downtime



ThermoFisher SCIENTIFIC

## Proven industry standard adsorbents

- Standard ITEX DHS adsorbent:
  - Tenax TA 80/100 mesh (volatile and semivolatile compounds)
- Additional ITEX DHS adsorbents:
  - Carbopack C, 80/100 mesh
  - Carboxen 1000, 60/80 mesh
  - Carbosieve S III, 60/80 mesh
  - Tenax GR, 80/100 mesh
  - Tenax GR, 80/100 mesh / Carbosieve S III, 60/80 mesh



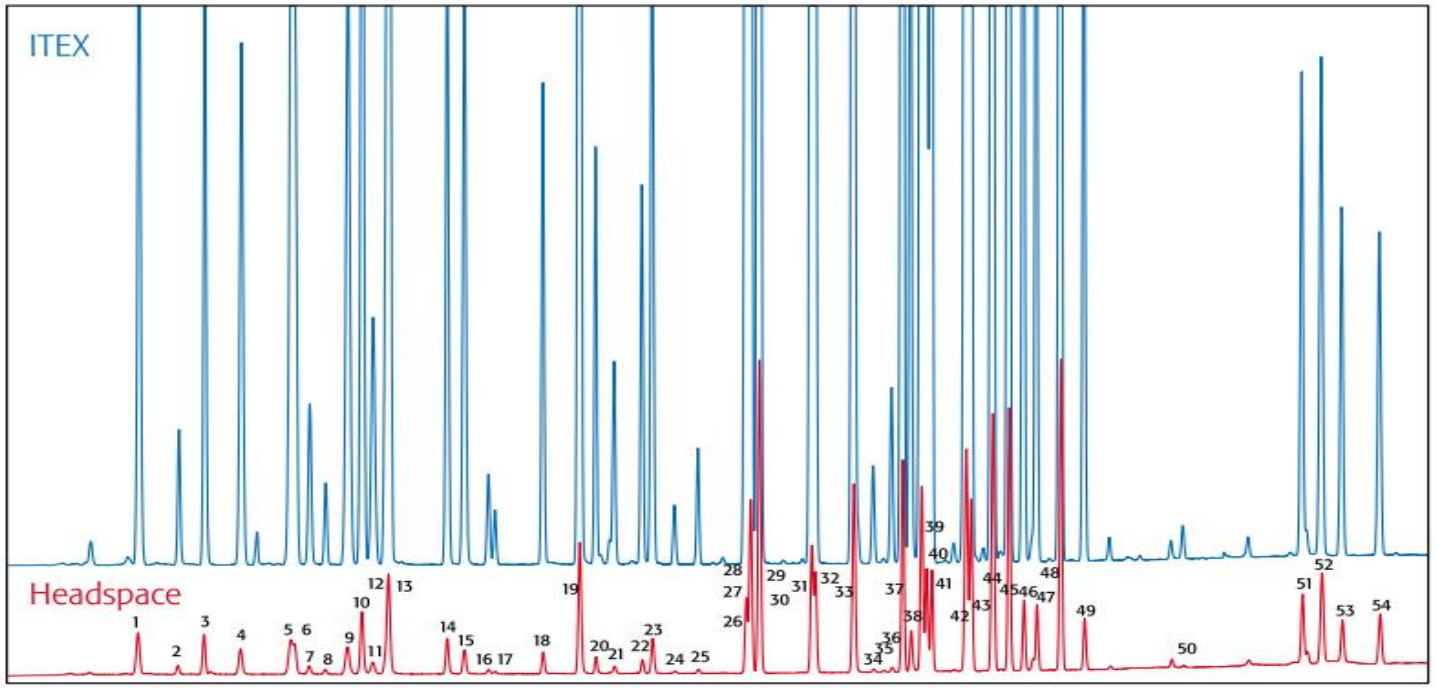
***SUGGESTED APPLICATIONS:***

| | |
|---|---|
| Tenax TA: | Volatile and semivolatile compounds, temperature limit of 350°C |
| Carbopack: | Hydrophobic properties minimized sample displacement by water |
| Carbosieve/Carboxen: | For very volatile compounds, e.g. Vinylchloride, Freon compounds |

Reference: **Optimization strategies of in-tube extraction (ITEX) methods**
*J. Laaks et al. Anal Bioanal Chem (2015) 4017:6827-6838*

# TriPlus RSH: ATC Automatic Tool Change

- Multiple injection methods on one instrument: Flexibility and Productivity
- Intelligent Switch to Dynamic Headspace if Static Headspace is not sensitive enough




ITEX Dynamic Headspace

Static Headspace

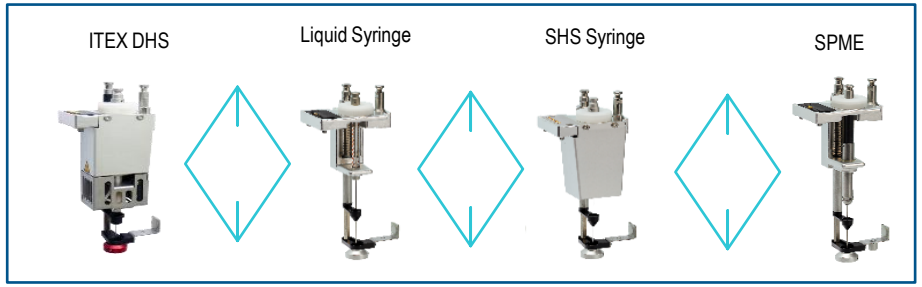
EPA 502.2: Increased sensitivity towards Headspace by magnitudes, **Easily reaching threshold values of US-EPA Methods for VOC's**



ThermoFisher SCIENTIFIC

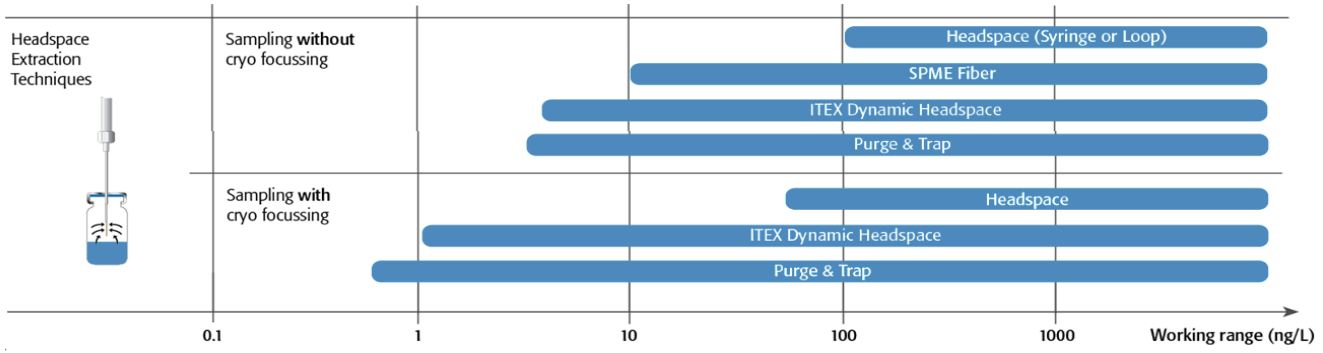
# TriPlus RSH: ATC Automatic Tool Change

- Switching of sample injection techniques on the same instrument
- TriPlus RSH is compatible with a wide range of syringe volumes
- ATC station enables **unattended** syringe exchange **during a sequence**

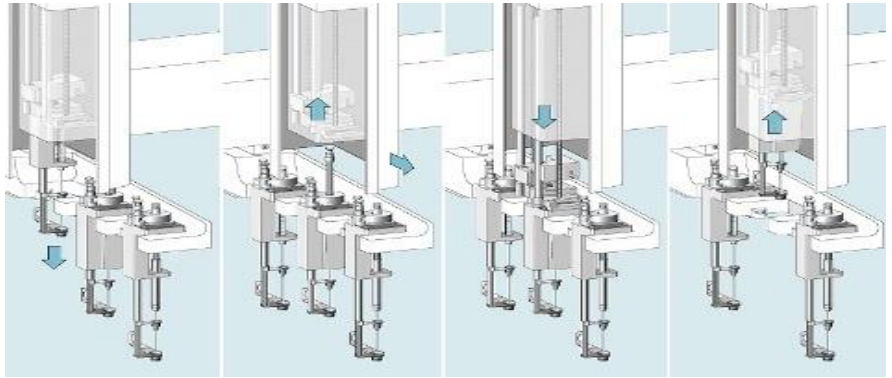



ATC (Automatic Tool Change)


**TriPlus RSH: ATC (Automatic Tool Change)**




Achievable sensitivities by sampling technique

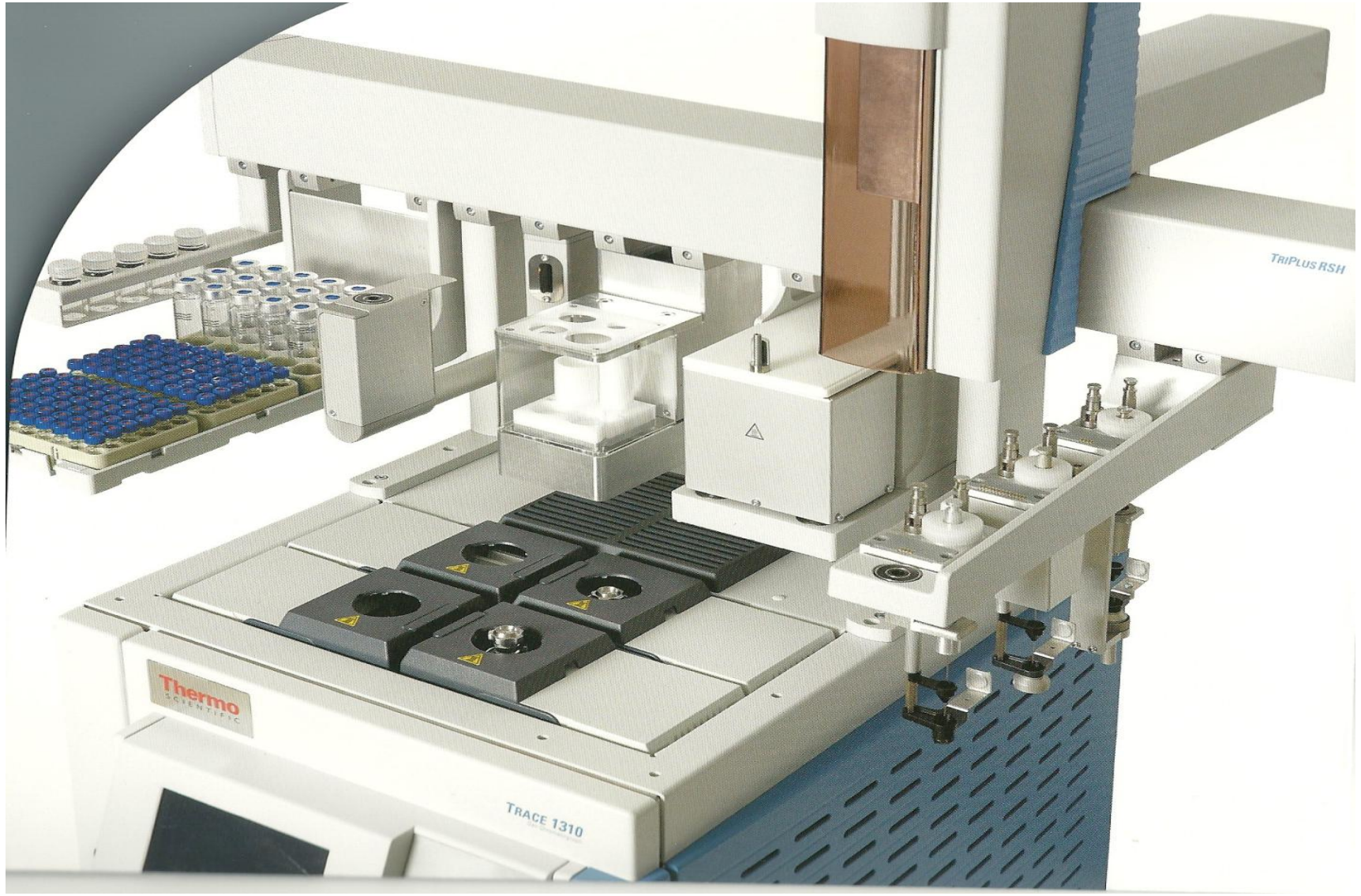


ATC (Automatic Tool Change)



ThermoFisher SCIENTIFIC

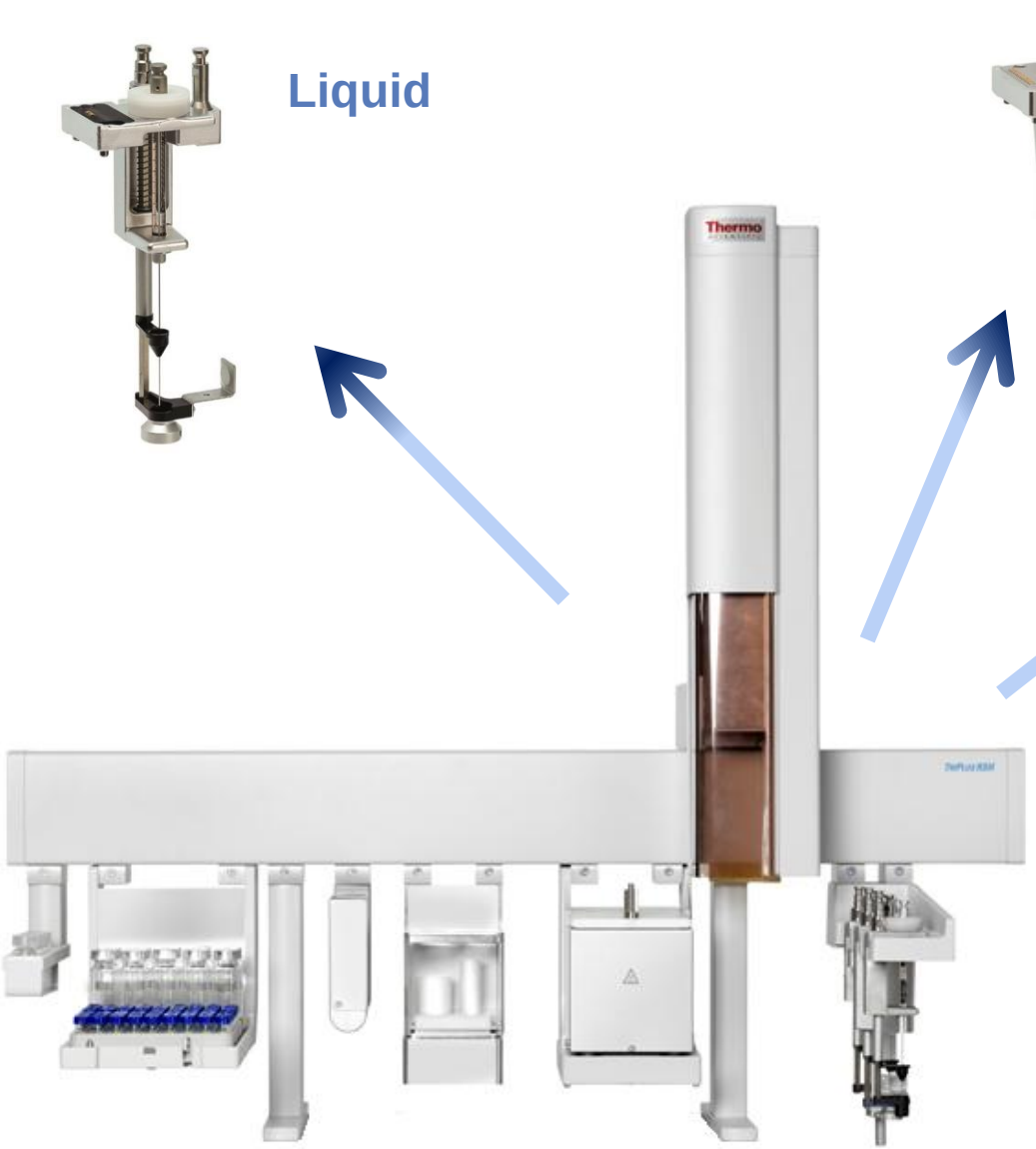
# Triplus RSH






ThermoFisher SCIENTIFIC

# Triplus RSH expanded options for VOC and SVOC market





Liquid

Static Headspace

ITEX- Dynamic Headspace

SPME


NEW

**SPME ARROW**

***To boost sample capacity and robustness***

***....Coming in Q4 !***



ThermoFisher SCIENTIFIC

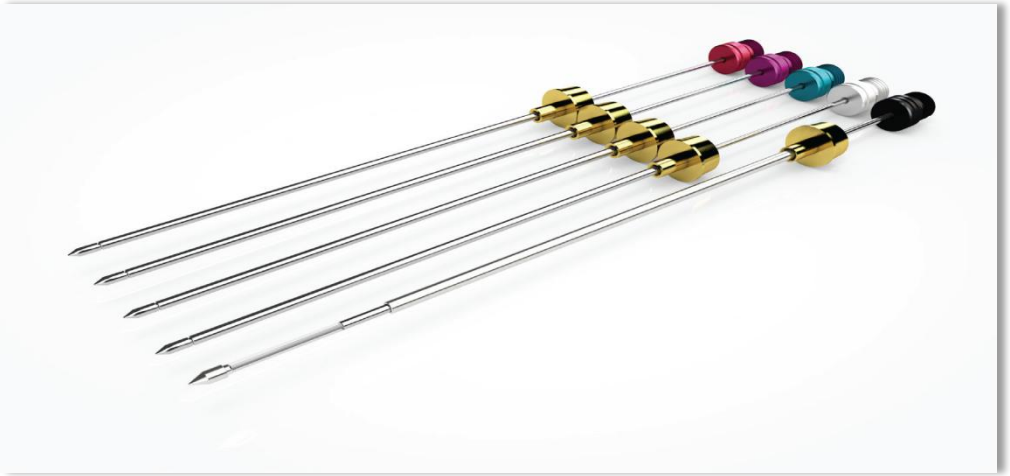
# SPME Arrow tools

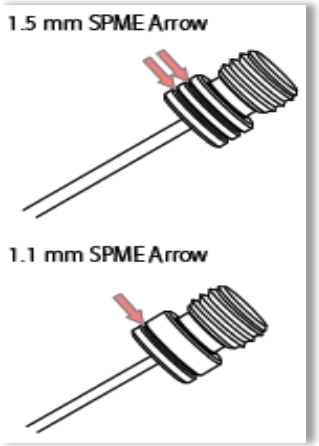
- SPME Arrow tool


- Heatex-Stirrer

- SPME Arrow conditioning module

# SPME Arrow Fiber collection

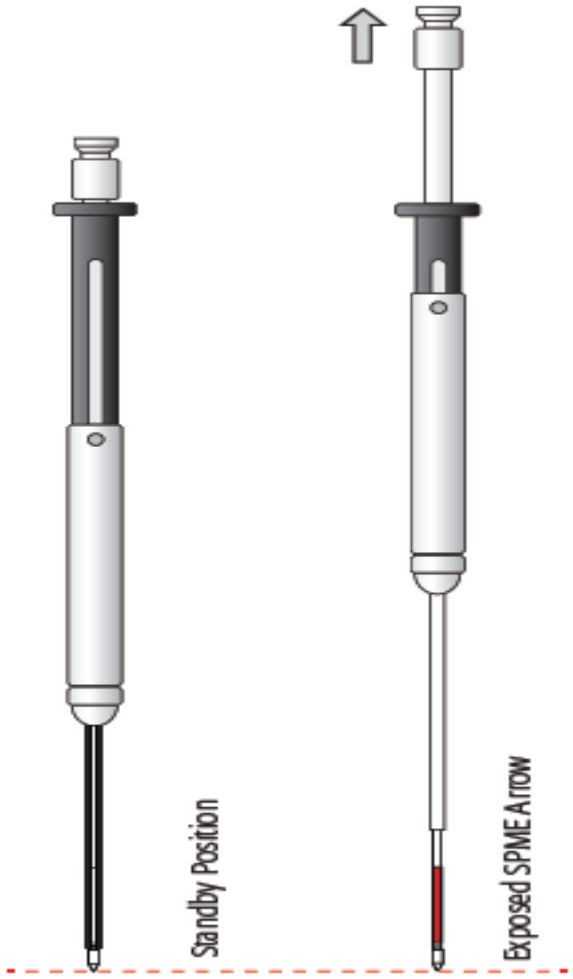





- A full range of fibers is available with different diameter and thickness
- Diameter is coded
- All SPME Arrow fibers have 20 mm phase length

| Color code | Phase | Diameter | Phase Thickness |
|---|---|---|---|
| Red | PDMS | 1,1 mm | 100 um |
| Grey | Acrylate | 1,1 mm | 100 um |
| Light Blue | Carbon WR/PDMS | 1,1 mm | 120 um |
| Violet | DVB/PDMS | 1,1 mm | 120 um |
| Black | PDMS | 1,5 mm | 250 um |

# Increased robustness




- Due to the larger needle diameter, an SPME Arrow adaption kit for the Split/Splitlessinjector is necessary:
  - Adaptation kit for TRACE 1300 Series GC Split/Splitless injector
  - Adaptation kit for TRACE Ultra GC Split/splitless injector
- A specific liner (1.8 or 1.3 mm i.d. depending on the fiber diameter) is suggested for optimal performance

# Increase sensitivity

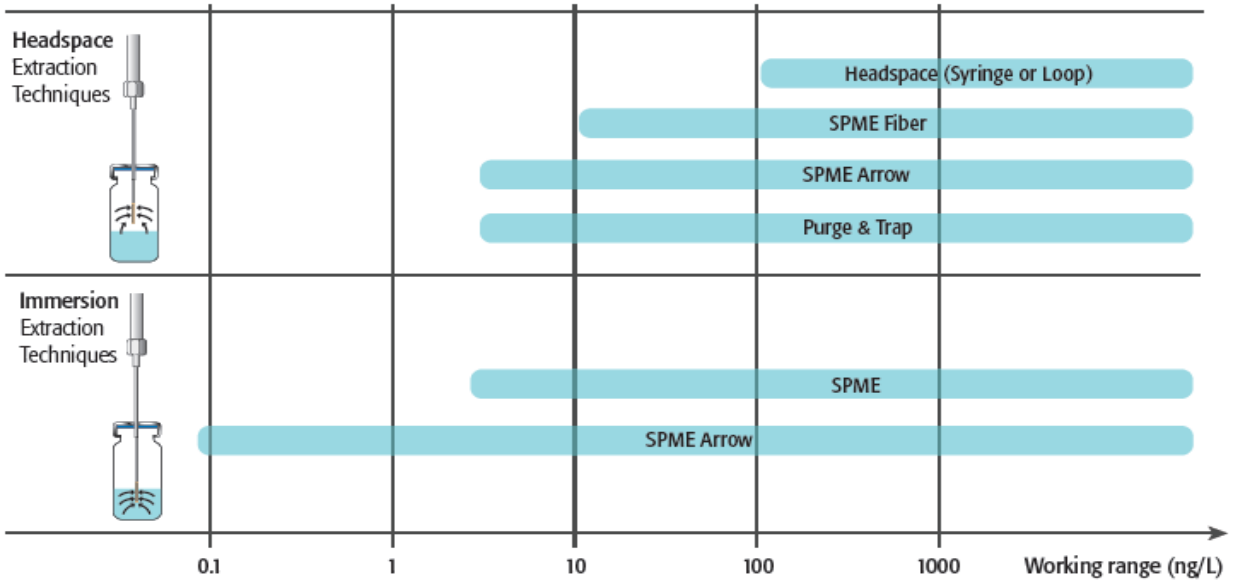
Higher volume = Up to 10 times more sensitivity

The table below shows the dimension of a PAL SPME Arrow 1.5 mm (a), 1.1 mm (b) and a SPME Fiber (c) in comparison:

| | | Sorption phase surface | Sorption phase volume |
|---|---|---|---|
| a |  | 62.8 mm² | 11.8 µL |
| b |  | 44.0 mm² | 3.8 µL |
| c |  | 9.4 mm² | 0.6 µL |

# SPME Arrow

- Larger surface, faster extraction >> *2x higher sample throughput*
- More sorption phase, superior sensitivity*>>up to 10 times more sensitivity, wider dynamic range*
- Optimized geometry, greater robustness*>>SPME Arrow and injector septa last at least 2 x times longer*
- Designed for reliable automation via TriPlus RSH autosampler

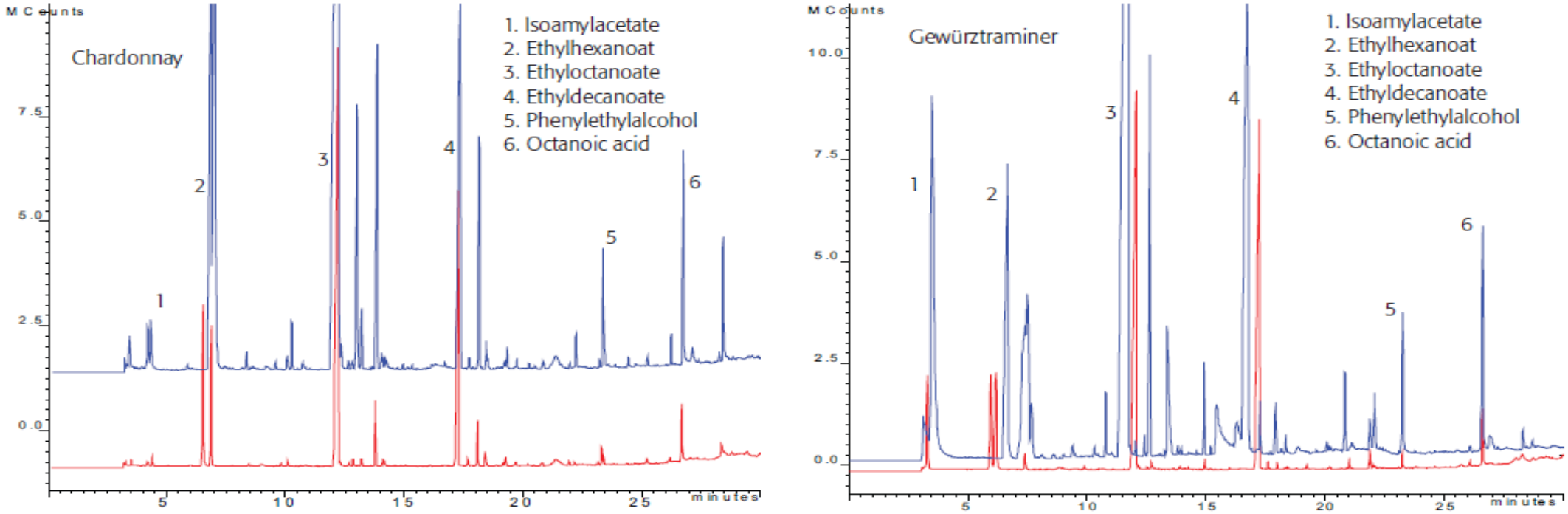





ThermoFisher SCIENTIFIC

# SPME Arrow vs SPME fiber

- Headspace extraction: aroma analysis in white wine




(SPME Arrow 100 µm, 20 x 1.1 mm compared to SPME 100 µm, 10 x 0.3 mm)

# SPME Arrow vs SPME vs SBSE

MDL and RSD obtained with SPME Arrow (250 umx 20 mm) for PAHs in water in comparison with literature data for classical SPME and SBSE bars

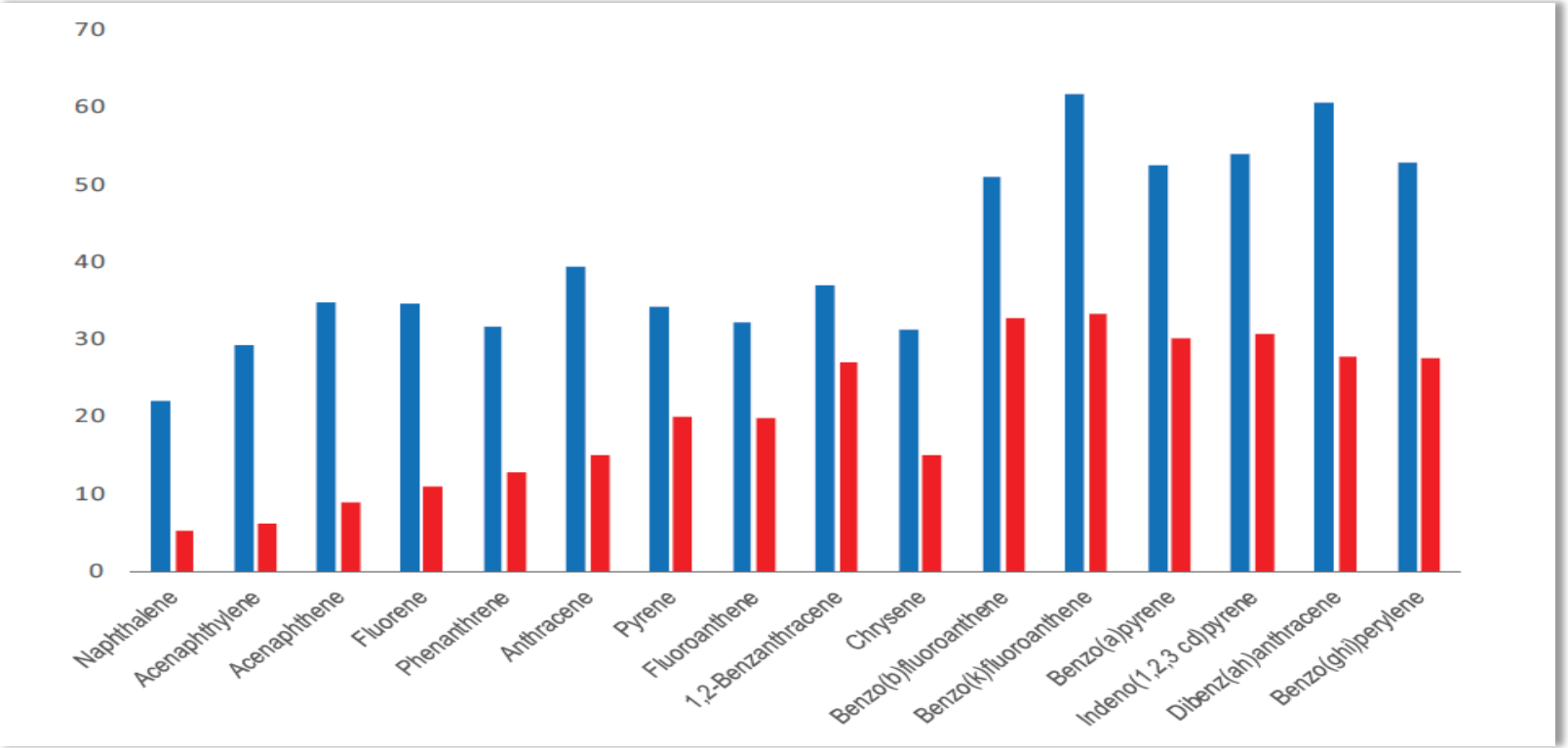
| Compound | PAL SPME Arrow | | SPME (Cheng et al.) [15] | | SBSE (Carrera et al.) [22] | |
|---|---|---|---|---|---|---|
| | MDL (ng $L^{-1}$) | RSD (%) (at 10 ng $L^{-1}$) | LOD (SD X 3) | RSD (conc. at S/N=3×3) | LOD (conc. at S/N=3×3) | RSD (%) (at 50 ng $L^{-1}$) |
| Naphthalene | 0.3 | 5.7 | 2.7 | 9.0 | / | / |
| Acenaphthylene | 0.2 | 6.0 | 1.8 | 6.0 | 0.1 | / |
| Acenaphthene | 0.1 | 7.1 | 0.9 | 3.0 | / | / |
| Fluorene | 0.2 | 5.6 | 3 | 10.0 | 0.1 | 8.3 |
| Phenanthrene | 0.2 | 5.5 | 2.1 | 7.0 | 0.1 | 1.1 |
| Anthracene | 0.3 | 7.6 | 2.1 | 7.0 | 0.2 | 2.1 |
| Pyrene | 0.2 | 6.4 | 3.6 | 12.0 | 0.2 | / |
| Fluoroanthene | 0.2 | 6.2 | 2.1 | 7.0 | 0.2 | / |
| 1,2-Benzanthracene | 0.1 | 6.2 | 2.1 | 7.0 | 0.2 | 6 |
| Chrysene | 0.1 | 11.0 | 1.5 | 5.0 | 0.2 | 10.6 |
| Benzo(b)fluoroanthene | 0.2 | 10.5 | 2.7 | 9.0 | 0.1 | / |
| Benzo(k)fluoroanthene | 0.2 | 8.6 | 1.8 | 6.0 | 0.1 | / |
| Benzo[a]pyrene | 0.3 | 7.2 | 3.6 | 12.0 | 0.1 | / |
| Indeno(1,2,3 cd)pyrene | 0.8 | 9.2 | 3.6 | 12.0 | 0.3 | / |
| Dibenz(ah)anthracene | 0.6 | 11.3 | / | / | 0.3 | / |
| Benzo(ghi)perylene | 0.8 | 11.9 | 1.8 | 6.0 | 0.3 | / |

MDL values calculated with a 99 % confidence interval
/ not determined

SPME Arrow - Evaluation of a Novel Solid-Phase Microextraction Device for Freely Dissolved PAHs in Water; Kremser A. et al 2016, 408, 943-952

# Immersion extraction: PAHs in water

Extraction yields for water samples containg 50 ng/L PAHs after 70 min




**SPME Arrow** 20 mm x 250 um carbon WR

**SPME fiber** 10 mm x 100 um Carbon WR

SPME Arrow - Evaluation of a Novel Solid-Phase Microextraction Device for Freely Dissolved PAHs in Water; Kremser A. et al 2016, 408, 943-952

## Sampling techniques comparison chart

| Analytical quality | HS | | | DHS/Purge & Trap | | SPME | SPME Arrow | ITEX-DHS | SBSE/HSSE |
|---|---|---|---|---|---|---|---|---|---|
| | Loop | syringe | P bal | headspace | sparkling | Immersion/ headspace | Immersion/ headspace | headspace | Immersion/ headspace |
| Sensitivity | + | + | + | ++ | +++ | ++ | ++++ | +++ | ++++ |
| Regulation compliance | Yes | Yes | Yes | Yes | Yes | Yes | Yes | Yes | Yes |
| EPA methods | Yes | Yes | Yes | Yes | Yes | Yes | Yes | Yes | No |
| EU methods | Yes | Yes | Yes | Yes | Yes | Yes | Yes | Yes | No |
| Ease of use | +++ | +++ | +++ | ++ | ++ | +++ | +++ | +++ | +++ |
| Sample handling | +++ | +++ | +++ | ++ | + | +++ | +++ | +++ | ++ |
| Analytes discrimination | low | low | low | low | med | med/high | med/high | low | high |
| Risk of contamination | low | very low | low | low | high | very low | very low | low | low |

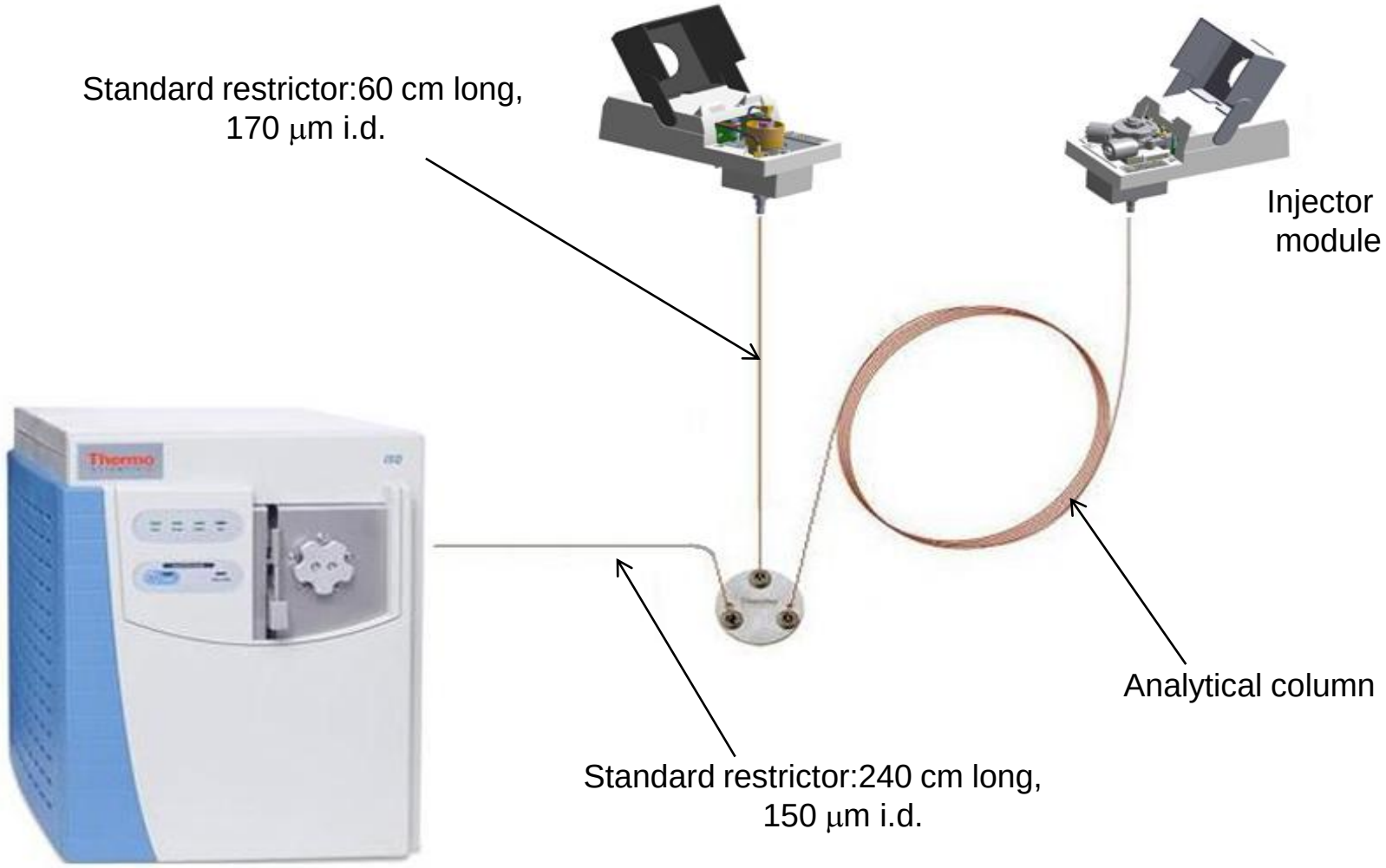
| Hardware related | HS | | | DHS/Purge & Trap | | SPME | SPME | ITEX-DHS | SBSE/HSSE |
|---|---|---|---|---|---|---|---|---|---|
| Modularity | No | Yes | No | No | No | Yes | Yes | Yes | Yes |
| Cost of device | high | low | high | high | high | low | low | low | high |
| Automated | Yes | Yes | Yes | limited | Yes | Yes | Yes | Yes | Yes |
| Space requirement | high | low | high | high | high | low | low | low | low |
| GC installation needs | high | low | high | high | high | low | low | low | low |
| GC injector blocked | Yes | No | Yes | Yes | Yes | No | No | No | No |
| Flexible w injection modes | No | Yes | No | No | No | Yes | Yes | Yes | Yes |

# Head Space TriPlus 300 –transfer line

- **Instrument configuration**
  - TRACE 13XX GC
  - Dual column system
  - TriPlus 300 Head Space Autosampler
  - FID
  - Chromeleon 7.2 CDS

# Dual detectors confirmation analysis

- Screening with GC detector; confirmation with MS detector






ThermoFisher SCIENTIFIC


ThermoFisher
SCIENTIFIC

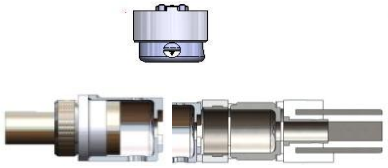
# 2016 GCMS Single Quadrupole

# Mass Spec Components Same for All Product Offerings

**Designed With Intention** ***ISQ Series*** - ***I***ntelligent ***S***ingle ***Q***uad

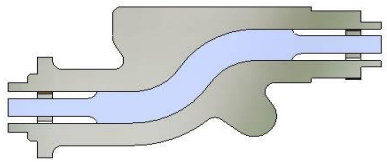



**Unique Dual-Filament**

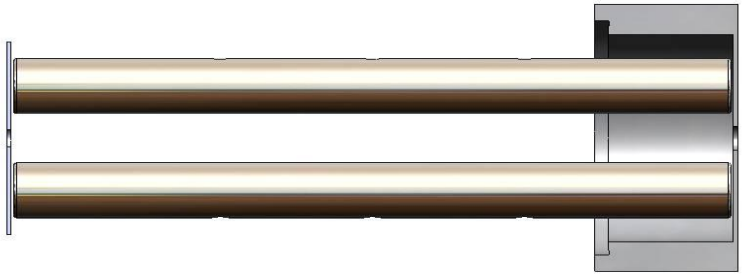


**ExtractaBrite™ ion**

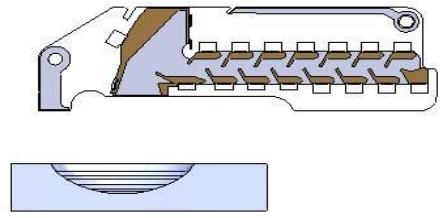
**s-shaped ion guide**



**Solid, homogeneous, and maintenance-free metal quadrupole rods**



**DynaMax™ XR detection**





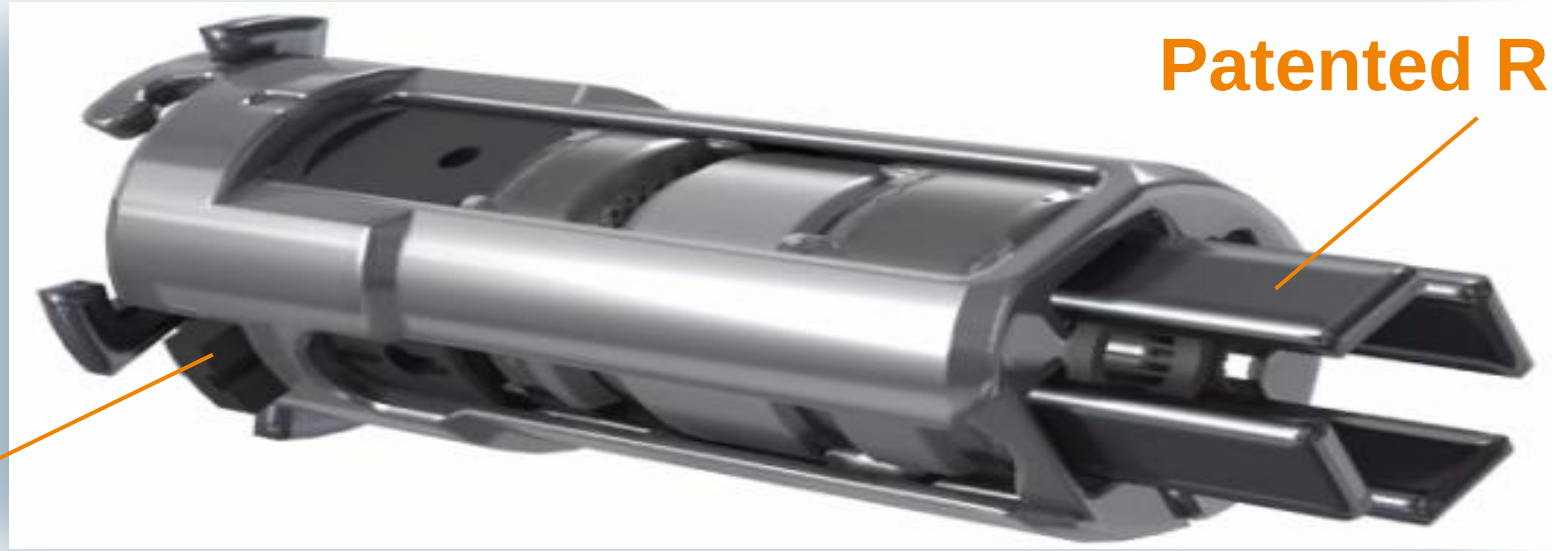
ThermoFisher SCIENTIFIC

# *ISQ Series* Technical Specifications

| Specification | *ISQ QD* | *ISQ QD 300* | *ISQ LT* |
|---|---|---|---|
| In **EI** mode, 1 µL of 1 pg/µL OFN m/z 272 , scanning from 50 – 300 Da **(*)** | **750:1 (*)** | **2000:1 (*)** | **2000:1 (*)** |
| In **PCI** mode, 1 µL of 100 pg/µL BZB m/z 183, scanning from 80 – 230 Da | Not Available | Not Available | 300:1 |
| In **NCI** mode, 2 µL of 100 fg/µL of OFN m/z 272, scanning from 50 – 300 Da | Not Available | Not Available | **2000:1** |
| IDL for m/z 272 in SIM mode in EI | **≤ 10 fg** | **≤ 5 fg** | **≤ 1,5 fg** |
| Ionization Modes | EI only | EI only | EI and CI |
| Carrier Gas Choice | He only | He or $H_2$ | He or $H_2$ |
| Instant Connect Helium Saver Injector | Compatible | Compatible | Compatible |
| Turbomolecular High Vacuum Pump | 66 L/s | 300 L/s | 300 L/s |
| Vacuum Probe Interlock | Not Available (No Direct Probes) | Not Available (No Direct Probes) | VPI as standard Optional Direct Probes |
| Automation Features | Optional t-SIM/AutoSIM | t-SIM/AutoSIM | t-SIM/AutoSIM |
| Quadrupole Scanning Speed | 20,000 Da/s | 20,000 Da/s | 20,000 Da/s |

**(*) demonstrated at installation**

# ExtractaBrite Ion Source




- Patented RF lens protects ion guide and quads
- RF lens is removed  with source cartridge without venting
- RF lens kept hot to keep clean
- Repeller designed to overcome ion burn once it forms

# ExtractaBrite Ion Source

***ExtractaBrite Ion Source***

Lenses 1, 2 and 3 plus the RF lens, along with the repeller and ion volume are contained in a sleeve, all of which can be removed from ***ISQ LT*** while the system is under vacuum.

The ability to remove the entire ion source from ***ISQ LT*** without venting means you are never down and always productive.




ThermoFisher SCIENTIFIC

# Removable Source Under Vacuum




ThermoFisher SCIENTIFIC

# GCMS Analyzer Kits

- Aim to target routine Environmental Laboratories with proven robustness, sensitivity and high sample throughput
- Compatible with ISQ QD and ISQ LT
- Ready to use package with method, troubleshooting and reporting
- Dedicated consumables and spares to complete the package
- Compatible with both Chromeleon and TraceFinder
- Compatible with Helium Saver

Dedicated to **semivolatile contaminants in environmental samples**

*(EPA 8270D)*

*Target Launch Q3*

Dedicated to **semivolatile contaminants in drinking water**

*(EPA 525.3)*

*Target Launch Q4*

thermo scientific

# One Minute GC & GC-MS Highlight

## New Product: U.S. EPA 8270D Analyzer Kit

**Update your lab and overcome the challenges of semivolatile (SVOC) analysis**

Get a complete solution designed to provide seamless migration to Thermo Scientific GC-MS instrumentation for semivolatile organic compound (SVOC) analysis. The Thermo Scientific™ U.S. EPA 8270D Analyzer Kit removes the need for new method development offering a validated methodology that includes instrument and processing methods, as well an EPA environmental specific report package. All components of the kit were developed to fulfill EPA methods requirements.


Click the links below to learn more about the new EPA 8720D Analyzer Kit:

Link to One Minute Highlight



ThermoFisher SCIENTIFIC

# Web page

ThermoFisher SCIENTIFIC

Contact Us | Sign In | Quick Order 5

Recently Viewed Items

Applications & Techniques | Shop All Products | Services & Support | About Us | Cloud

Mass Spectrometry Instruments & Equipment › Mass Spectrometry Systems & Components › EPA 8270D Analyzer Kit

## EPA 8270D Analyzer Kit


Thermo Scientific™ **Related applications:** Industrial Mass Spectrometry

Get a complete solution designed to provide seamless migration to Thermo Scientific™ GC-MS instrumentation for semi-volatile organic compound (SVOC) analysis. The Thermo Scientific™ EPA 8270D analyzer kit removes the need for new method development offering a validated methodology that includes instrument and processing methods, as well an EPA environmental specific report package. All components of the kit were developed to fulfill EPA methods requirements.

Contact us for support ›

| Catalog number | Product Size | Description | Software | For Use With | Price (GBP) |
|---|---|---|---|---|---|
| 1R120400-8270 | - | 88 Validated Compounds<br>Linearity Range: 0.2-200ppm (with same column and liner) | Chromeleon 7.2 SR4 MUB or newer;<br>TraceFinder EFS 4.1 or newer | Thermo Scientific™ ISQ™ QD Single Quadrupole GC-MS System and Thermo Scientific™ ISQ™ LT Single Quadrupole GC-MS System | Request A Quote |

EPA 8270D Web page



ThermoFisher SCIENTIFIC

# EPA 8270D kit is a new, ready-to-use application solution delivering maximum up-time and more reliable results to Environmental customers


## Kit concept

- Ready to use with Method 8270D, includes:
  - Set of consumables (column, liner, septa, etc.)
  - Pre-loaded processing methods, templates and e-workflows
  - Videos with training on most common sw activities
  - App note AN10522, troubleshooting guide

## Product offering

- Available with ISQ QD and ISQ LT
- Chromeleon (SR4 Mub HF) or TraceFinder  EFS compatible
- Compatible with Helium Saver
- Splitless method 0.2-50ppm and split method 2-200ppm (same column and liner)

# EPA 8270D kit p/n **1R120400-8270** BOM (Bill Of Materials)

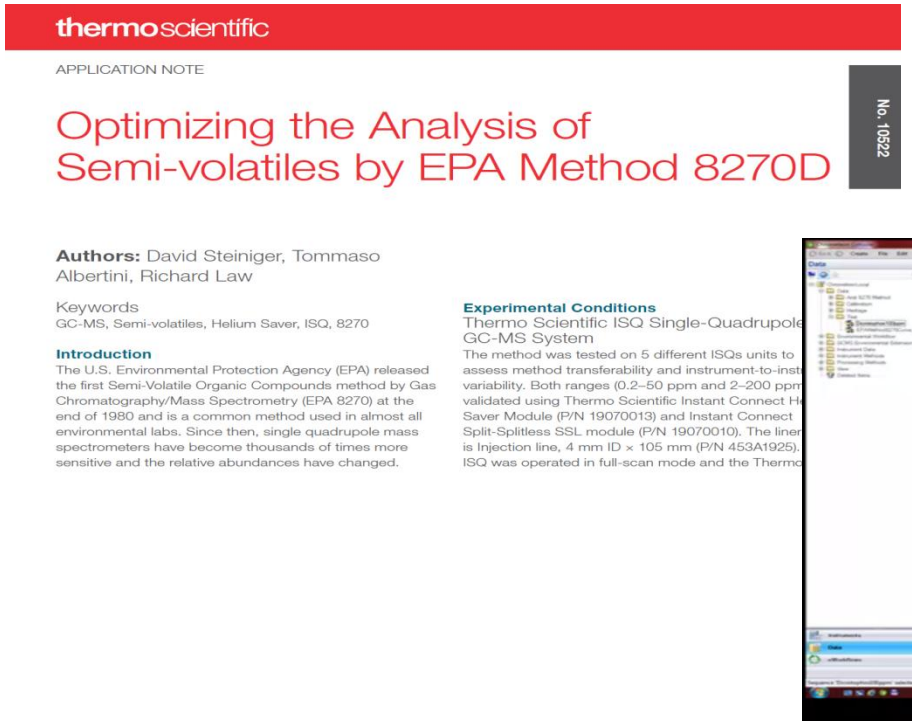
| Part number | Description | GRP, $USD |
|---|---|---|
| 26098-1425 | Column, TG-5MS w/ 5m guard,30m X 0.25mm X 0.25µm | $637,00 |
| 453A1925 | Injection liner,4mm ID x 105 mm, pack of 5 | $109,00 |
| 290VA191 | Graphite/Vespel Ferrule, 0.1 - 0.25 mm, pack of 10 | $48,00 |
| 31303233 | Septa BTO Coated, 11 mm, pack of 50 | $81,00 |
| 1R120400-SCA | System Conditioning Agent | $85,41 |
| 1R120479-0060 | EPA 8270D CD (contains methods, user guide, video training, app note, troubleshooting guide) compatible with TF and CM | $500,00 |
| | Total Reference Price **of all parts** | $1460.41 |
| **1R120400-8270** | **EPA 8270D Kit Global Reference Price** | **$800,00** |




ThermoFisher SCIENTIFIC

# EPA 8270D CD 1R120479-0060

- TraceFinder methods and templates
- Chromeleon e-Workflow (with methods and reports)
- EPA 8270D user guide
- EPA 8270D application note
- Tutorial Video



thermoscientific

APPLICATION NOTE

Optimizing the Analysis of Semi-volatiles by EPA Method 8270D

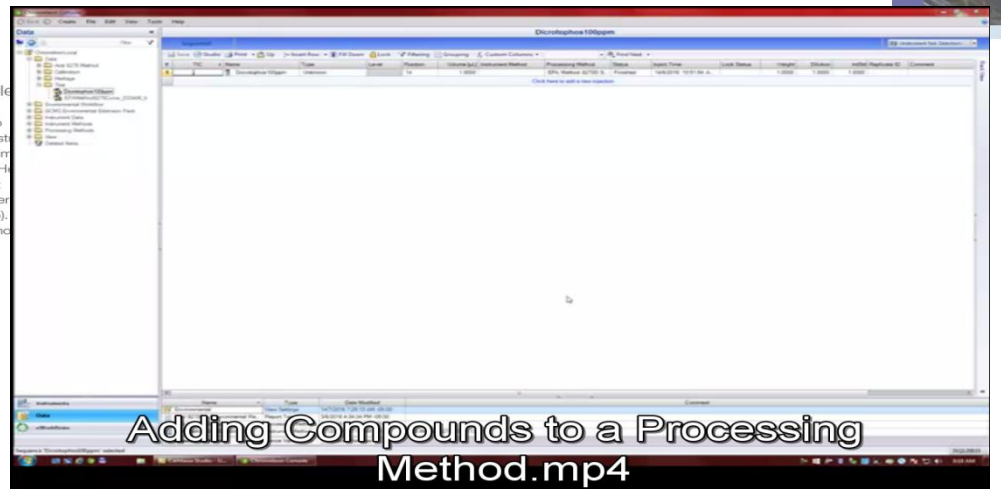
No. 10522

**Authors:** David Steiniger, Tommaso Albertini, Richard Law

Keywords
GC-MS, Semi-volatiles, Helium Saver, ISQ, 8270

**Introduction**
The U.S. Environmental Protection Agency (EPA) released the first Semi-Volatile Organic Compounds method by Gas Chromatography/Mass Spectrometry (EPA 8270) at the end of 1980 and is a common method used in almost all environmental labs. Since then, single quadrupole mass spectrometers have become thousands of times more sensitive and the relative abundances have changed.

**Experimental Conditions**
Thermo Scientific ISQ Single-Quadrupole GC-MS System
The method was tested on 5 different ISQs units to assess method transferability and instrument-to-inst variability. Both ranges (0.2–50 ppm and 2–200 ppm validated using Thermo Scientific Instant Connect He Saver Module (P/N 19070013) and Instant Connect Split-Splitless SSL module (P/N 19070010). The liner is Injection line, 4 mm ID × 105 mm (P/N 453A1925). ISQ was operated in full-scan mode and the Thermo




EPA 8270D Kit for ISQ Series Mass Spectrometers

**User Guide**

1R120555-0010 Revision A July 2016

thermo scientific



ThermoFisher SCIENTIFIC

# How to order EPA 8270D kit

1° • Select GC mainframe for GC/MS (Trace 1300 or Trace 1310)

2° • Optional stage, select auto sampler

3° • Select  GC injector module (SSL or He Saver)

4° • Select SW (TraceFinder EFS or Chromeleon) and Computer

5° • Select MS detector (ISQ QD or QD 300 or LT)

6° • Select EPA 8270D kit (p/n **1R120400-8270**)

7° • If needed or requested  select application support at customer site

**LINK TO SALES TRAINING WEBINAR**

# Chromeleon 7.2 SR3 – New GCMS Functionality



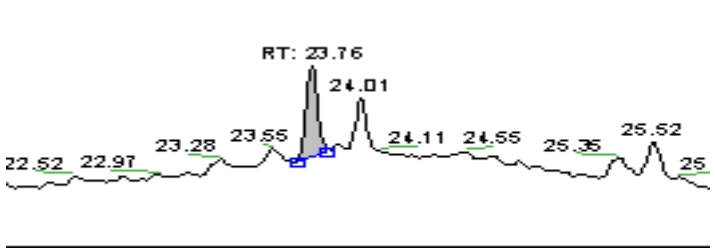
- Integrated control for TSQ8000Evo
  - Performance Improvements with Large Datasets
- Pesticides Analyzer
  - Update to GCBU Pesticides Analyzer DVD
  - Will include method templates, report templates, compound database and workflow instructions
- GCMS EPA Water Analysis
  - Environmental Extension Pack containing eWorkFlows, method templates and report templates, view settings, custom variables
- Deconvolution SW for unknowns and RI
  - Target release  in Q4 2016


ThermoFisher
SCIENTIFIC

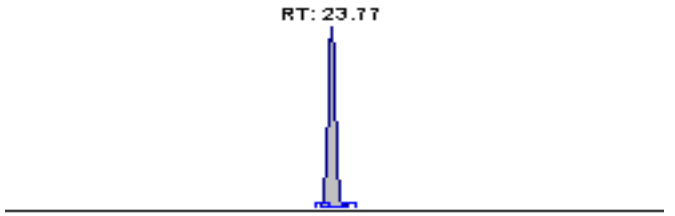
# 2016 GCMSMS TSQ 8000 EVO , TSQ 8000 DUO

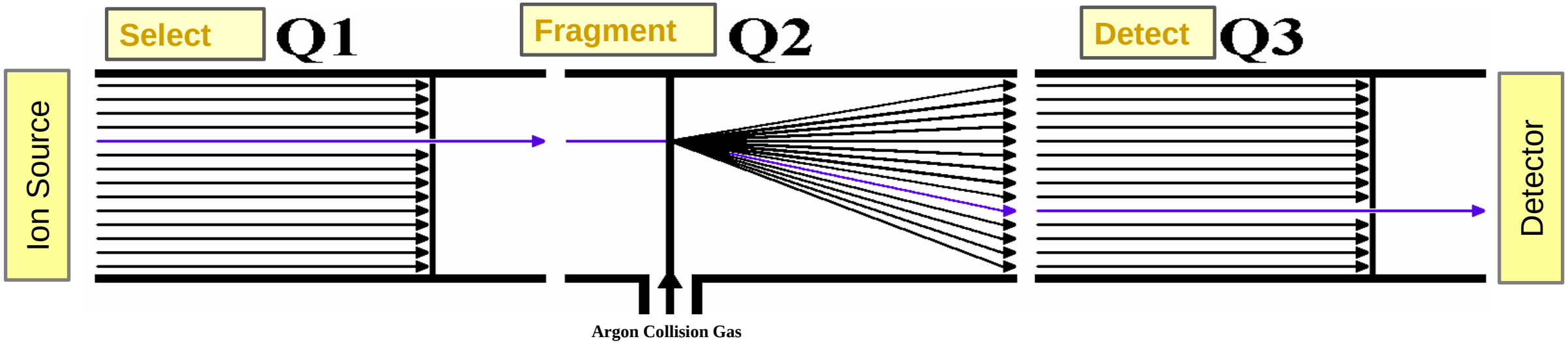
# Triple Quadrupole MS – Principle of Operation

## Quantitation of target compounds in matrix samples




SRM: selected reaction monitoring-transitions




Q1 selects the *precursor ion*
***TCDD ion: m/z* 319.90**

Q3 selects the *product ion*
**fragments to *m/z* 256.90**



ThermoFisher SCIENTIFIC

# GCMSMS Analyzer Kits

- Aim to target routine Environmental and Food Safety Laboratories with proven robustness, sensitivity and high sample throughput
- Compatible with TSQ DUO and TSQ8000EVO
- Ready to use package with method templates, report templates, compound database and workflow instructions
- Dedicated consumables and spares to complete the package
- Compatible with both Chromeleon and TraceFinder
- Compatible with Helium Saver

## Pesticide Analyzer

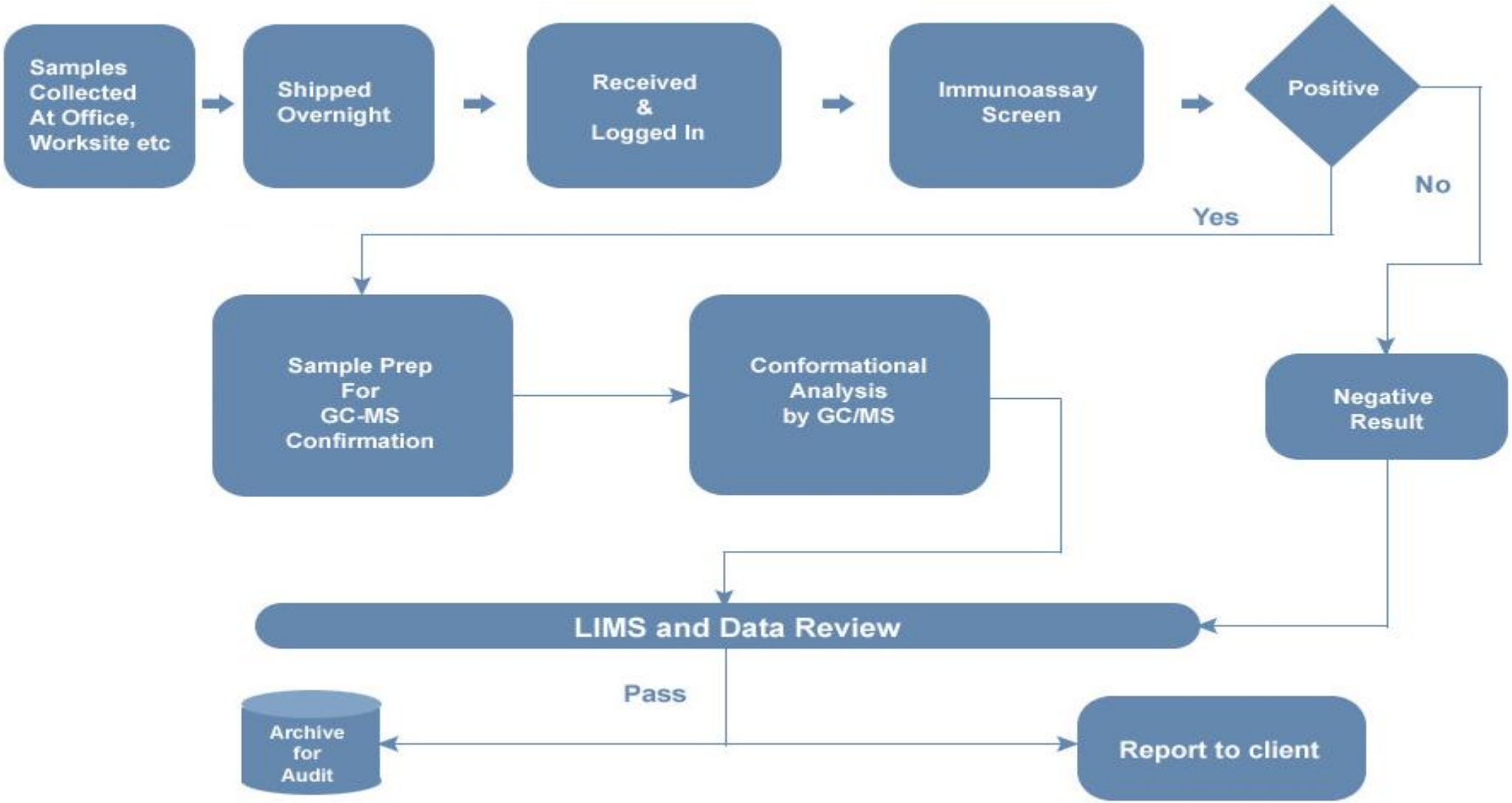
CDB extended to 1001 compounds with 3 optimized transitions

## Dioxins Analyzer

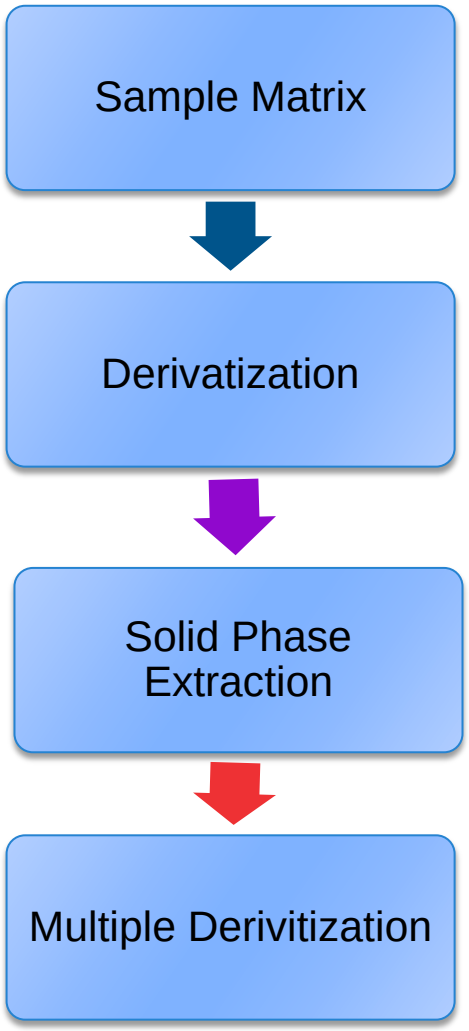
Dedicated workflow and SOP for Dioxins Analysis

*Target Launch Q3*

# Drugs of Abuse Testing Laboratory Workflow



# Sample prep: injecting blood, sweat and tears on a GC




- Sample preparation reagents and solutions for various matrices
  - Blood, Urine, Oral Fluid hair and other bodily fluids
- Accurate separation of components analogues
  - Avoid misinterpretation of target compounds
  - Avoid metabolic product exclusion or interference
    - Opioids - Keto-moeity derivitization
- Removal of noise associated with sample matrix components
  - Higher recovery, Better reproducibility
  - Less noise = Better chromatography
    - Hyper Sep Verify - CX
- Enhance target compound stability
  - Better detection

# Determination THCA in Hair

- **Why test THCA?**

Delta 9 THC (THC) is the most commonly abused illicit drug.
The metabolite THCA indicates the ingestion of THC as opposed to passive contamination of the hair through the air.

- **Why test Hair?**

Long detection time windows

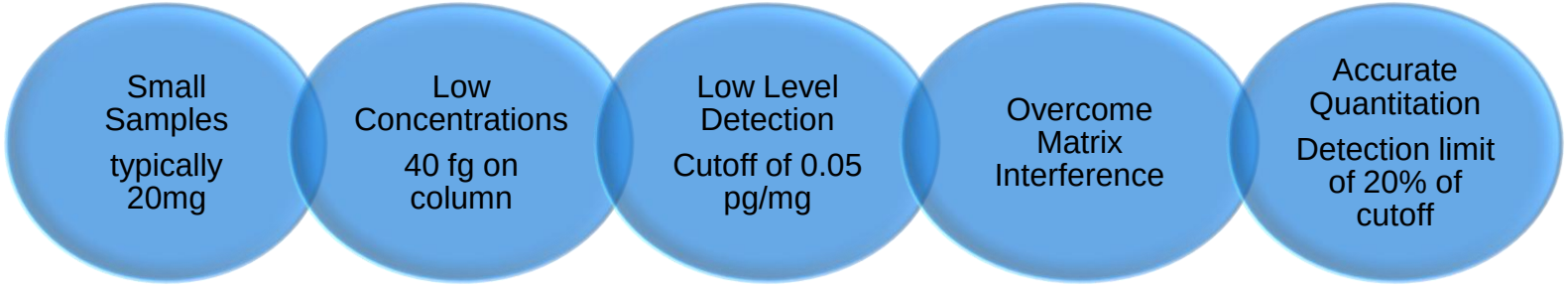
*Urine/blood/oral fluid*: minutes to days detection widow
*Hair: months to years detection window*

- **Applications for Hair testing**

Death investigations
Workplace drug testing
Drug-facilitated crimes
Violation of probation or parole
Drivers license re-instatement

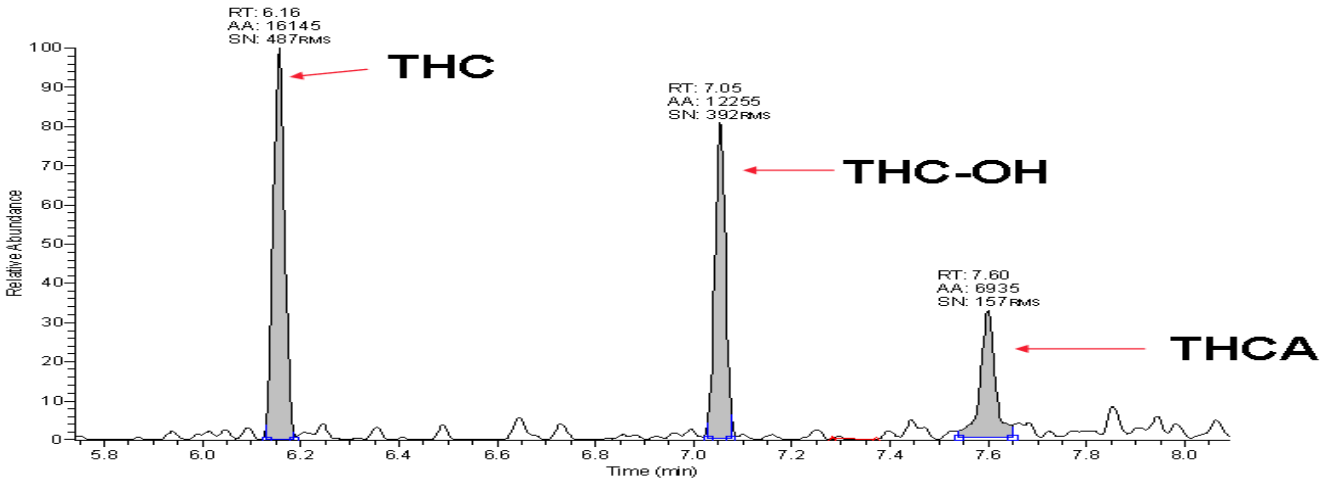
# Determination THCA in Hair

- Delta 9 THC (THC) is the most commonly abused illicit drug.
- The metabolite THCA indicates the ingestion of THC as opposed to passive contamination of the hair through the air.
- Hair is a very complex and variable matrix even after sample cleanup




| Agency/Organization | Cutoff Level |
|---|---|
| Society of Hair Testing (SoHT) | 0.20 pg/mg |
| Gesellschaft fur Forensische und Toxikologische Chemie (GFTCh) | 0.05 pg/mg |
| Substance Abuse and Mental Health Services Administration (SAMHSA) | 0.05 pg/mg |

# Determination THCA in Hair



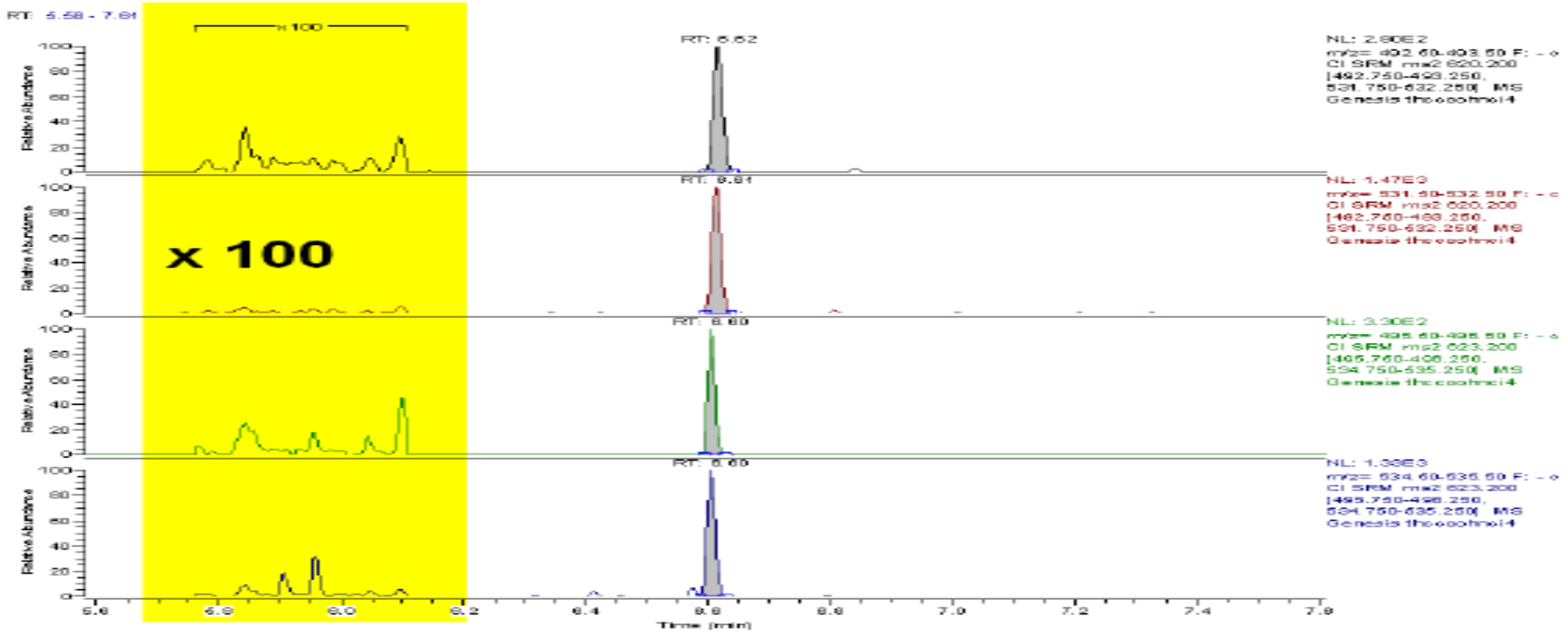

MSTFA Derivatized, EI, SRM Transition: 371 > 289

- **Sensitivity of GC TSQ 8000 EVO to THCA**
- On-Column Injection of 8fg
- Use of a 0.05 pg/mg cutoff
- Demonstrates the sensitivity sufficient for published cutoffs

- **NCI** - Specific transitions can be defined in NCI (Methane used as reagent gas), enhancing selectivity for both THC-COOH and the corresponding ISTD D3

| Compound | Precursor ion (m/z) | Daughter ion (m/z) | Coll cell (mtorr) | Width | Time | CE | Q1 PW | Q3 PW |
|---|---|---|---|---|---|---|---|---|
| THC-COOH | 620.2 | 493 | 1.5 | 0.5 | 0.05 | 15 | 0.7 | 0.7 |
| THC-COOH | 620.2 | 532 | 1.5 | 0.5 | 0.05 | 15 | 0.7 | 0.7 |
| THC-COOH d3 | 623.2 | 496 | 1.5 | 0.5 | 0.05 | 15 | 0.7 | 0.7 |
| THC-COOH d3 | 623.2 | 535 | 1.5 | 0.5 | 0.05 | 15 | 0.7 | 0.7 |

# THCA in Hair - NCI transitions




PFAA Derivatized, Negative Ion Chemical Ionization - **50 fg** THCA and ISTD-D3

- Demonstrates very low noise level relative to the signal
- Zoom in the baseline by 100 times before we start seeing significant noise
- Possible to drop the concentration by a factor of 10 and still achieve the selectivity to accurately quantitate THCA


ThermoFisher
SCIENTIFIC

# 2016 Qexactive GC & Exactive GC Orbitraps

# Exactive GC / Q Exactive GC


Thermo Scientific Exactive GC
Orbitrap GC-MS System

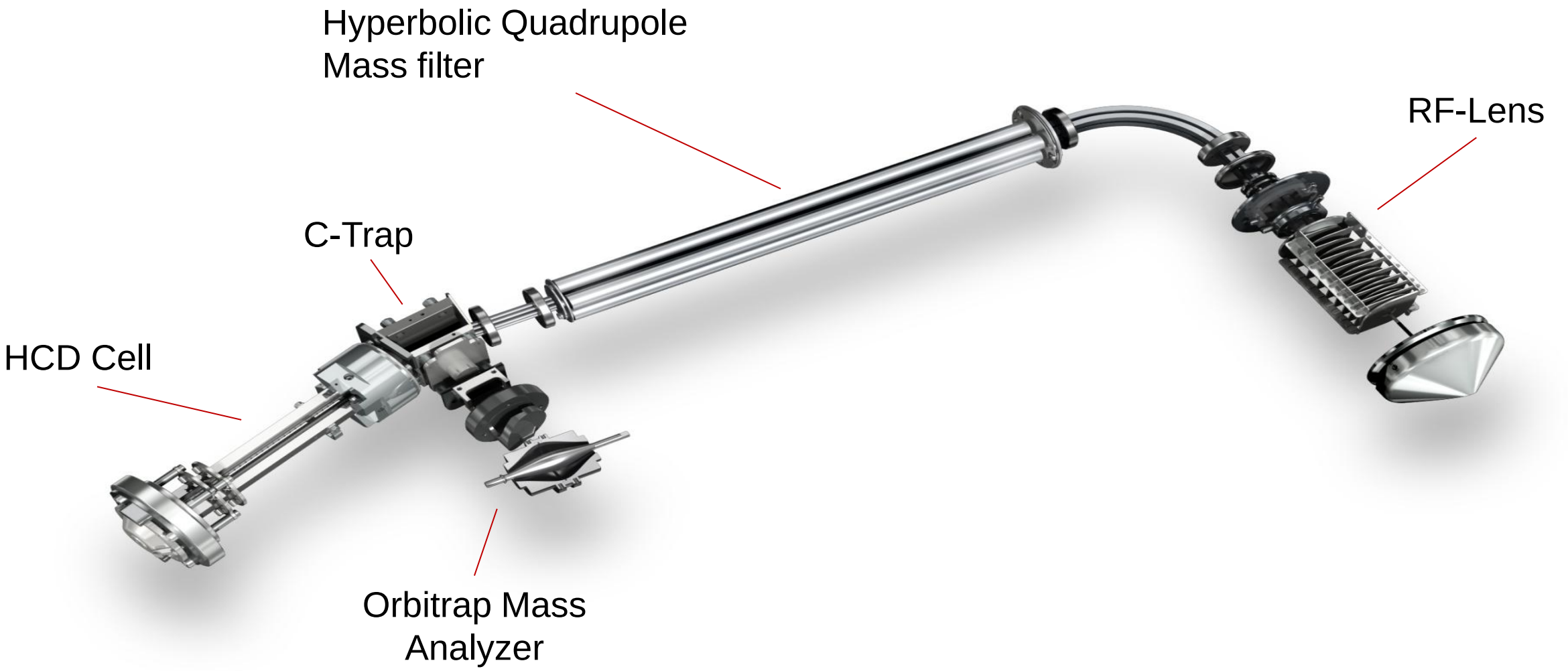
| | |
|---|---|
| | 50,000 maximum Resolution |
| | 18 Hz maximum speed |
| Mass Accuracy | <1ppm RMS for Internal Calibration<br>< 3ppm RMS for External Calibration |

| | |
|---|---|
| | 100,000 maximum Resolution |
| | 18 Hz maximum speed |
| Mass Accuracy | <1ppm RMS for Internal Calibration<br>< 3ppm RMS for External Calibration |



ThermoFisher SCIENTIFIC

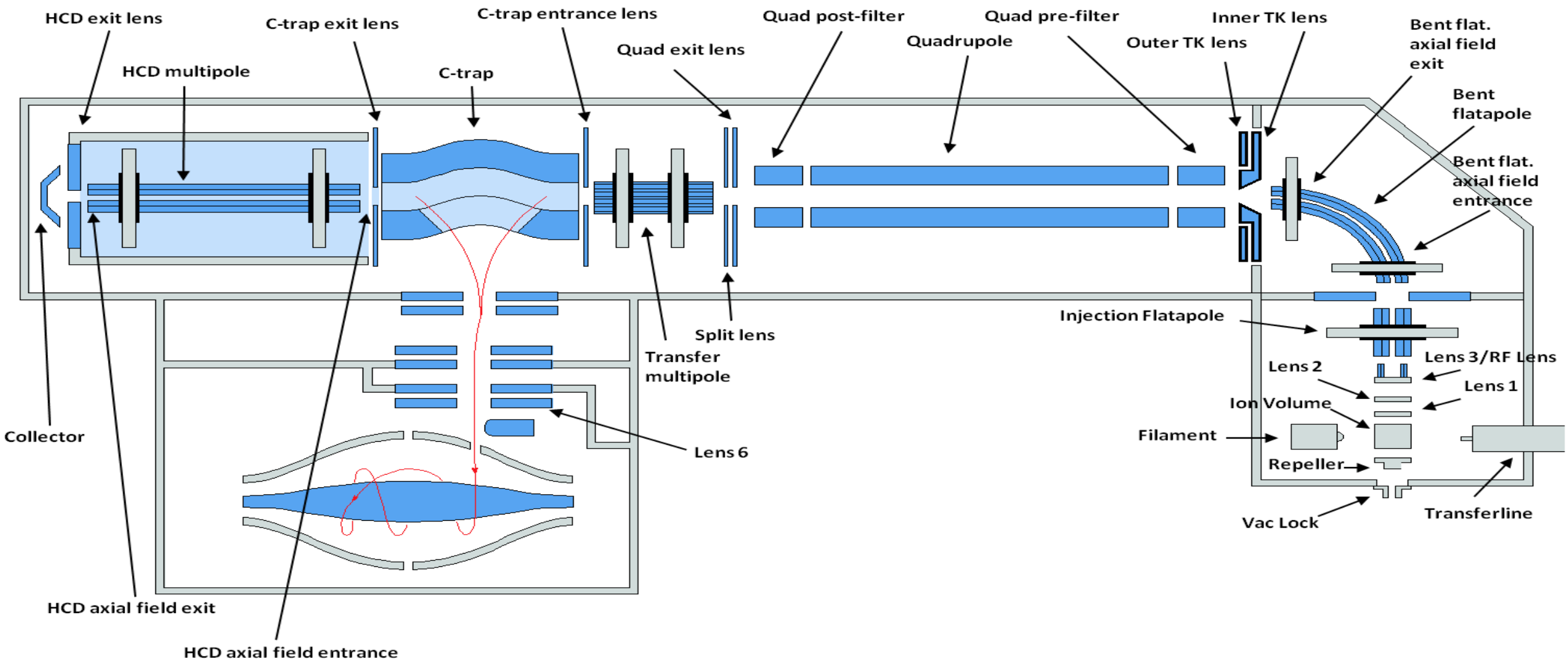
# Q Exactive GC



# Exactive GC Internal Components


Note for reasons of internal product positioning, AQT quadrupole won't be highlighted in marketing material

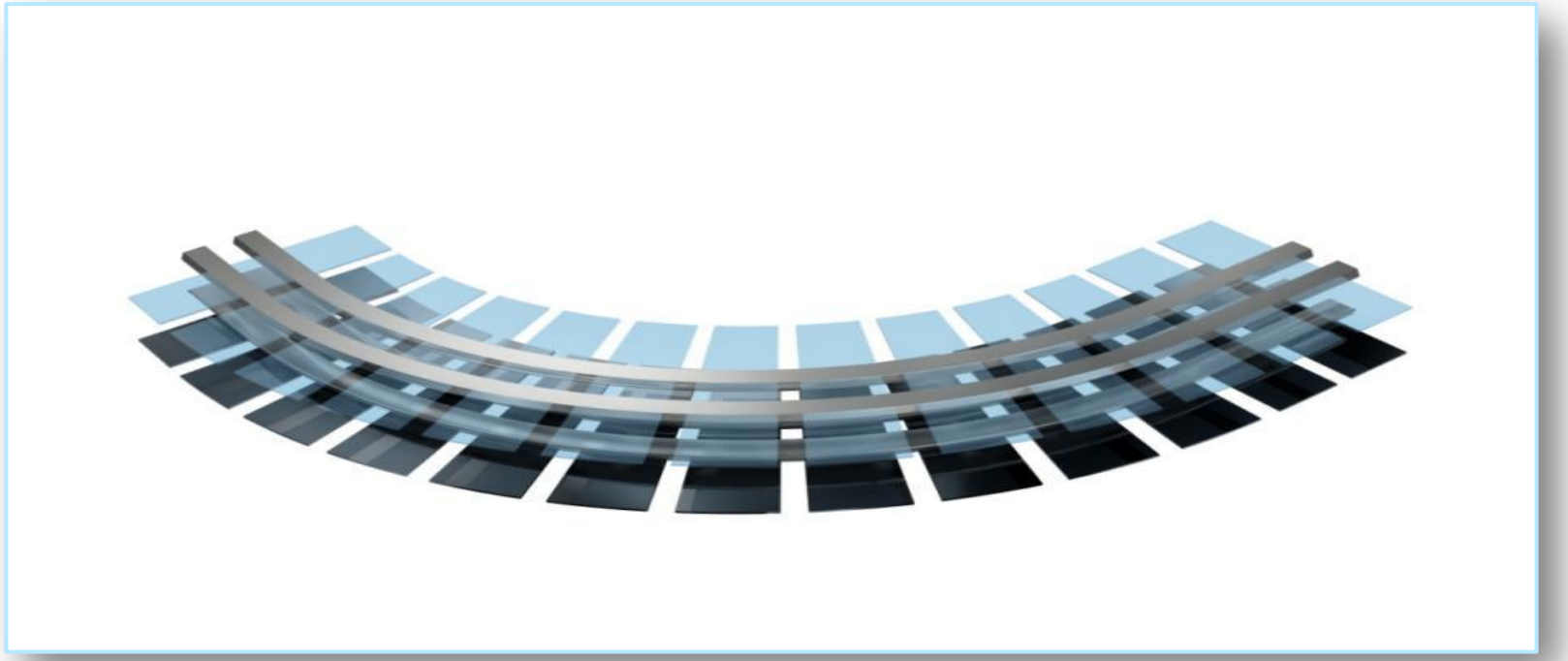
# Instrument Overview





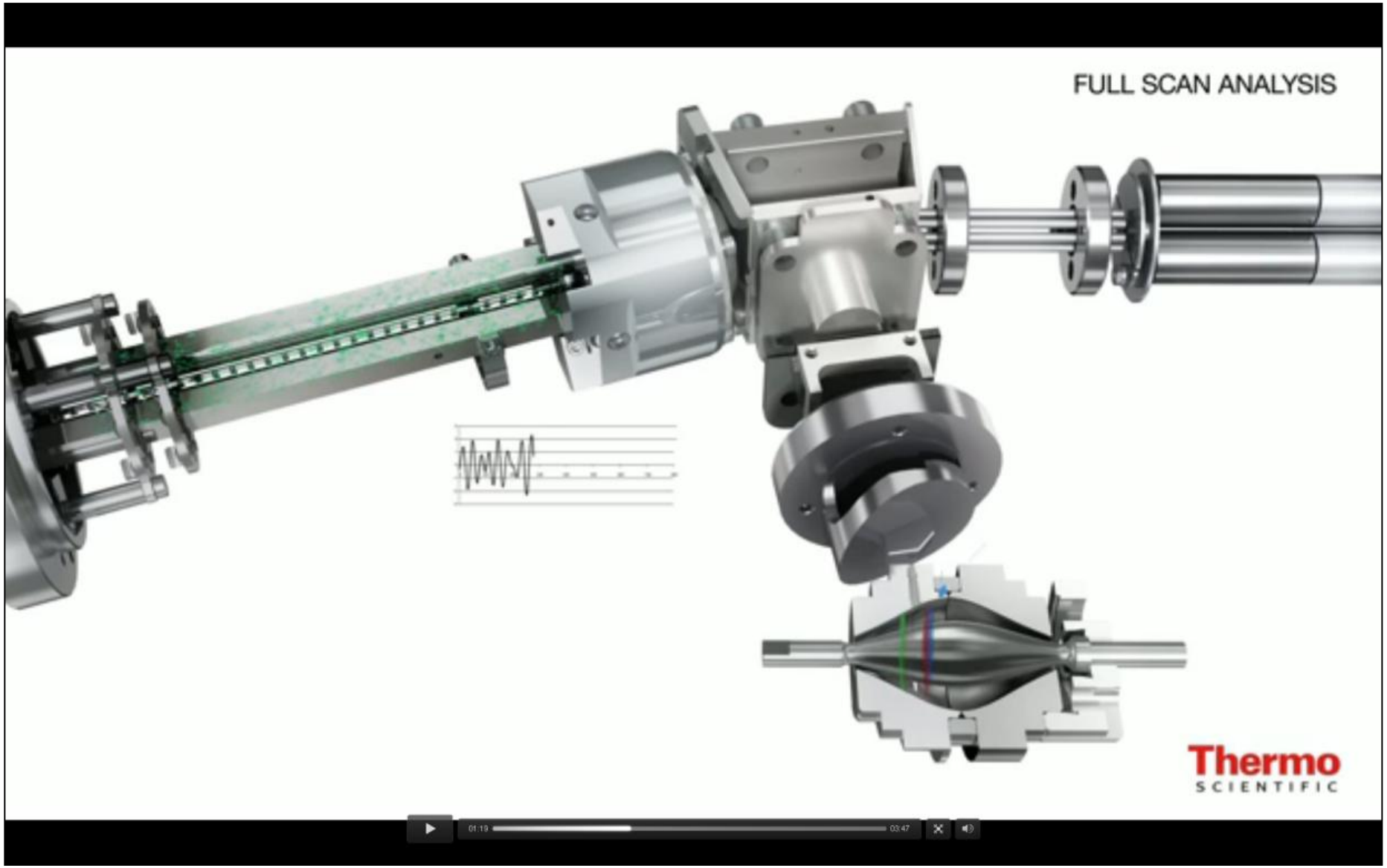

ThermoFisher SCIENTIFIC

# 90° Bent Flatapole



- Similar design to Q Exactive Plus and Q Exactive HF
- Axial field to optimize ion transfer
- Neutrals are removed from ion beam

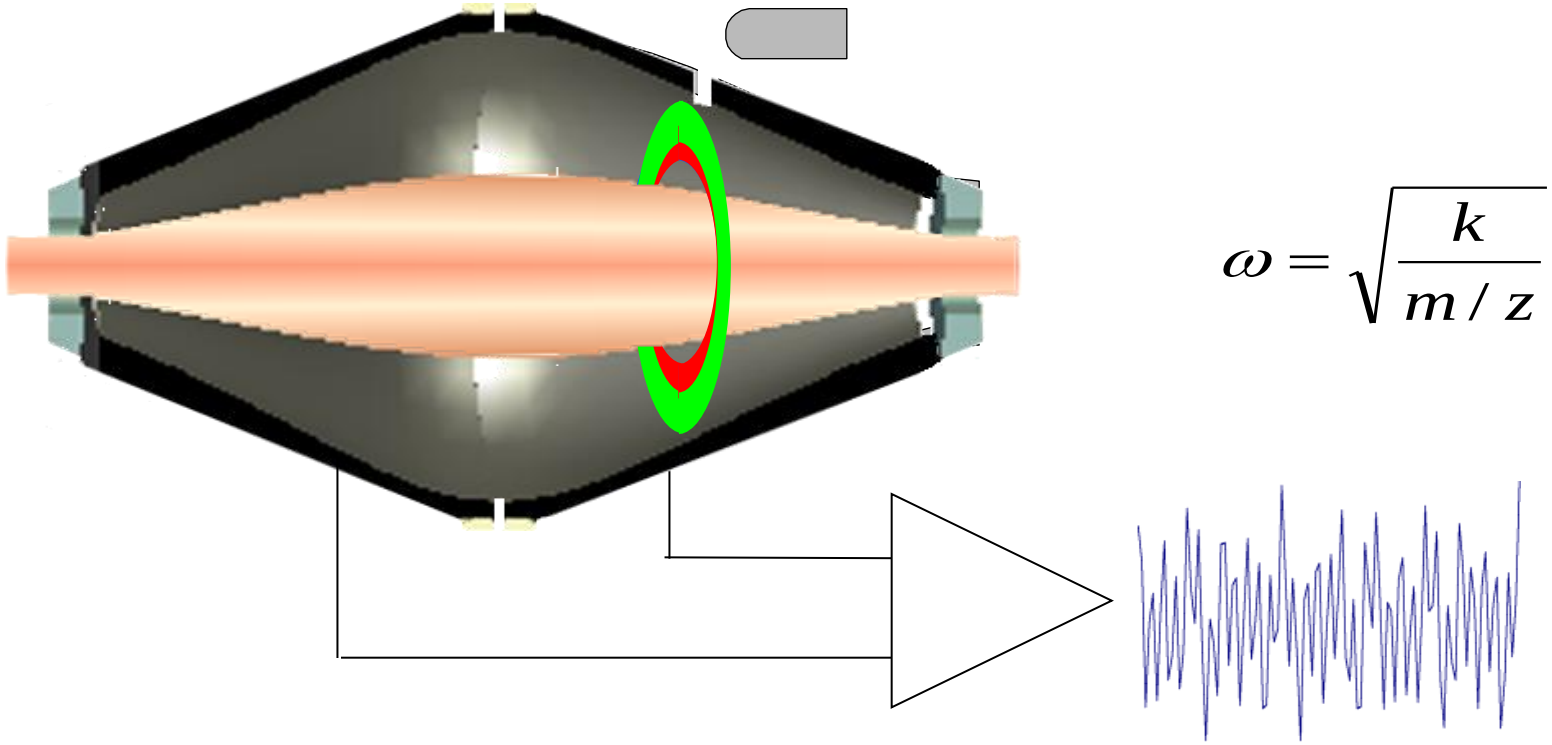
# Video of Basic Orbitrap Scan Modes






ThermoFisher SCIENTIFIC

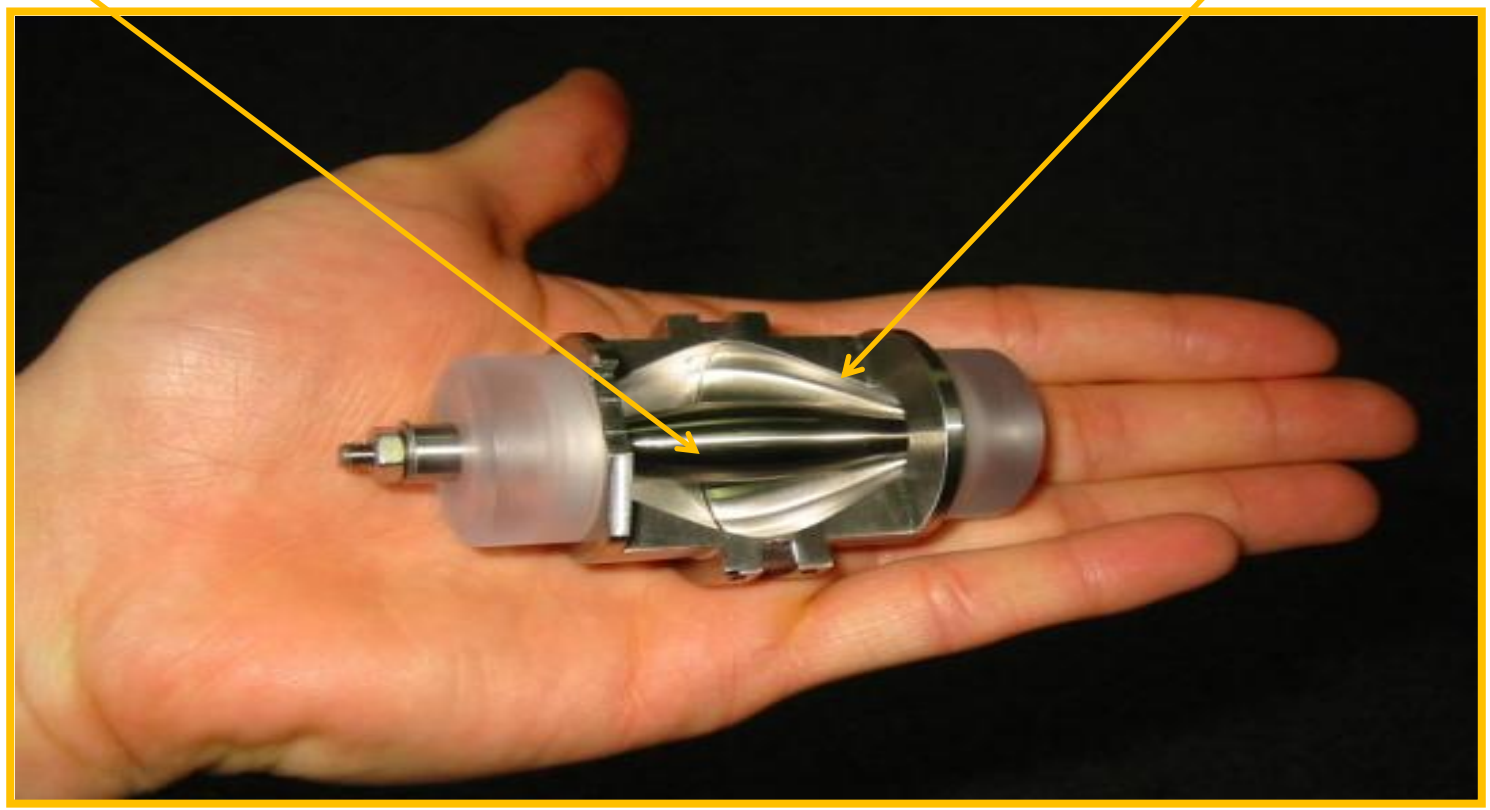
# Retaining the Ions in the Orbitrap



$$\omega = \sqrt{\frac{k}{m/z}}$$

- Frequency of axial oscillations are independent of initial conditions of ions entering trap
- Therefore these oscillations used for mass determination
- Image current measured by outer split electrodes (no electron multiplier to replace!)
- Ion frequencies determine by complex superposition of measured ring oscillations through Fourier transform

# What the Orbitrap Looks like



# Definitions to remember

- **Nominal mass**: the mass of an ion calculated using the *integer mass of the most abundant isotope of each element.*
  - ignores the mass defect, where H=1, C=12, O=16

- **Monoisotopic mass**: the mass of an ion calculated using the *exact mass of the most abundant isotope of each element.*
  - includes the mass defect, where $^{1}$H=1.**0078**, $^{12}$C=12.**0000**, $^{16}$O=15.**9949**

- **Average mass**: the mass of an ion calculated using the *relative average isotopic mass of each element.*
  - where C=12.0111(12.000000) (0.9890) + (13.003355) (0.0110) = 12.011 Da
  - H=1.00797, O=15.9994

- **Isotopic abundance**: the naturally occurring distribution of the same element with different atomic mass.
  - ex: $^{12}$C=12.0000 = 98.9%
    $^{13}$C=13.0034 = 1.1%

# How accurate is your mass?

- Mass accuracy

$$\Delta m / z = \frac{m_{meas} - m_{true}}{m_{true}} \cdot 10^6$$

- Quadrupole MS

$$\Delta m / z = \frac{500.1 - 500.0}{500} \cdot 10^6 = 200\,ppm$$

- Orbitrap MS

$$\Delta m / z = \frac{500.10314 - 500.10214}{500.10314} \cdot 10^6 = 2\,ppm$$

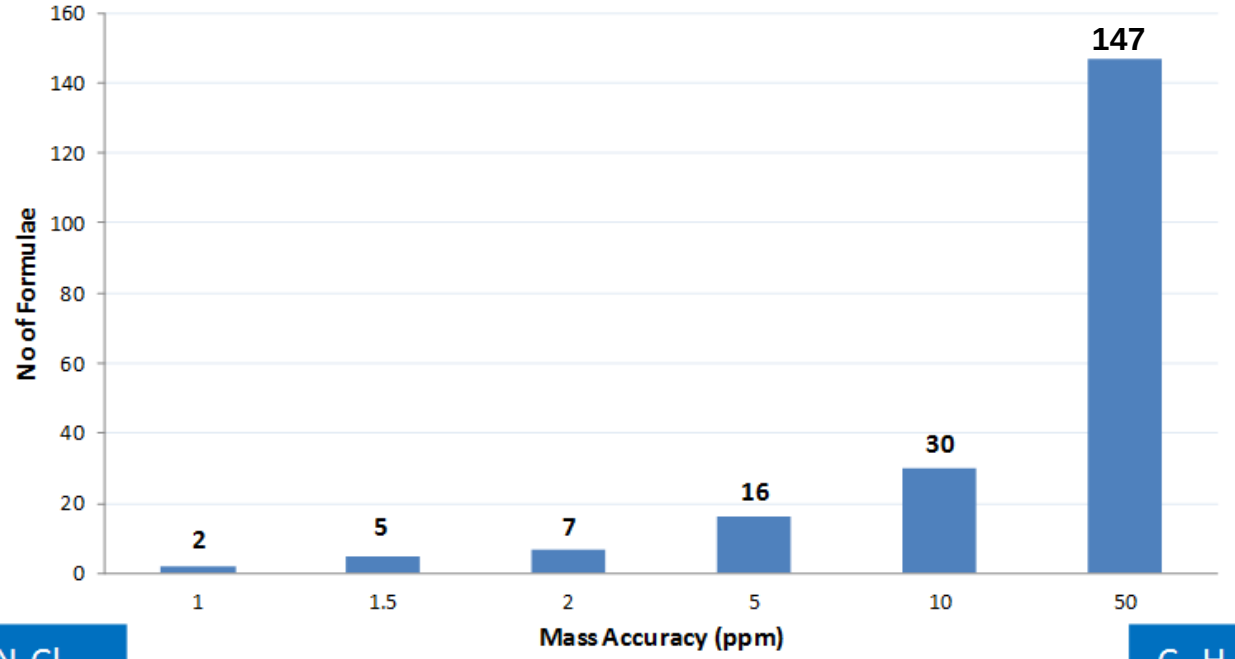
# Mass Accuracy

- Typical mass accuracy capability for various MS types:

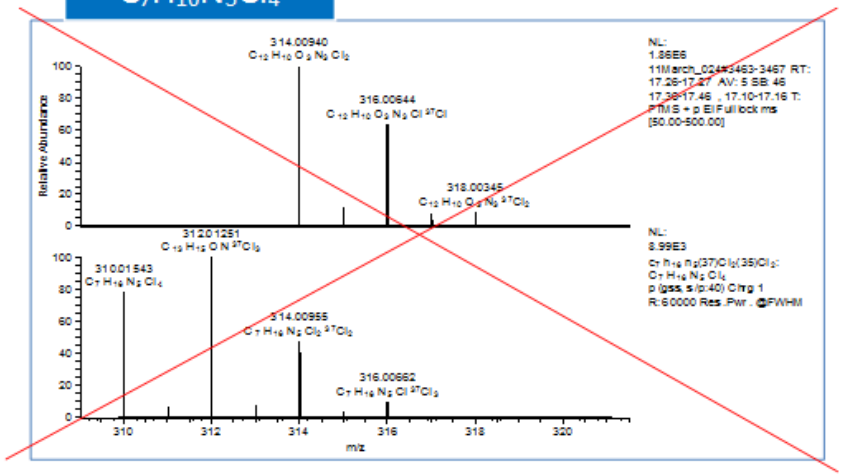
| Type | Mass Accuracy |
|---|---|
| FT-ICR-MS | 0.1 - 1 ppm |
| Orbitrap | 0.5 - 1 ppm |
| Magnetic Sector | 1 - 2 ppm |
| TOF-MS | 3 - 5 ppm |
| Q-TOF | 3 - 5 ppm |

*Source: Metabolomics Fiehn's lab*

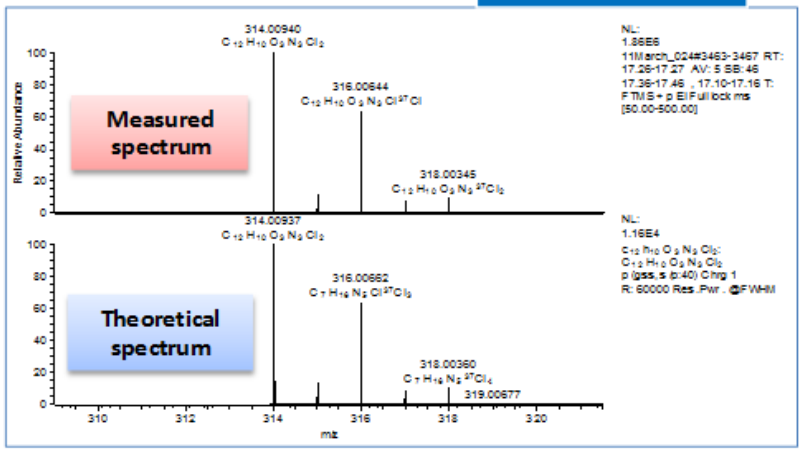
# Compound ID confirmation




$C_7H_{16}N_5Cl_4$



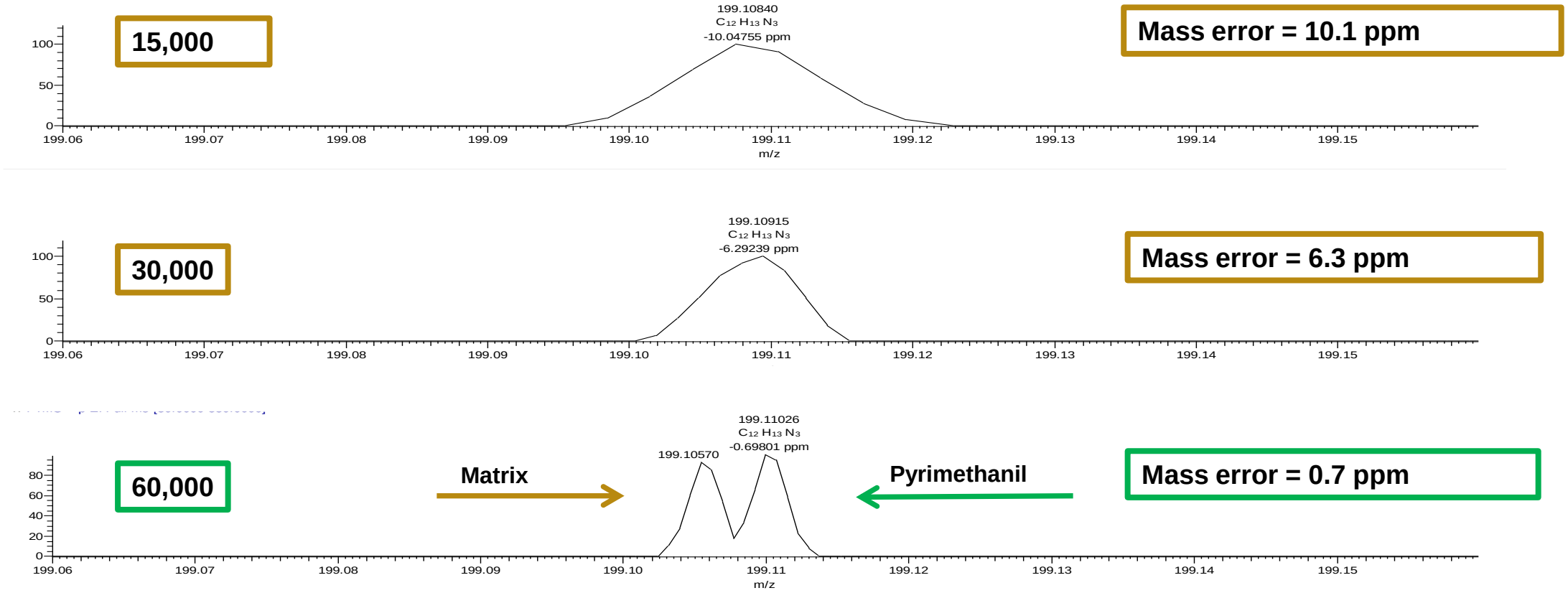
$C_{12}H_{10}N_5O_3Cl_2$






ThermoFisher SCIENTIFIC

# The Need for High Resolution

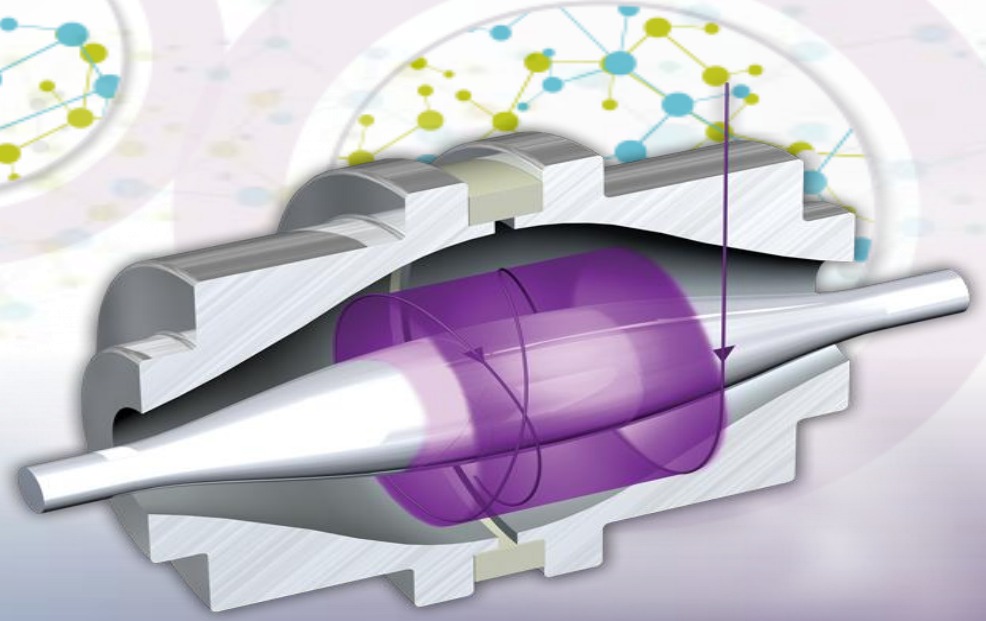





ThermoFisher SCIENTIFIC

## Thermo Scientific Q Exactive GC
## Hybrid Quadrupole-Orbitrap GC-MS/MS System

### Unprecedented Depth in GC-MS Analysis

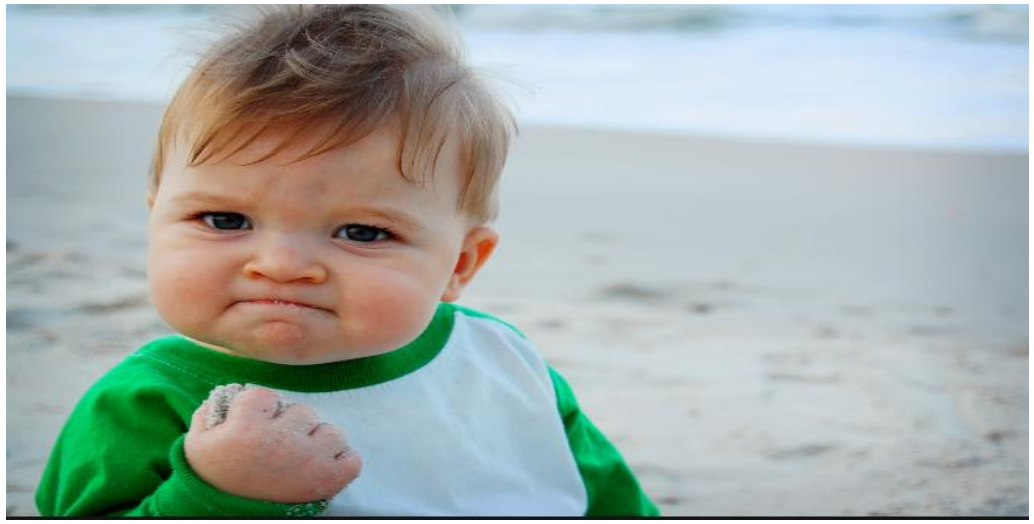




ThermoFisher SCIENTIFIC

# Q&A

- Thank you for your attention!
- Q&A



***We are changing the game!***