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Redefining Routine Analysis

Thermo Scientific Exactive GC
Orbitrap GC-MS System

Multi-award-winning Orbitrap GC-MS Technology

Metabolomics

Food & Beverage

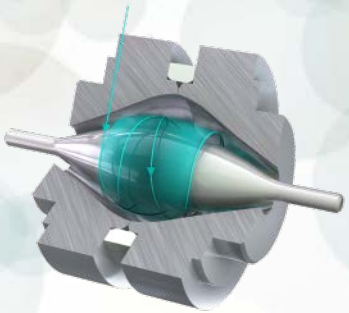
Industrial

Environmental

Pharmaceutical

Clinical & Toxicology

unknowns
discovery
research



Thermo Scientific™ Q Exactive™ GC system

Unprecedented Depth in Analysis

RP 120,000 (FWHM @ *m/z* 200)

EI/CI; Full-scan, timed-SIM

MS/MS capability

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Orbitrap GC-MS Technology: From the Experts

a game changer

Prof. Joshua Coon

University of Wisconsin, USA

a really powerful tool

Dr. Esteban Abad Holgado

CSIC Spain

clearly a major step forward

Dr. Hans Mol

RIKILT Netherlands

it feels like a step change

Dr. Karl Burgess

University of Glasgow, UK

a new level of performance

Prof. Jana Hajšlová

UTC Prague, CZ

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New Addition to the Orbitrap GC-MS Family

Redefining Routine GC-MS

RP 60,000 (FWHM @ *m/z* 200)

EI/CI; Full-scan; Timed-SIM

Thermo Scientific™ Exactive™ GC system

Thermo Scientific Q Exactive GC system

Unprecedented Depth in Analysis

RP 120,000 (FWHM @ *m/z* 200)

EI/CI; Full-scan, Timed-SIM

MS/MS capability

New Exactive GC Orbitrap GC-MS System

Redefining Routine GC-MS

RP 60,000 (FWHM @ *m/z* 200)

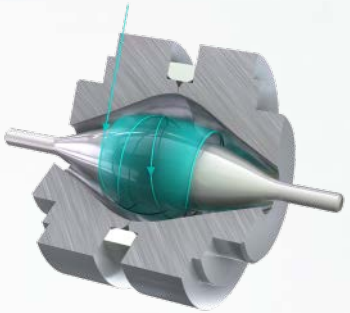
EI/CI; Full-scan; Timed-SIM

Thermo Scientific Exactive GC System

knowns
routine
screening

Food & Beverage

Environmental



Industrial

Clinical & Toxicology

The Frontier of Routine GC-MS

High Selectivity, Non-targeted Data Acquisition

- Fast instrument and method set-up
- Method consolidation
- Adjustable scope of analysis
- Quantitative and qualitative information in a single run
- High-efficiency data processing
- Retrospective data analysis

Exactive GC system: The Technology Inside

Orbitrap mass analyzer

Incredible HRAM performance

Highly regarded Q Exactive GC system platform

Thermo Scientific™ TRACE™ 1310 GC System

Unique modular injector and detector design

Rapid heat cycling

Thermo Scientific™ ExtractaBrite™ Ion Source technology

Routine grade robustness

Patented RF lens

Removable without breaking vacuum

Exactive GC system: The Technology Inside

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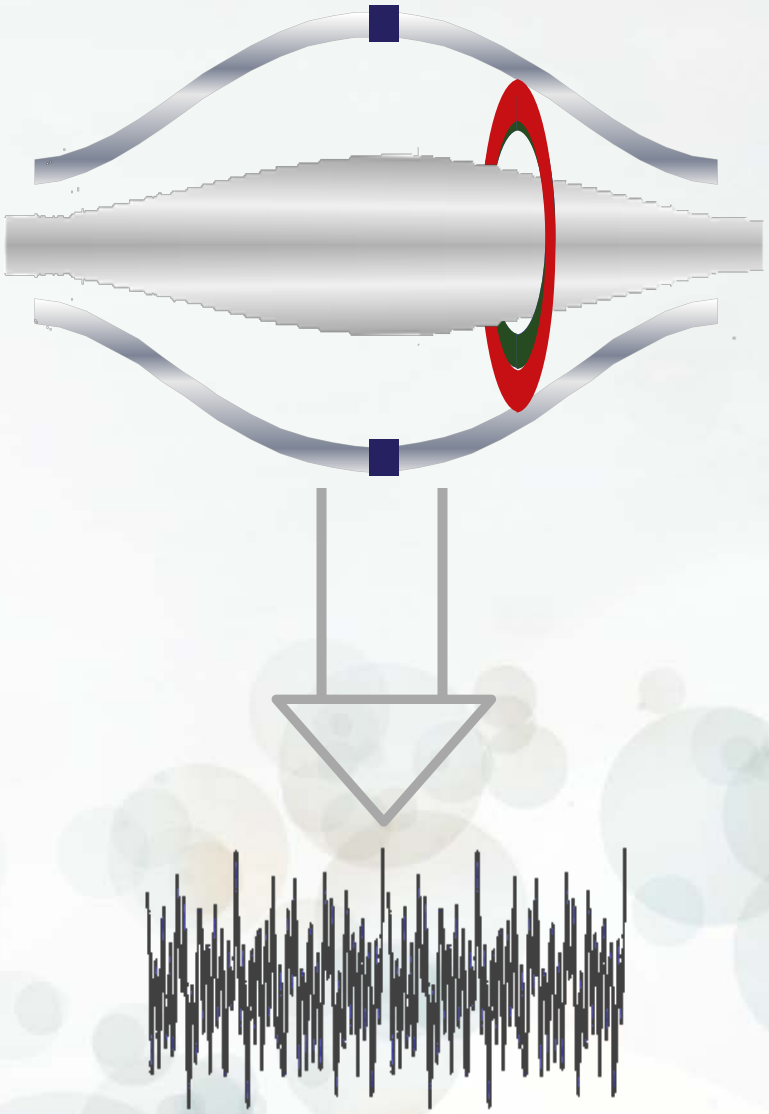
Orbitrap Mass Analyzer



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

- Ions injected into the Orbitrap are trapped in an electrostatic field
- Each ion oscillates axially with a frequency that is proportional to its mass
- An image current of these oscillations is measured using a split outer electrode
- This image is then converted to a mass spectrum using Fourier transform
- The longer a signal (transient) is measured, the higher the resolution

Exactive GC system Highlights

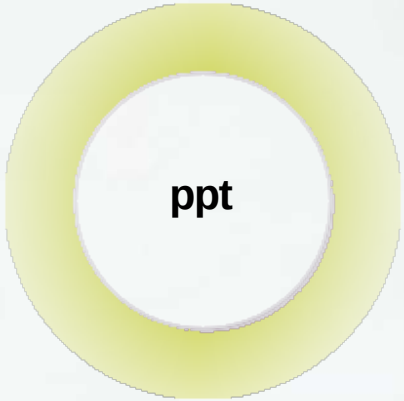
Resolving Power

- Maximum selectivity
- Fast enough for GC

Mass Accuracy

- Every scan
- All concentrations
- In complex matrix
- Across the mass range
- Everyday!

Sensitivity

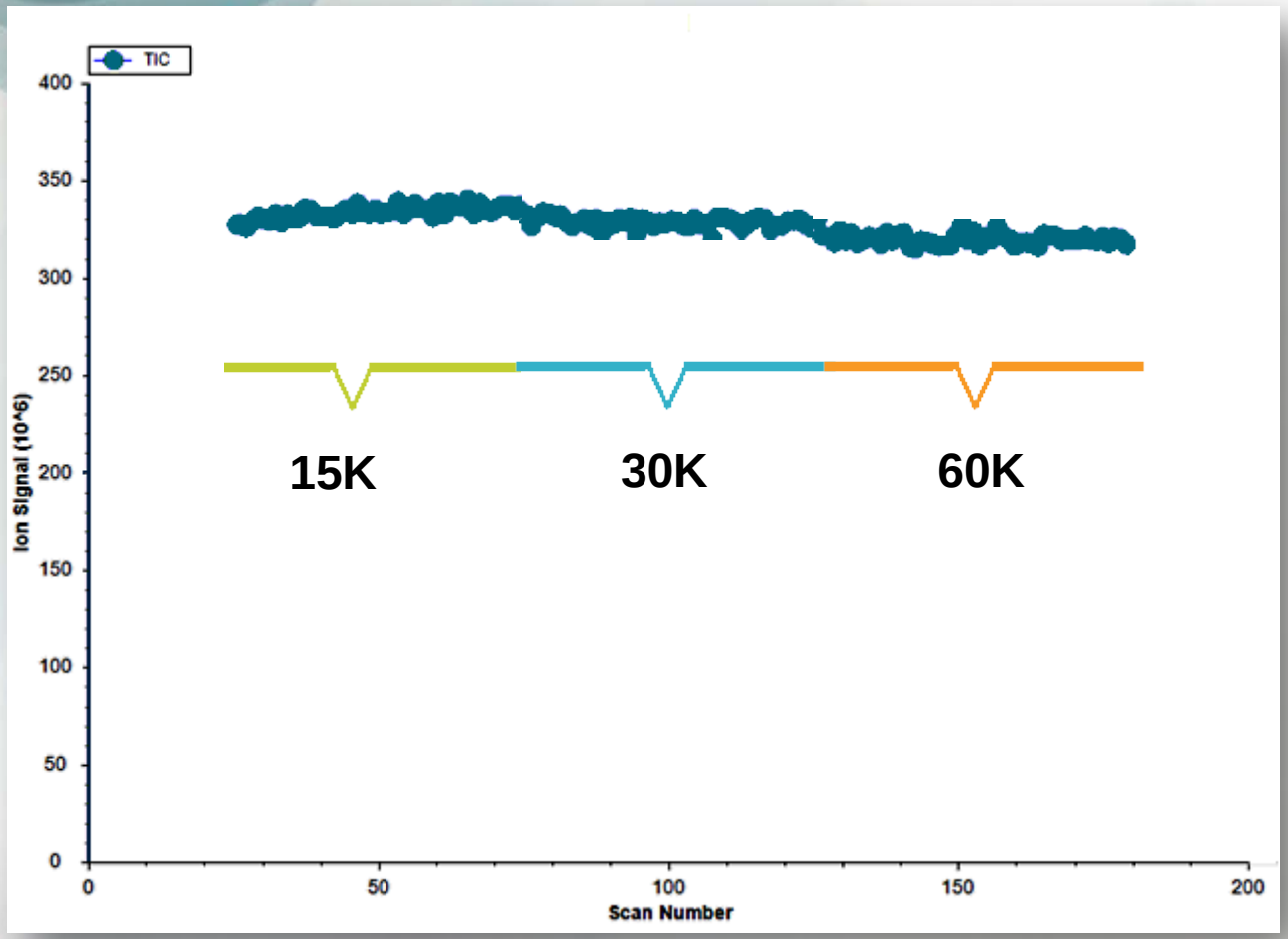


- In full-scan
- High selectivity
- High spectral fidelity

Dynamic Range

- Excellent coverage in sample profiling
- “Triple quad grade” quantitation in full-scan

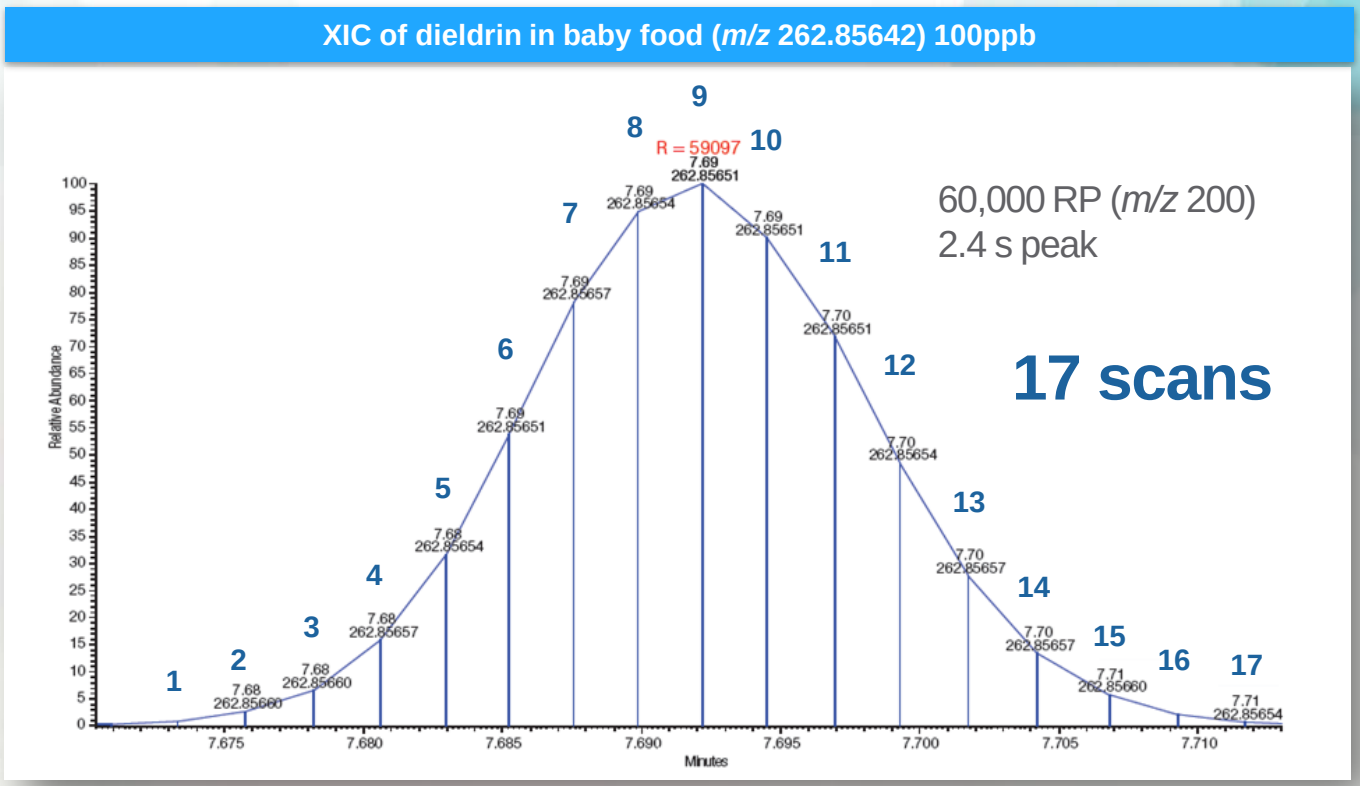
Resolving Power: Sensitivity



- TIC signal intensity vs. scan number
- Increase the resolving power during acquisition
- Negligible drop in sensitivity

High selectivity analysis all of the time

Resolving Power: Scan Rate @ 60K



- **Fast acquisition**
- Important for accurate profiling of narrow GC peaks
- Full-scan with resolving power of 60 (FWHM @ *m/z* 200) generates 17 scans

Fast enough for GC!

*Acquired on the Q Exactive GC system – the Exactive GC system provides equivalent performance

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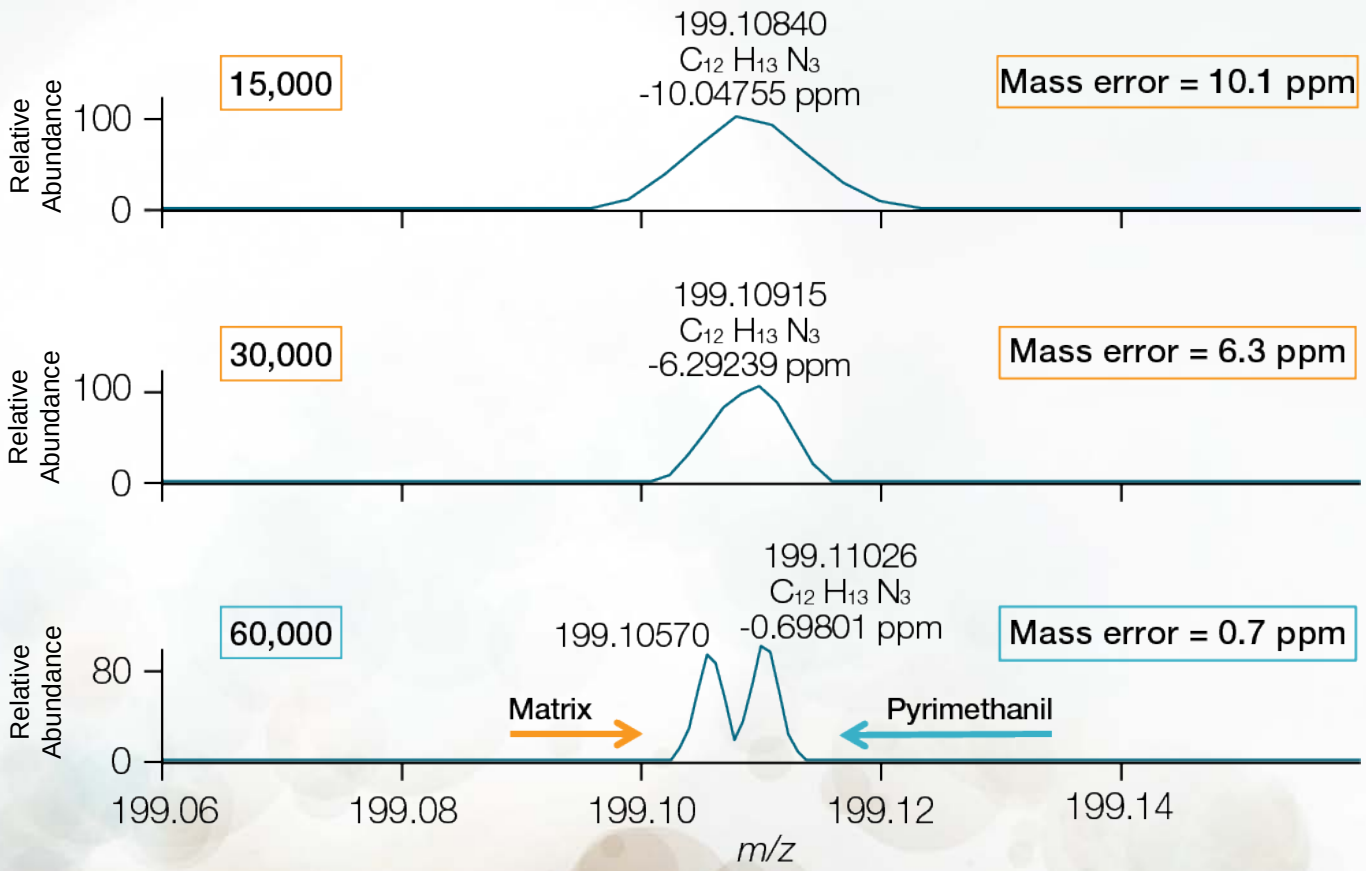
Resolving Power: Selectivity

Pyrimethanil in leek at 10 µg/Kg

< 5 ppm ID criteria



False negative

False negative

Positive Detection

High Selectivity ∴ high sensitivity *and* confidence in identification

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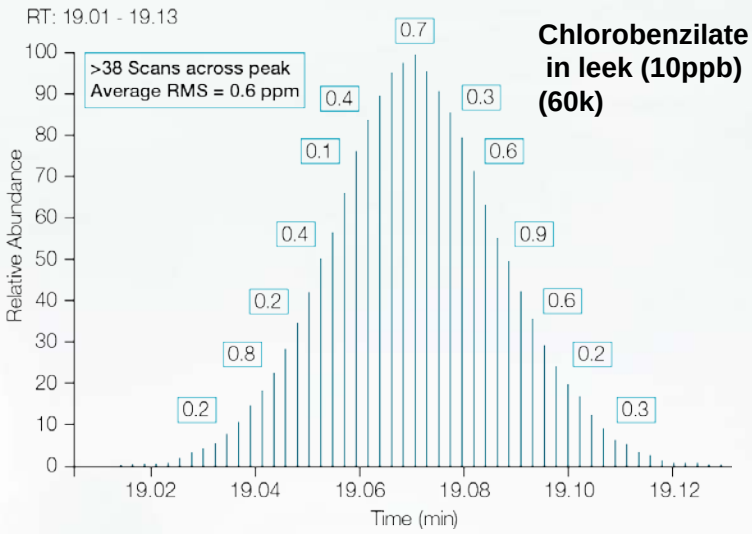
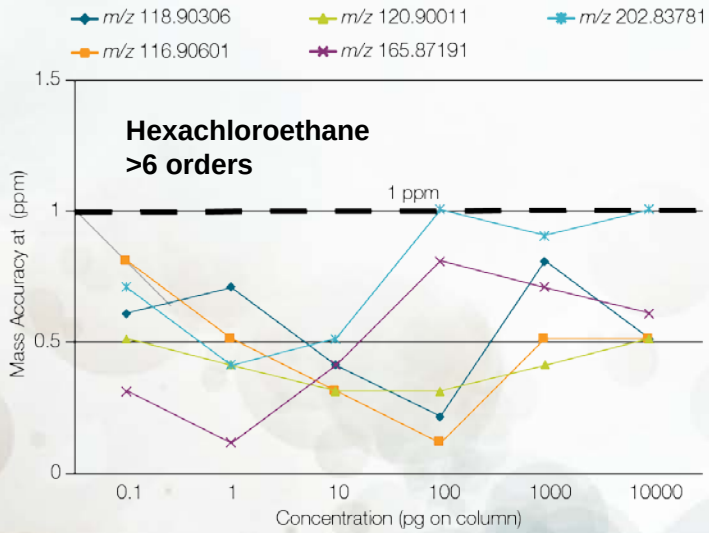
High Mass Accuracy

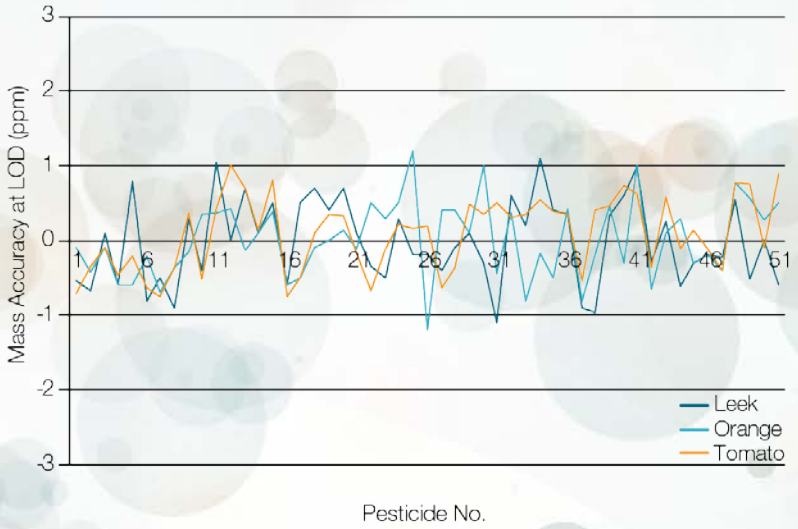


Chlorobenzilate in leek (10ppb) (60k)

- Typically <1ppm
- Across the peak
- Across the concentration range
- In matrix



50 pesticides in 3 different matrices



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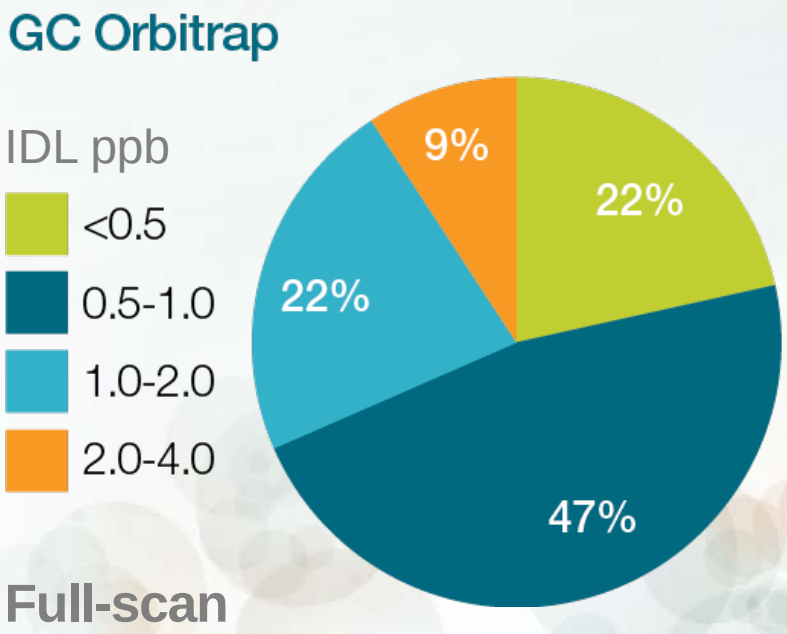
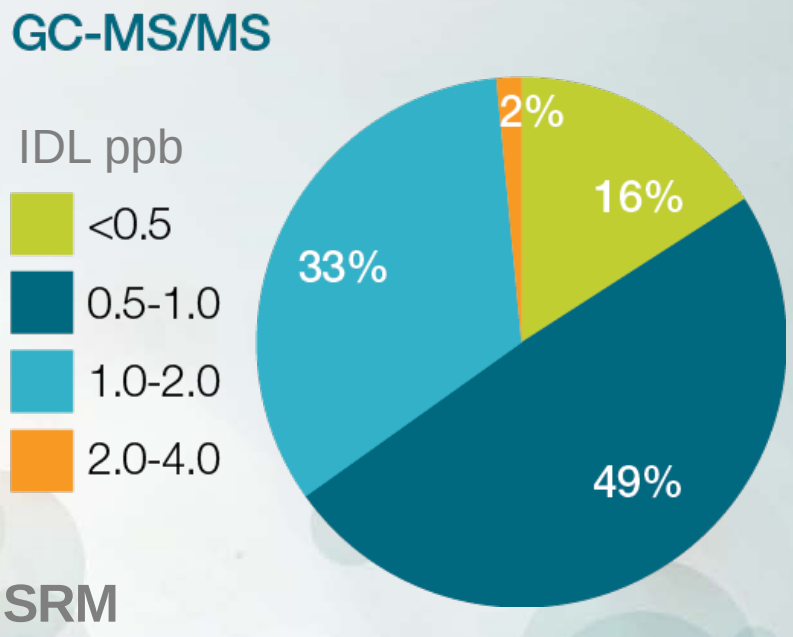
High Sensitivity Full-scan

150 compounds in mixed vegetable matrix





Triple quadrupole level sensitivity possible with a non-target acquisition

*Acquired on the Q Exactive GC system – the Exactive GC system provides equivalent performance

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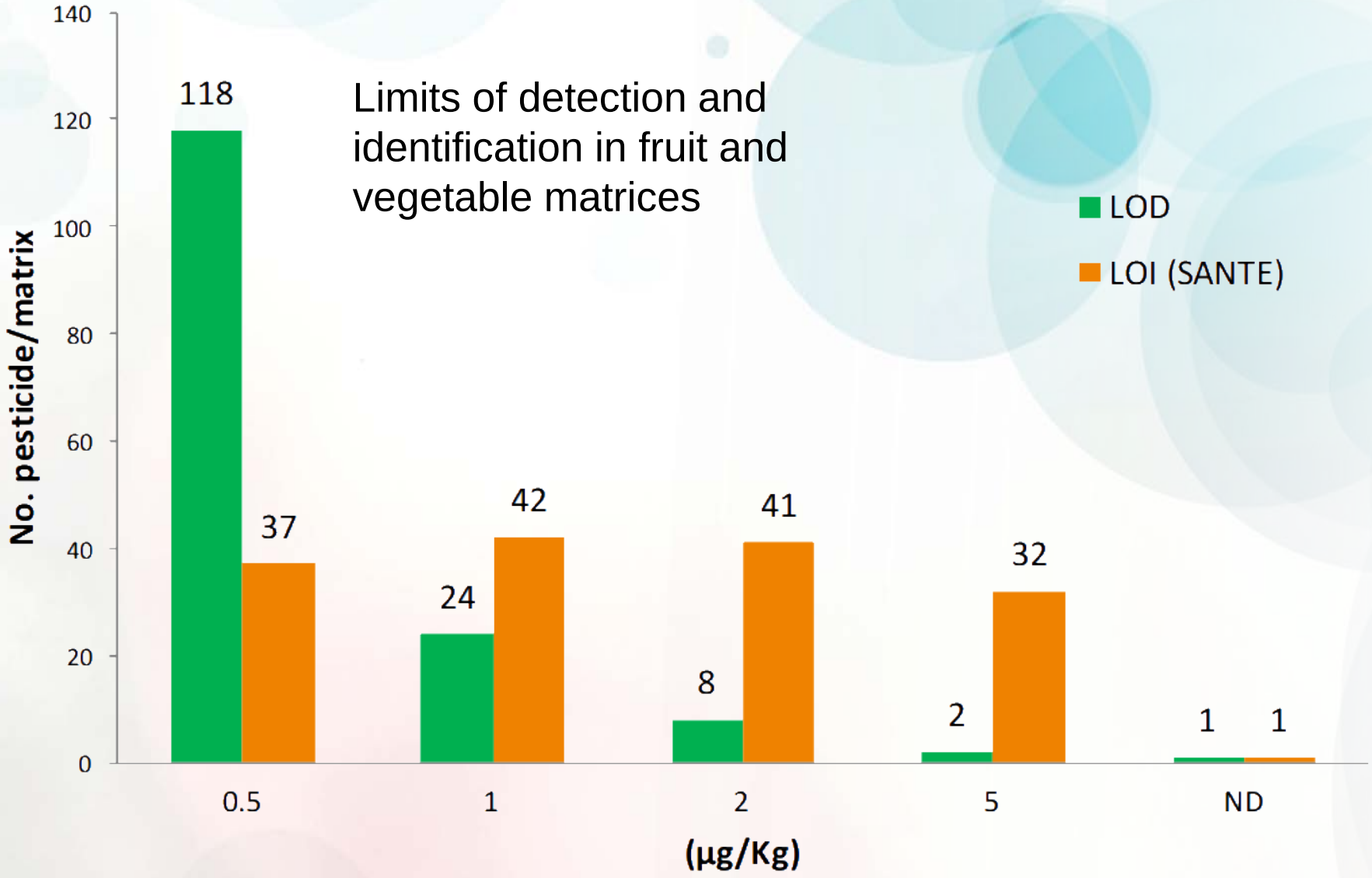
High Sensitivity Full-scan



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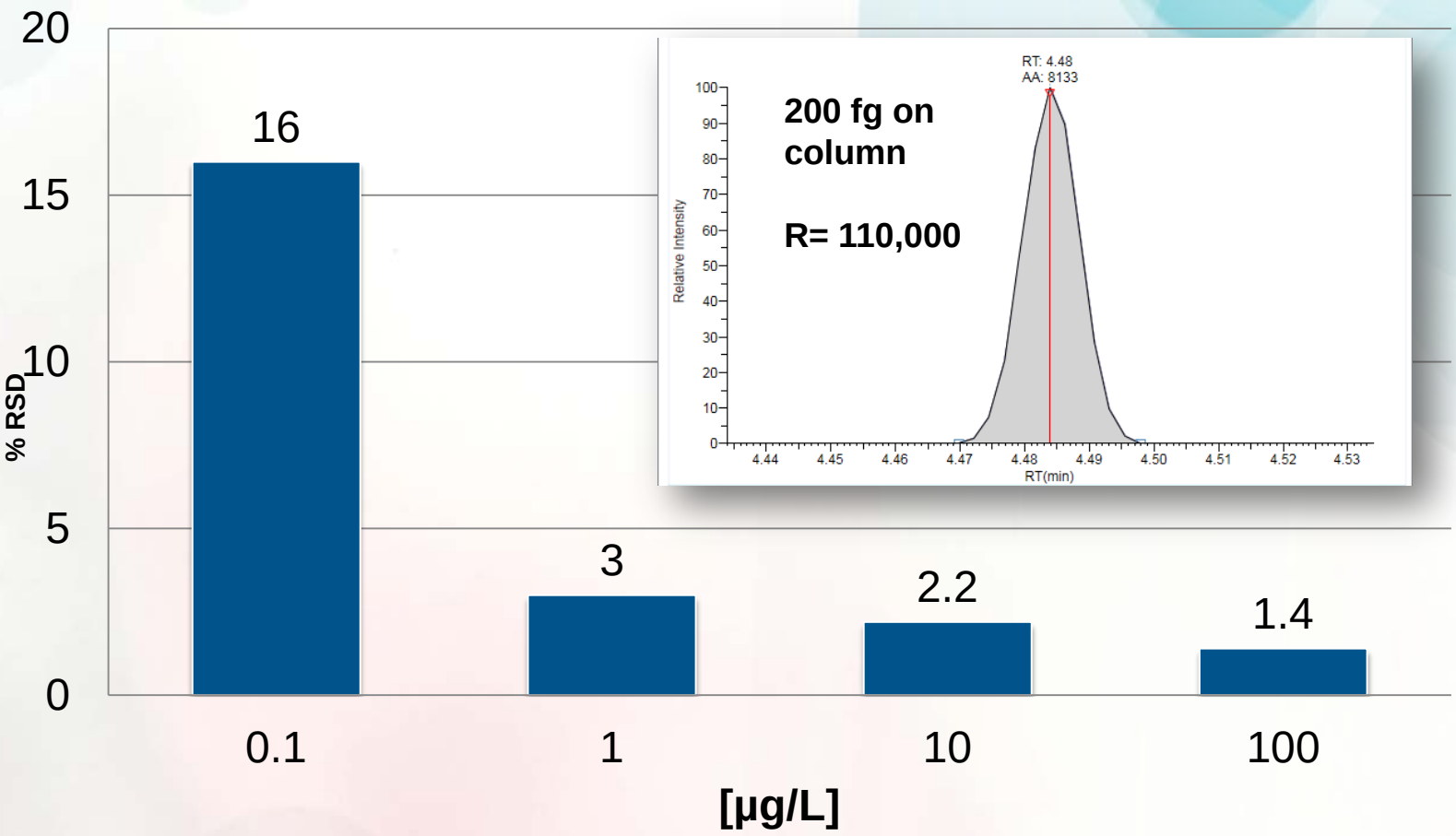
High Sensitivity Full-scan

N-Nitrosodimethylamine in tap water



* *n=5 injections per calibration standard were used except 1.0 µg/L level; where n=9 inj. were used*

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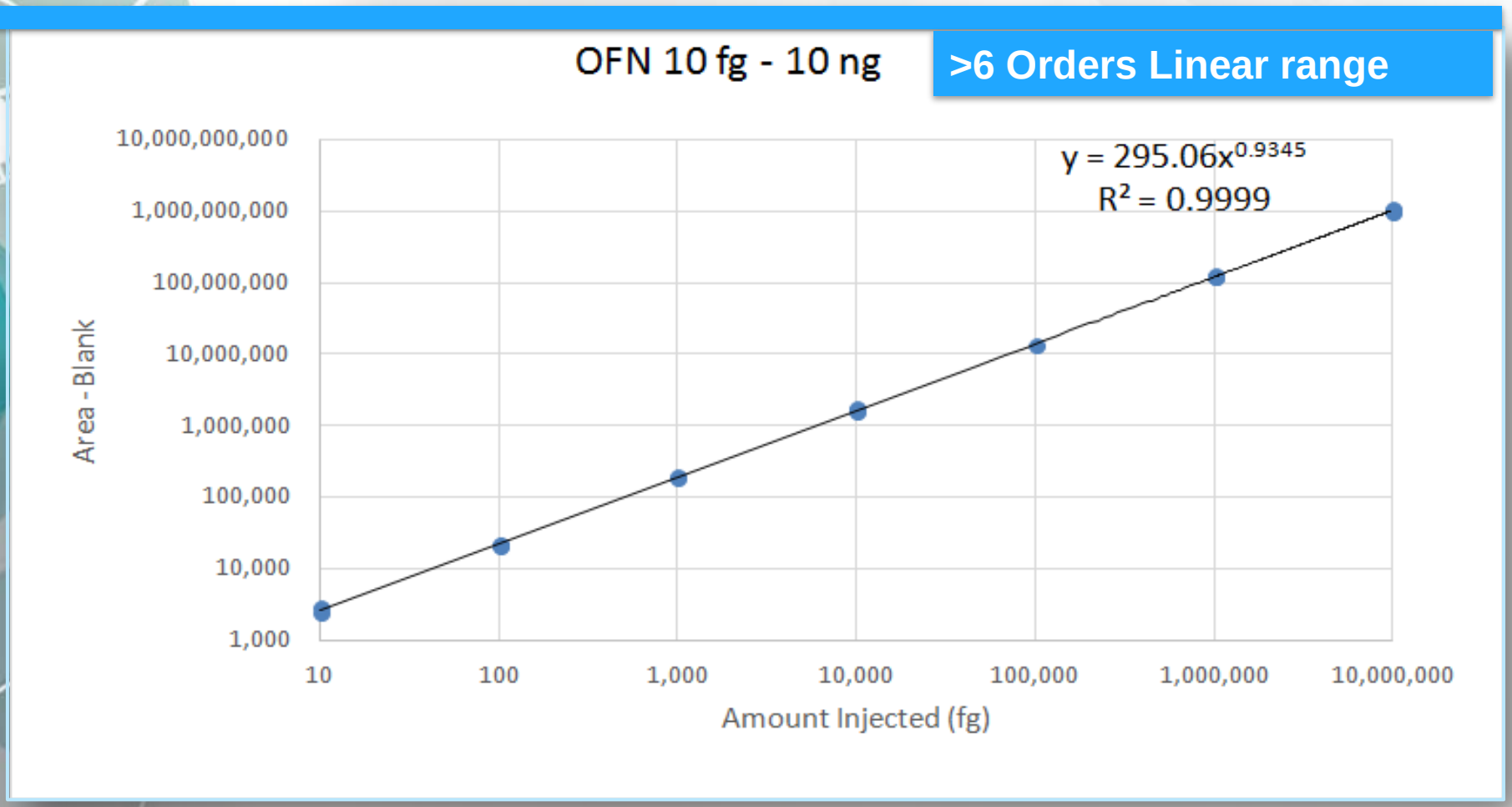
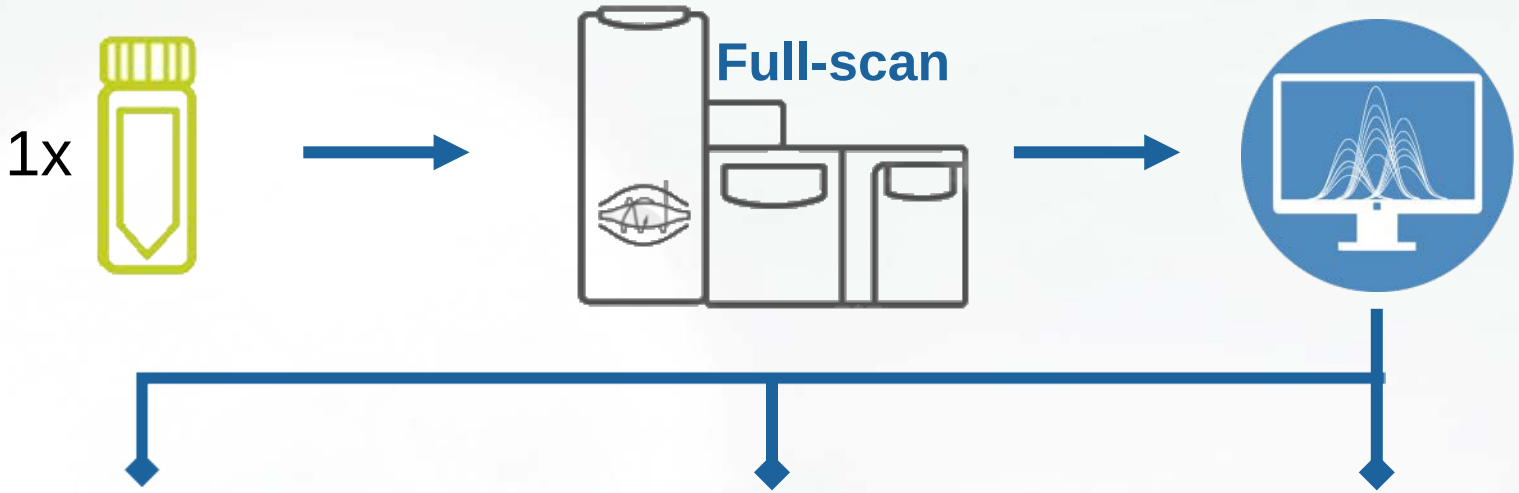
Dynamic Range



Triple quadrupole grade quantitation in full scan

*Acquired on the Q Exactive GC system – the Exactive GC system provides equivalent performance

Exactive GC System Main Workflows



expected

Targeted Quantitation

suspected

Targeted Screening

unexpected

Non-targeted Screening

Scope

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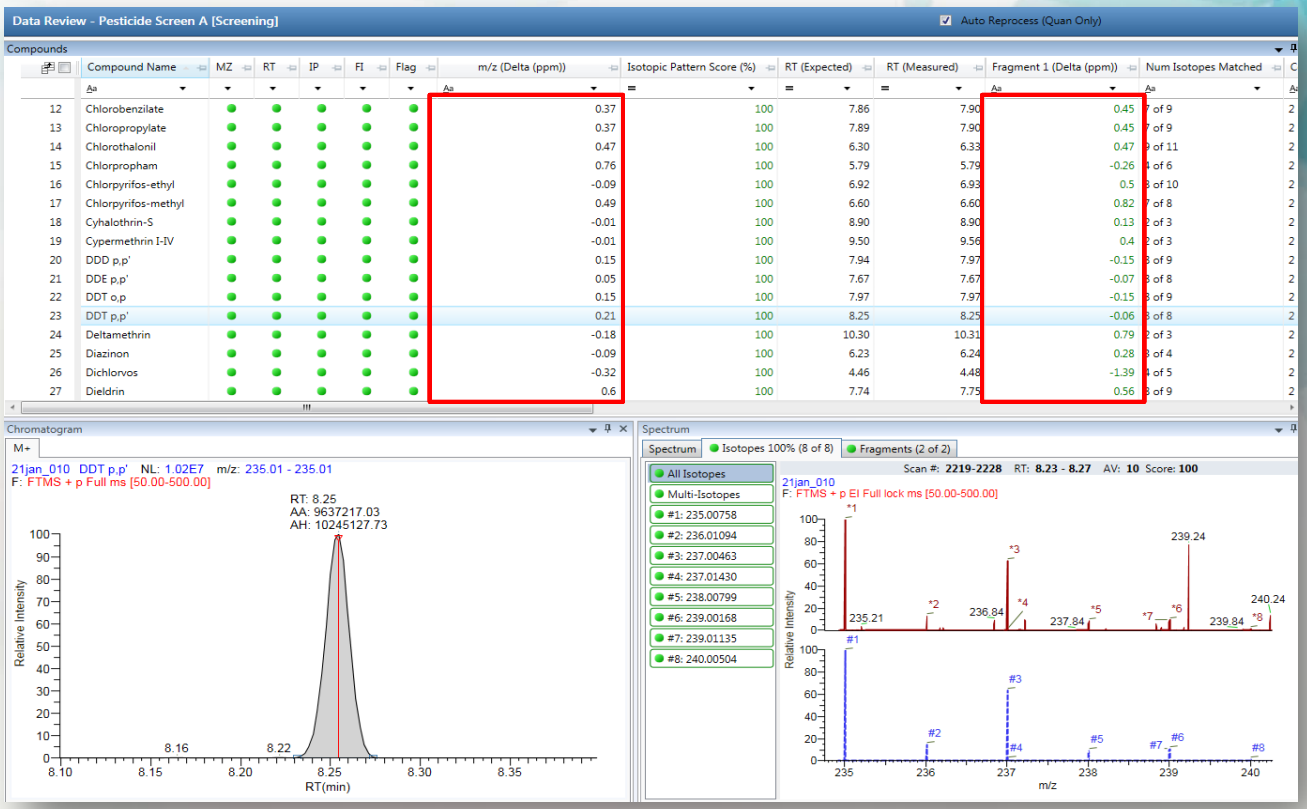
Orbitrap GC-MS Contaminants Library

- Fast start-up of screening and quantitation applications
- Thermo Scientific™ TraceFinder™ Compound Database >700 food and environmental contaminants
- HRAM Spectral Library of over 700 food and environmental contaminants
- User guide detailing how to install and make custom enhancements to library
- Compound classes V1:
  - Pesticides, PAHs, PCBs,Dioxins and Furans. Flame Retardants

Targeted Screening using Thermo Scientific™ TraceFinder™ Software



Positively identified example

- p,p'-DDT
- Accurate mass confirmation (2 ppm mass window)
- Isotopic pattern
- Fragment ions
- Sub ppm mass accuracy throughout

Automated screening and identification

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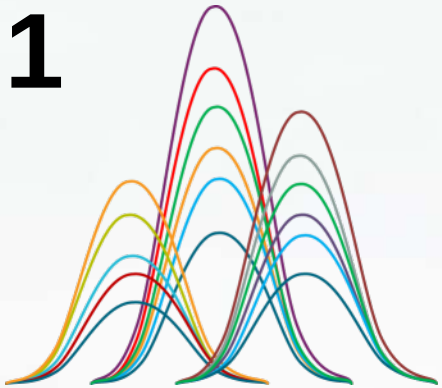
Non-targeted Screening Overview

detect and refine

1



- Sensitive and selective peak detection
- High resolution spectral deconvolution
- Clean spectrum

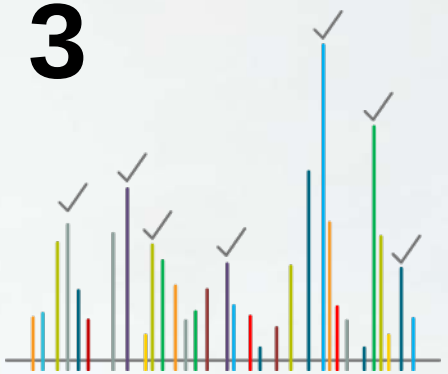
generate candidates

2

- Search spectra against spectral libraries
- HRAM or unit mass
- Candidates list generated

filter and identify

3

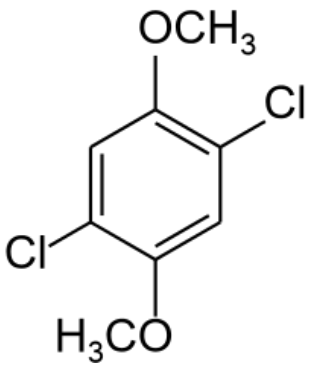


- High resolution filtering of candidates
- Putative identifications made

Process semi/fully automated as preferred

Non-targeted Screening HRF

Candidate



Subset formulae

$C_8H_8Cl_2O_2$

Acq m/z	Fragment ID	Theo m/z	Mass Error (ppm)
147.9477	$C_5Cl_2H_2O$	147.9477	0.20277
148.9369	$C_5Cl[37]ClHO$	148.9369	0.2679
149.9448	$C_5Cl[37]ClH_2O$	149.9448	0.06602
151.9419	$C_5[37]Cl_2\ H_2O$	151.9418	0.72528
154.9895	$C_7ClH_4O_2$	154.9894	0.38712
155.9974	$C_7ClH_5O_2$	155.9973	0.89745
157.9943	$C_7[37]ClH_5O_2$	157.9943	0.25381
159.9479	$C_6Cl_2H_2O$	159.9477	0.87529
161.9446	$C_6\ Cl[37]ClH_2O$	161.9448	0.80213
162.9711	$C6Cl_2H_5O$	162.9712	0.36816
163.9745	$C_5[13]CCl_2H_5O$	163.9745	0.3342
164.9682	$C_6Cl[37]ClH_5O$	164.9682	0.24186
165.9716	$C_5CCl[37]ClH_5O$	165.9716	0.02832

$$\text{HRF Score} = \frac{\sum (m/z * \text{Intensity})_{\text{explained}}}{\sum (m/z * \text{Intensity})_{\text{observed}}} \times 100\%$$

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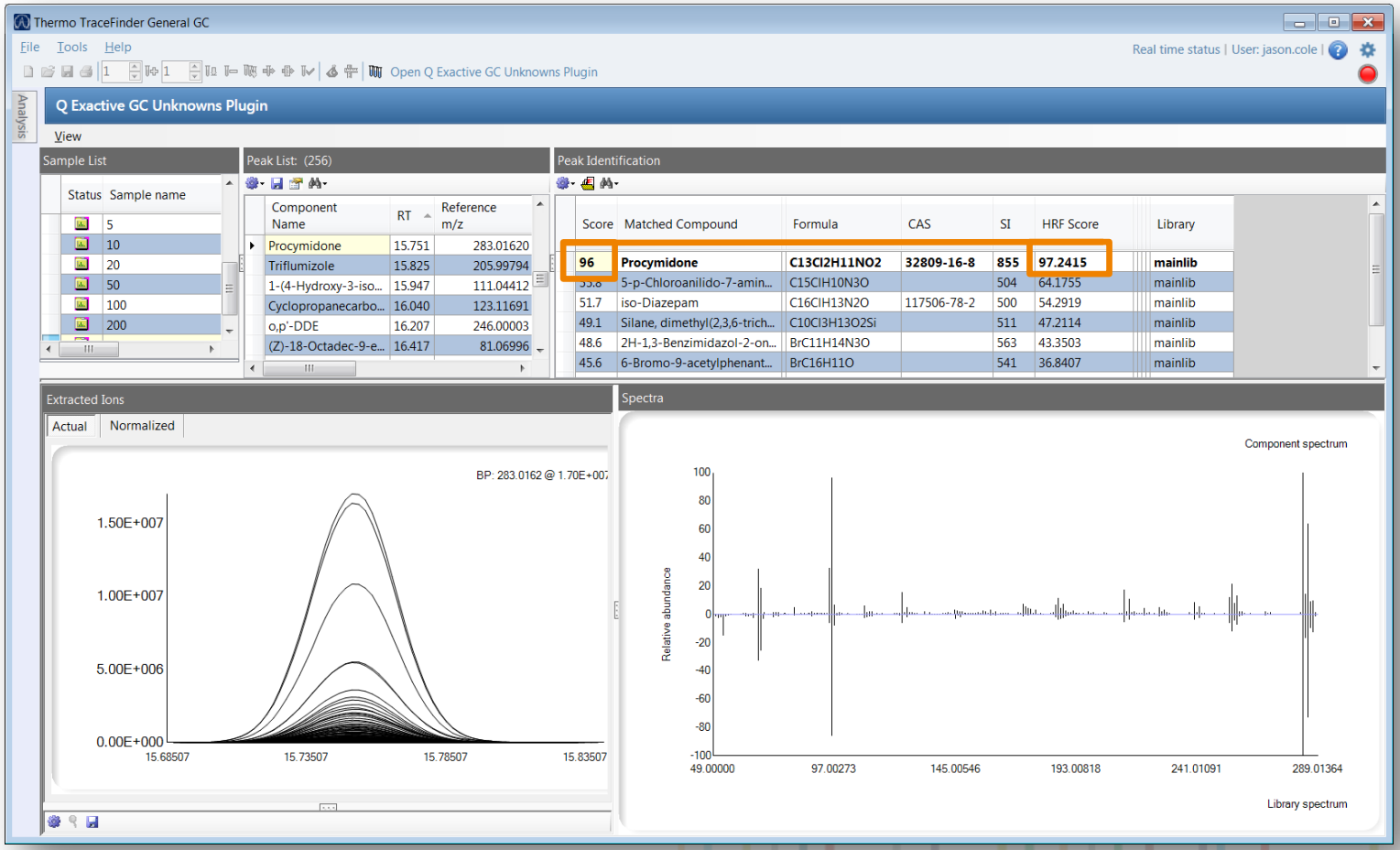
Non-targeted Screening Identification



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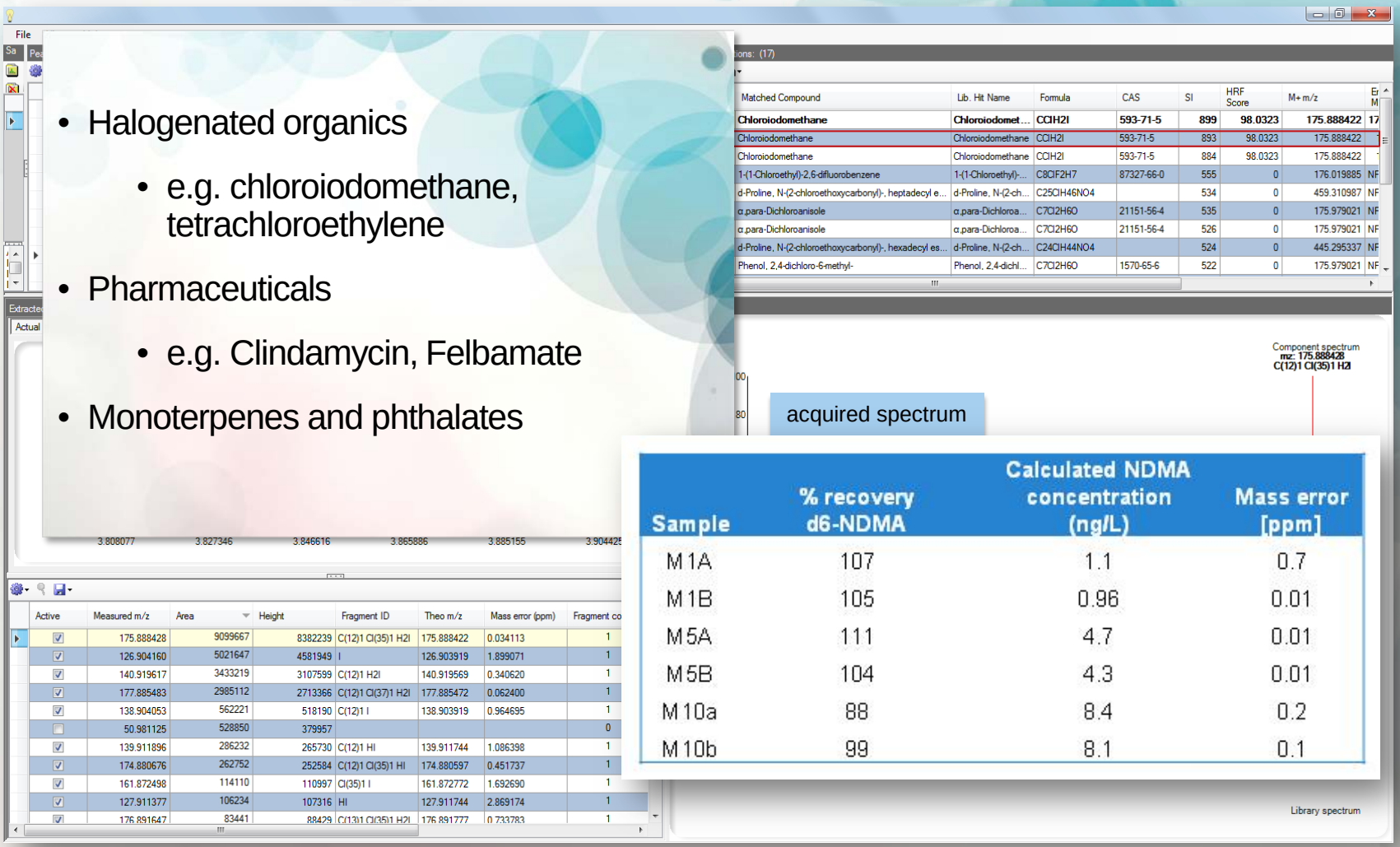
Non-targeted Screening Tap Water

Detected compounds in tap water during nitrosamine quantitation

- Halogenated organics
  - e.g. chloroiodomethane, tetrachloroethylene
- Pharmaceuticals
  - e.g. Clindamycin, Felbamate
- Monoterpenes and phthalates



Sample	% recovery d6-NDMA	Calculated NDMA concentration (ng/L)	Mass error [ppm]
M1A	107	1.1	0.7
M1B	105	0.96	0.01
M5A	111	4.7	0.01
M5B	104	4.3	0.01
M10a	88	8.4	0.2
M10b	99	8.1	0.1

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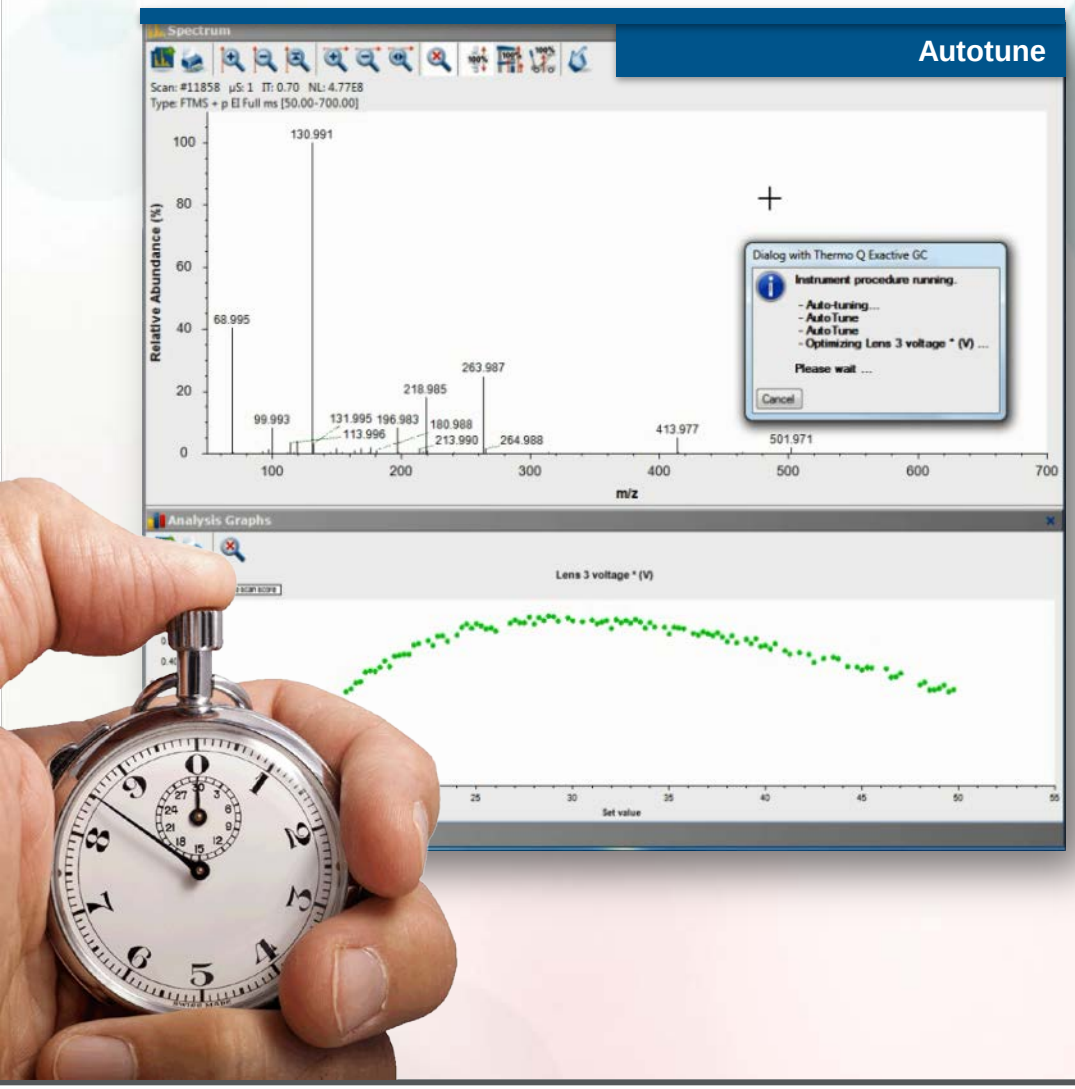
Fast and Automated Set-up



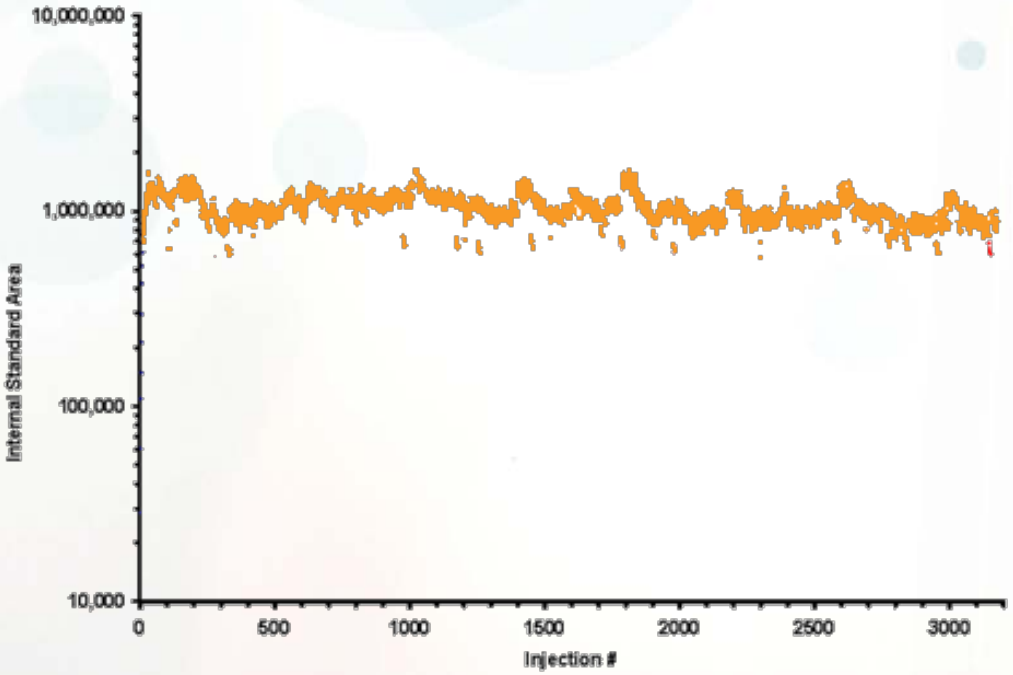
Tuning and Calibration

- Simple status
- Automated leak checking
- Automated tuning & calibration
- Source and lens tuning ~25 s
- Mass calibration ~30 s
- Ready to go < 1 min

Full-scan Simplicity

- Full-scan is really simple
- No setting of RT based windows
- Build sequence and hit start

Maximum Uptime: Routine-grade Robustness



Source Robustness in Matrix

- >3000 injections ExtractaBrite Ion Source
- BSTFA derivatized urine
- No source maintenance required during study

ExtractaBrite Ion Source Design

- Dual independent heated zones
- Patented RF lens protects post source ion optics
- Repeller designed to overcome any ion burn

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Maximum Uptime: “Never Vent”

“Never Vent” Philosophy

- Patented source plug
  - GC column change without venting
- ExtractaBrite Ion Source
  - Source change without venting
  - Including all areas where ion burn can form
- Minutes to use the vacuum probe interlock system

Acknowledgements

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