

# **Analysis of Organic Pollutants in Water and Sediment:**

## **Instrumental approaches for demanding problems**

- 1. Improved GC/MS sensitivity**
- 2. LC/MS solutions for new environmental problems**

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Environmental Industry Manager

Agilent Technologies



Agilent Technologies

# Definitions

- Sensitivity
  - Analytical definition: slope of the plot of amount of analyte (x-axis) versus signal response (y-axis)
  - Commonly used definition: minimum amount of analyte that gives an acceptable response (more correctly “limit of detection”)
- Sensitivity Specification (GC/MS)
  - S/N achieved for a very small amount of analyte injected under a carefully defined set of the instrument conditions using a “matrix-free” sample
- Useable Sensitivity
  - Instrument and method parameters and tools that enhance the signal response and reduced noise when **working with real sample matrices**

# Seminar Overview:

## Useful Sensitivity for Improved Environmental Analyses

### Technology Curve – Where is GC/MS Today?

#### Hardware Evolution

GC – Capillary Flow Technologies (Backflush)

MS – Triple-Axis Detector, Gain Normalization and Fast Electronics for Synchronous SIM/Scan

#### Software Evolution

MS – Trace Ion Detection and Deconvolution

GC – Retention Time Locking and New Databases

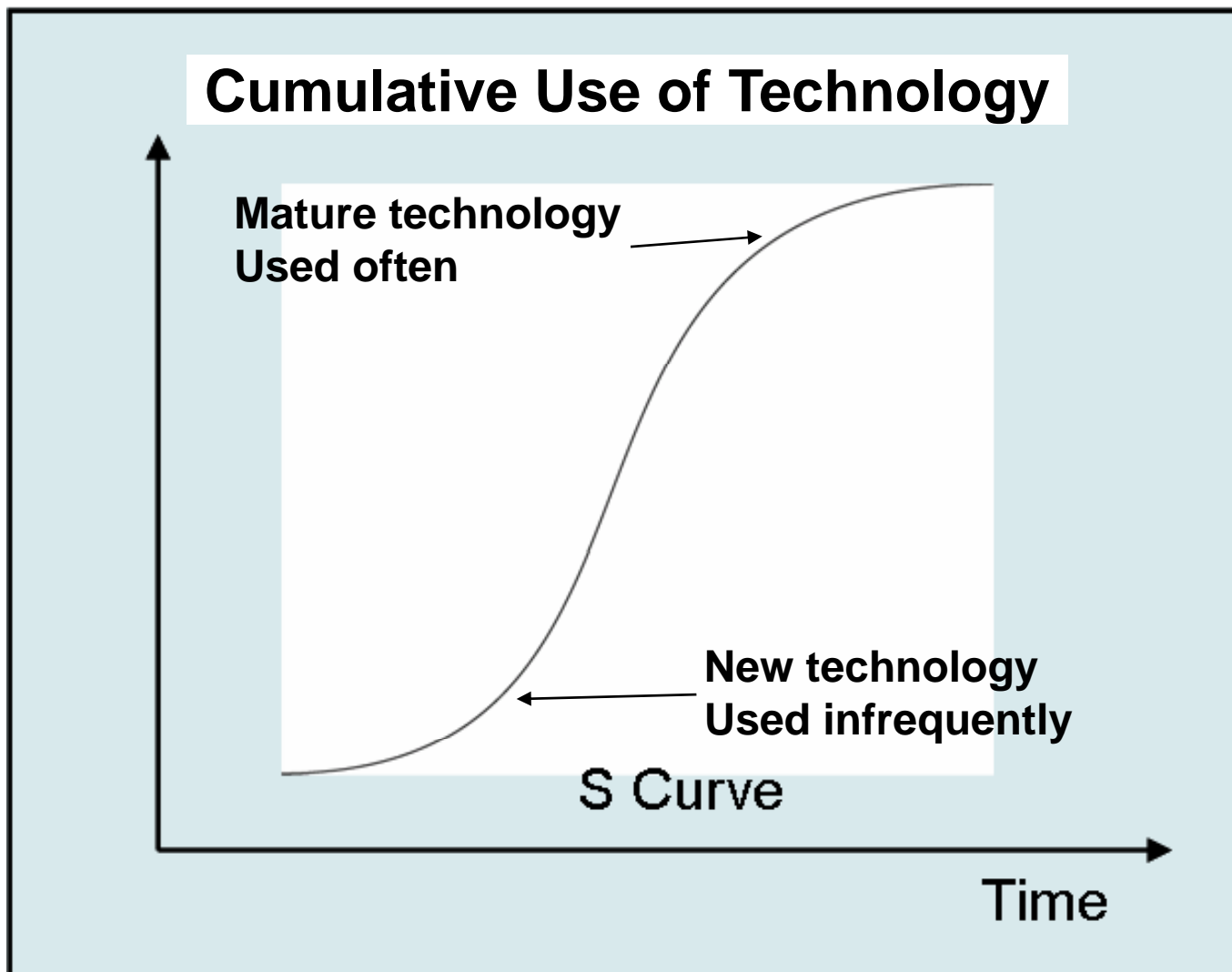
GC/MS: Detector sensitivity improves usable sensitivity

Agilent LC/MS solutions for Environmental Analysis

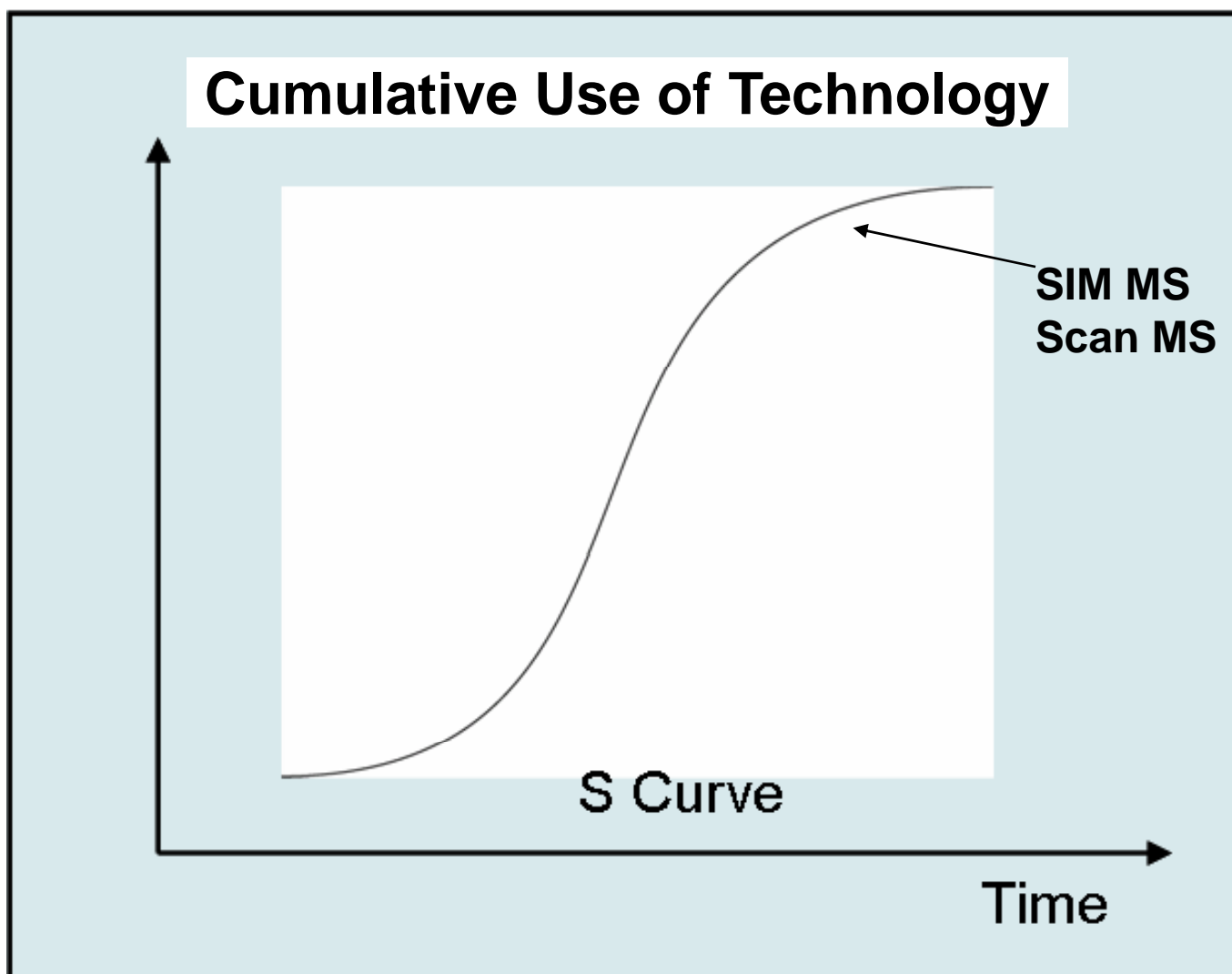
Perfluorinated Organic Compounds

Pharmaceutical compounds in water and sludge

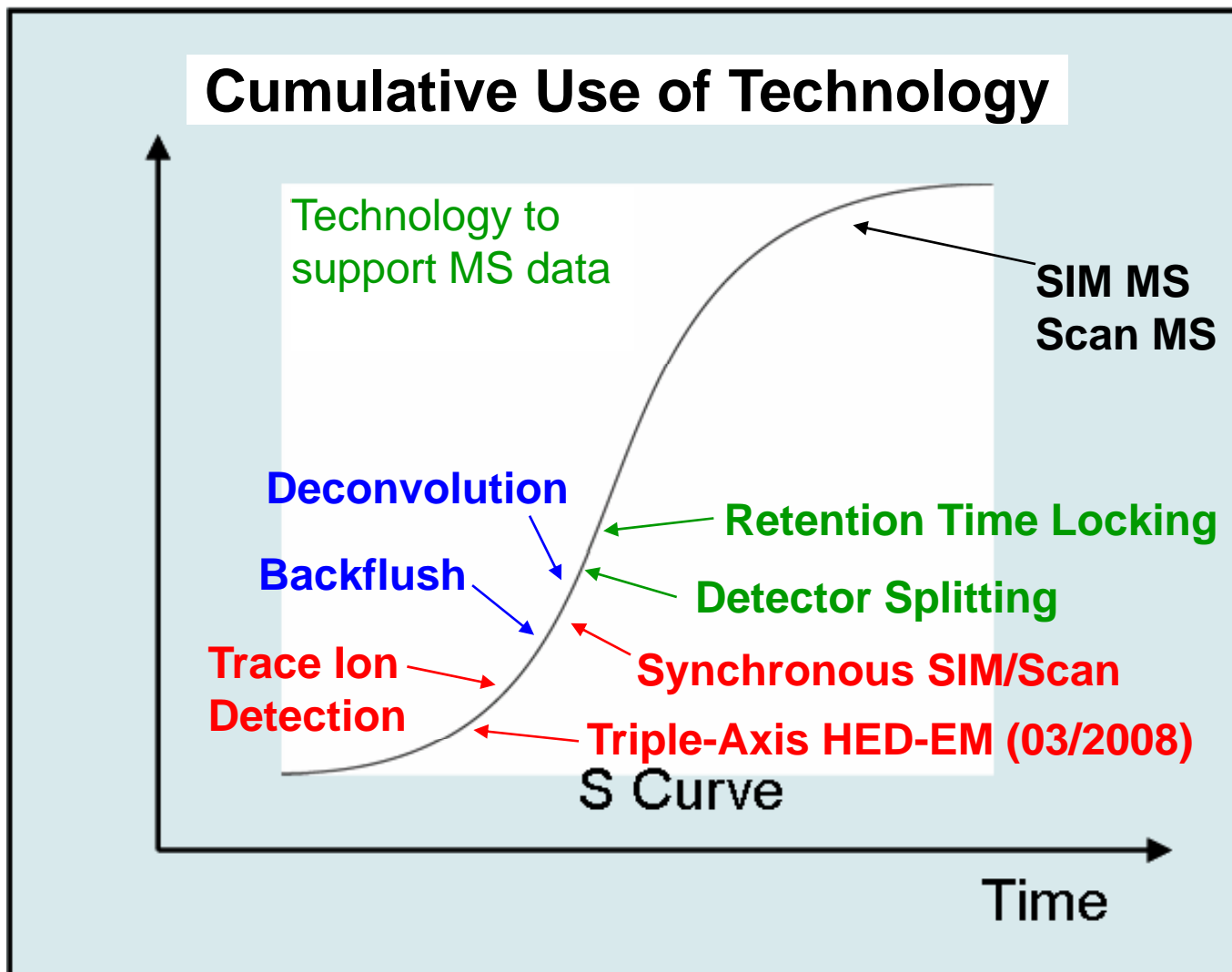
# Positioning of Basic GC/MS



# Positioning of Basic GC/MS



# The Benefits of Newer GC/MS Technologies



# Improve Productivity and Useable Sensitivity in Environmental Analysis with Agilent's 7890A/5975C GC/MSD

**Trace Ion  
Detection**

**Pollutant  
Retention Time  
Locked Databases**

**Deconvolution  
Reporting  
Software**

**Triple-Axis  
Detector**

**Backflush and  
other Capillary  
Flow Technologies**

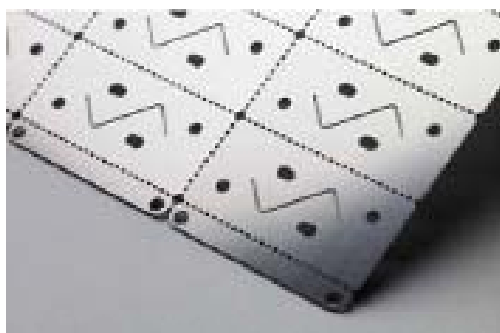
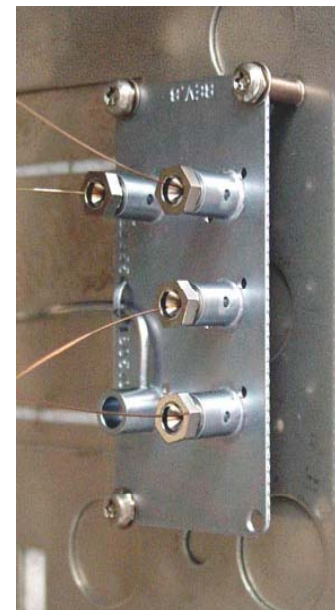


*Upgrades Available for All 5975 MSDs*

# Capillary Flow Technology

... a proprietary Agilent Technology

- Photolithographic chemical milling for **low dead volume**
- Diffusion bond two halves to form a single flow plate
- Small, thin profile provides **fast thermal response**
- Projection welded connections for **leak tight fittings**
- Deactivation of all internal surfaces for **inertness**
- SilTite (**metal**) ferrules





# 5<sup>th</sup> Generation Electronic Pressure Control (EPC)



- 3<sup>rd</sup>, 4<sup>th</sup> Generation EPC
- 0.01 psi
  - Diffusion bonded plate (2D)
  - one cable
  - three gas connectors
  - "credit card" size

6890N GC



- 1<sup>st</sup>, 2<sup>nd</sup> Generation EPC
- 0.1 psi
  - cables
  - gas lines & connectors
  - large size

5890 GC

7890A GC

The only GC to regulate pressure to 0.001 psi



- 5<sup>th</sup> Generation EPC
- Metal injection molded (3D)
  - Digital signal pathways

... improved reliability and precision

# Capillary Flow Technology for Environmental GC/MS Applications

- Detector splitting (detect peaks buried in matrix 'noise')
  - MS + ECD or ELCD
    - Confirmatory, selective, highly sensitive
  - MS + FPD or PFPD
    - Confirmatory, selective, highly sensitive
  - MS + NPD
    - Confirmatory, selective, highly sensitive nitrogen detection
  - MS + ECD + FPD
- Column backflush

**Not discussed in this seminar, but included in many literature references at the end of the slides**

# QuickSwap MSD Interface

Remove column w/o venting

- Air & H<sub>2</sub>O blocked

Safe disconnection of column from inlet for inlet maintenance

- Reversed flow through column during inlet maintenance

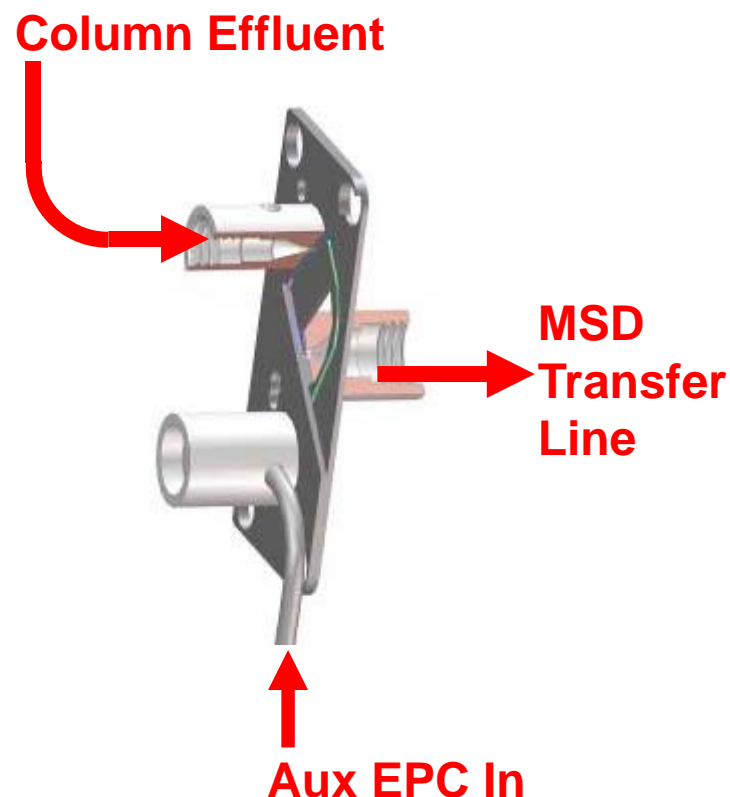
## Backflushing

- Removes heavies from column

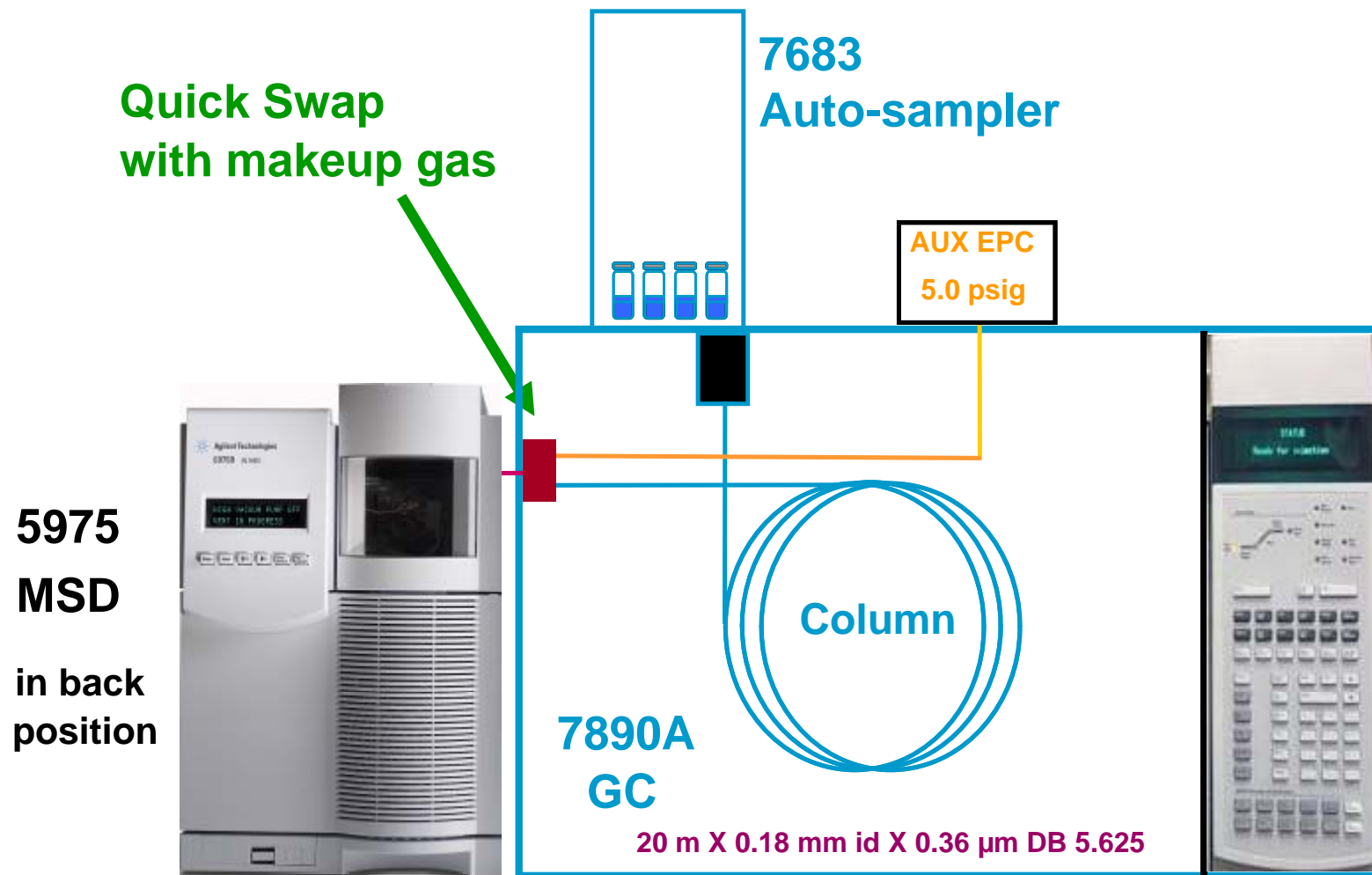
Maintain constant flow to MSD

Compensate for loss of sensitivity by making 10 µL injection

Turbo MSD required for backflushing

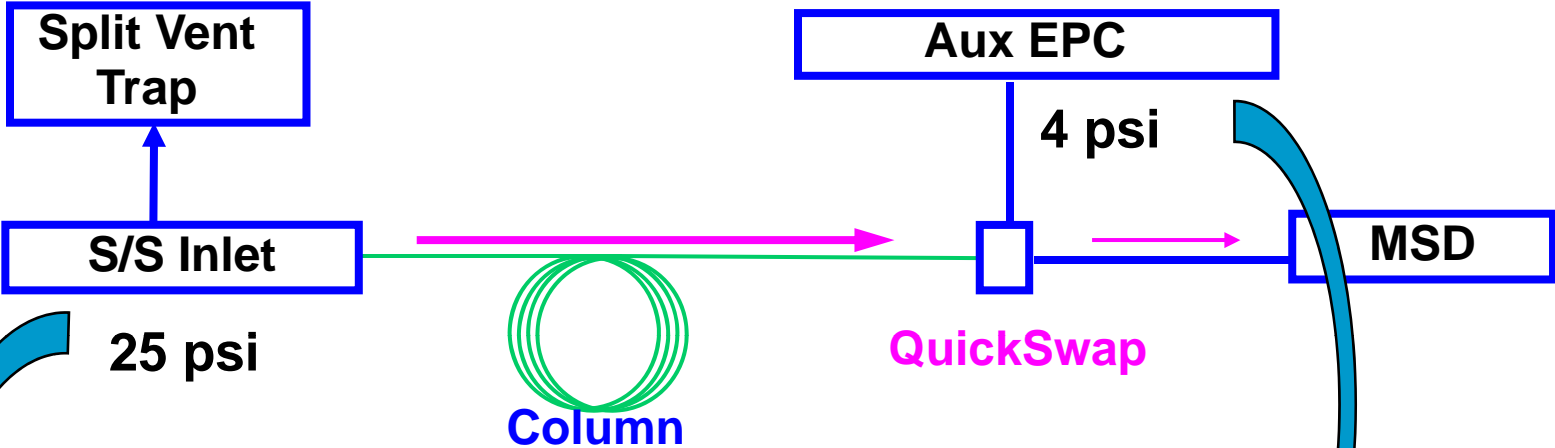


# Semivolatiles Instrument

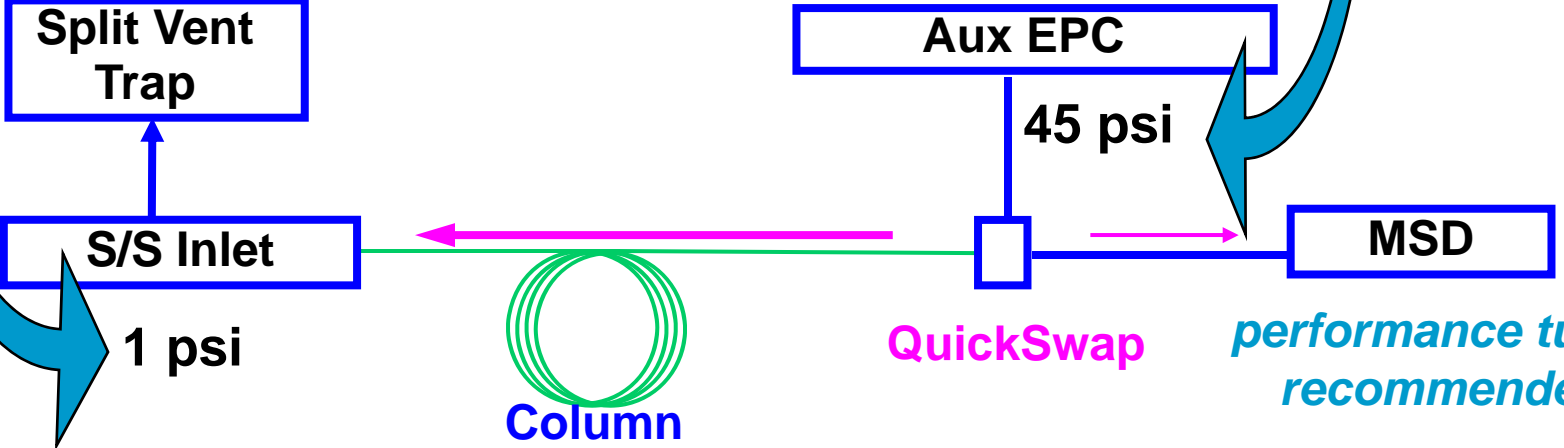


# Backflush with QuickSwap

## During GC Run



## After GC Run



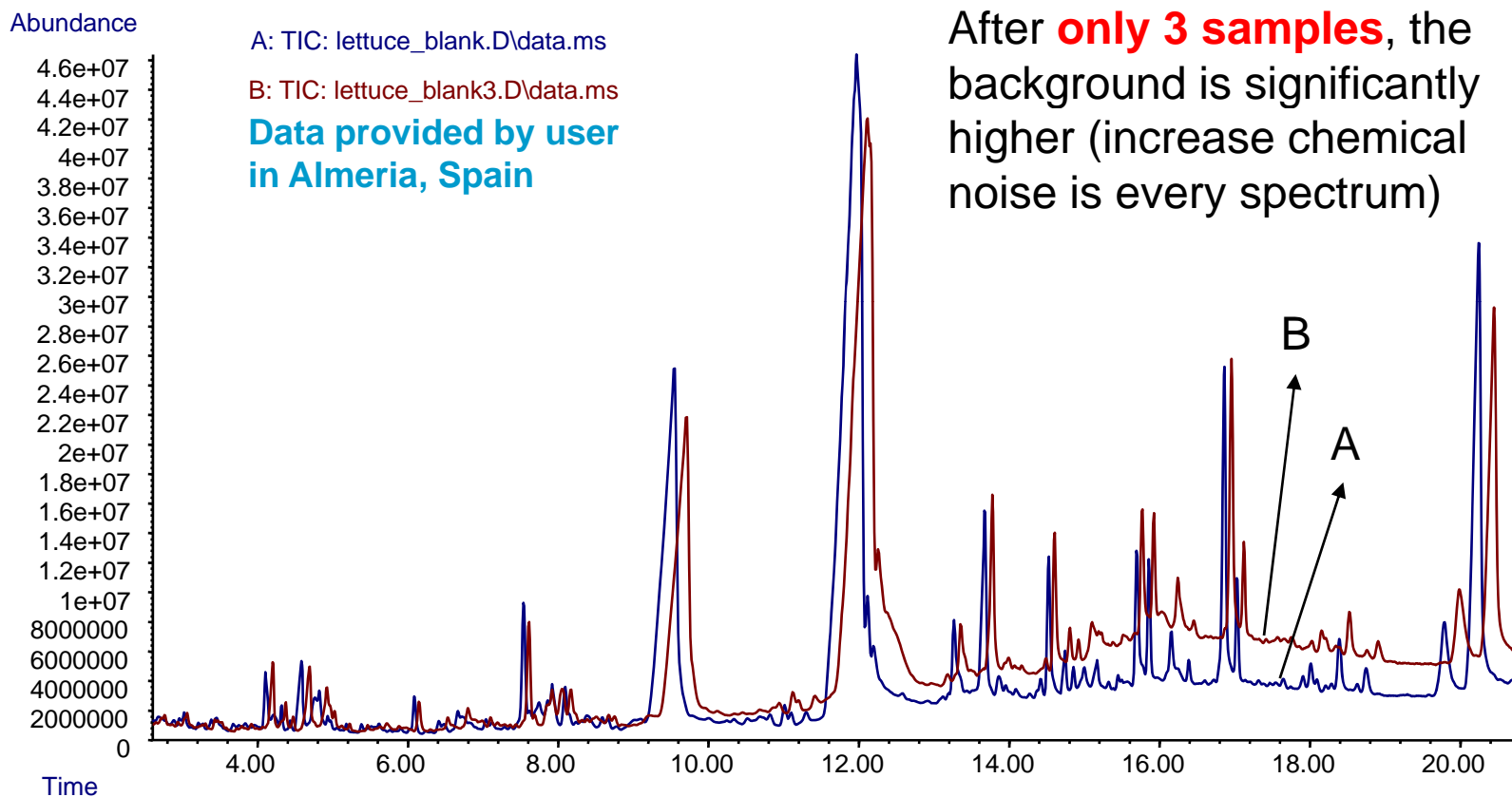
*performance turbo recommended*

# Benefits of Backflushing

- **Shorter analysis times**
  - More samples per day per instrument
- **Lower operating costs**
  - Longer column life
  - Less frequent and faster GC & MSD maintenance
- **Less chemical background ('noise' from matrix)**

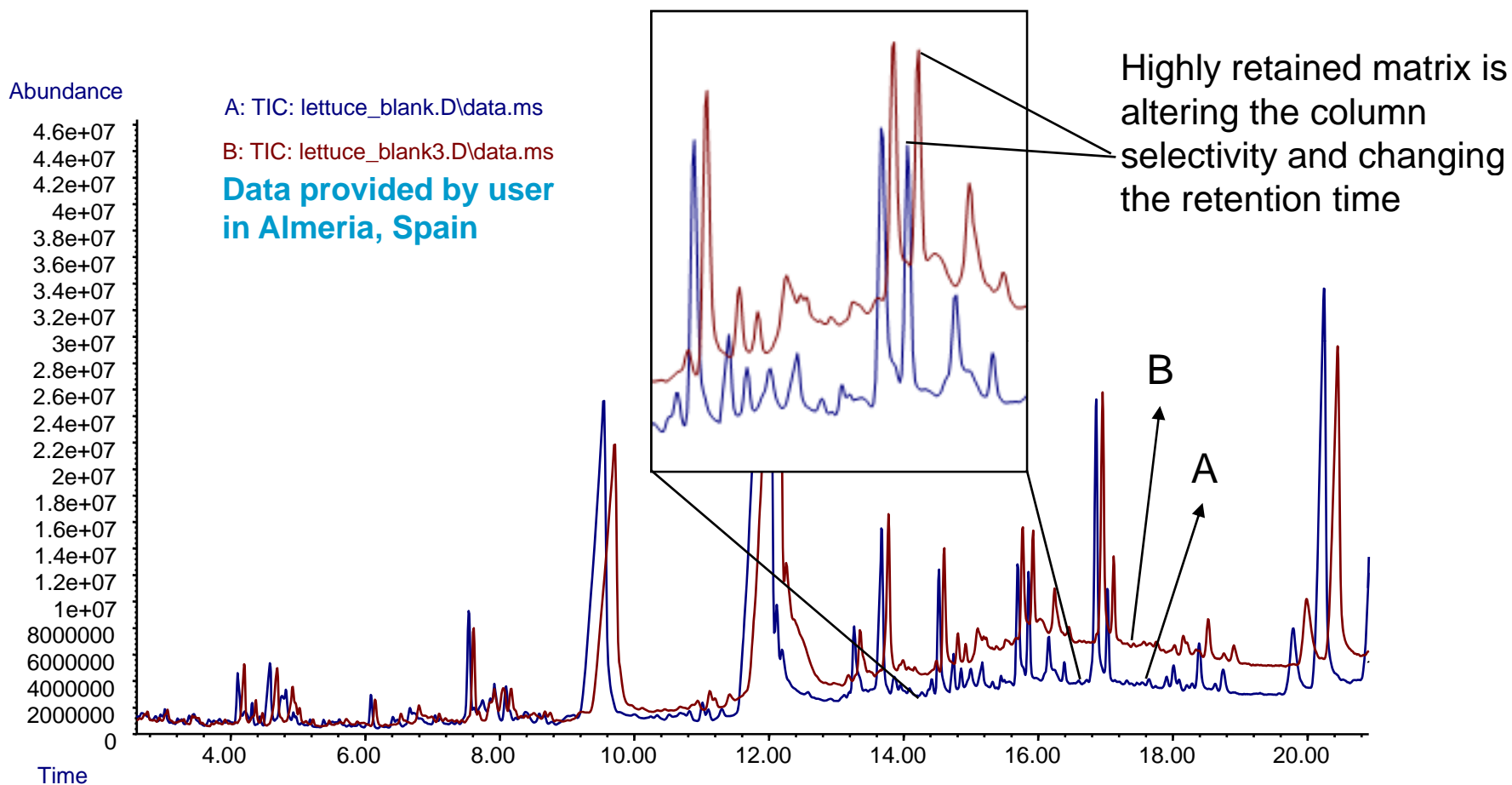


# Without Backflush: Increased Chemical Background (Spectral Noise) and Changes in Retention Time



Overlay of two chromatograms of a blank extract injected BEFORE (A) and AFTER (B) three injections without backflush

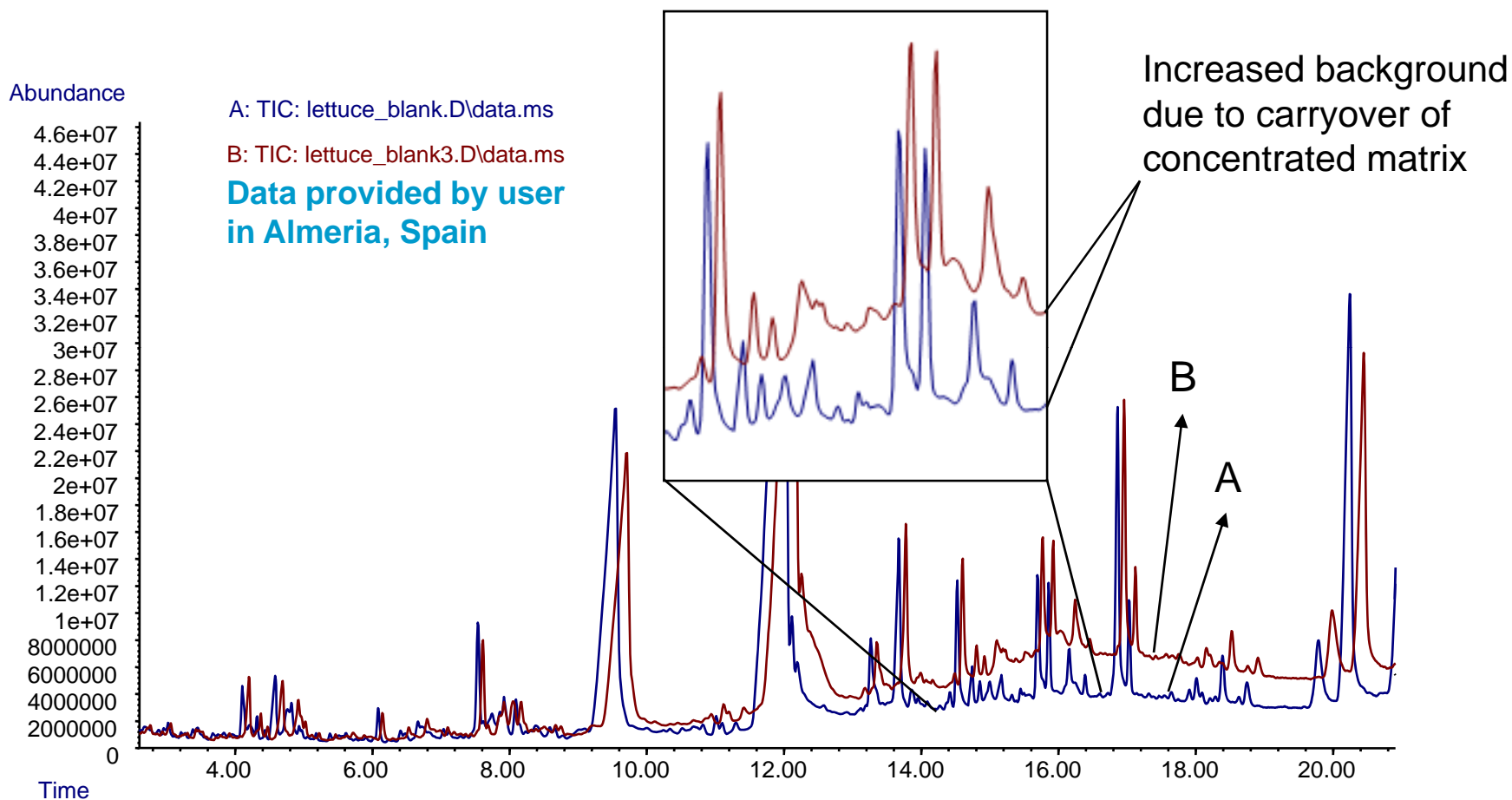
# Without Backflush: Increased Chemical Background (Spectral Noise) and Changes in Retention Time



Overlay of two chromatograms of a blank extract injected BEFORE (A) and AFTER (B) three injections without backflush

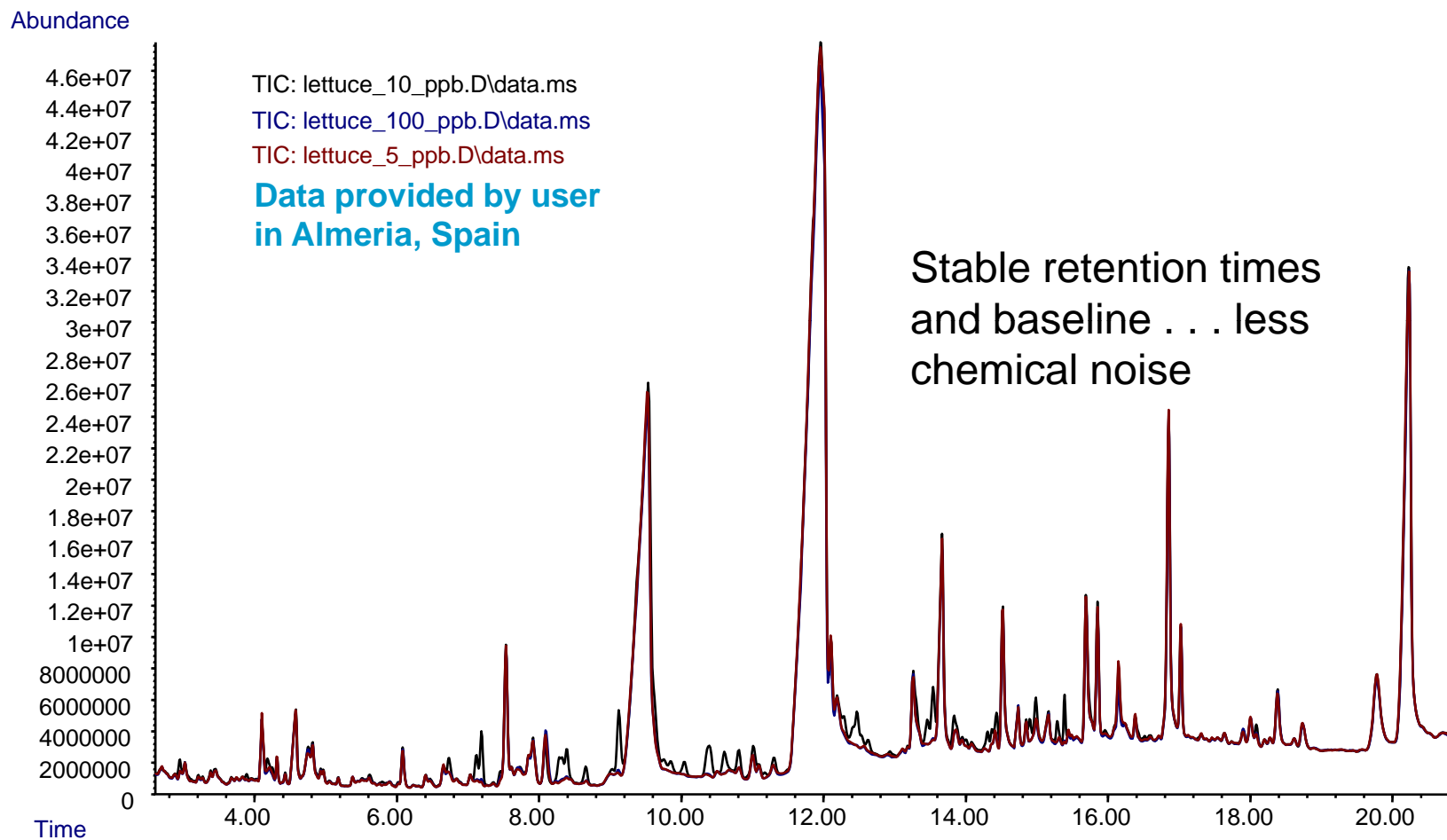


# Without Backflush: Increased Chemical Background (Spectral Noise) and Changes in Retention Time



Overlay of two chromatograms of a blank extract injected BEFORE (A) and AFTER (B) three injections without backflush

# With Backflush: No Increased Chemical Background (Spectral Noise) and No Change in Retention Time



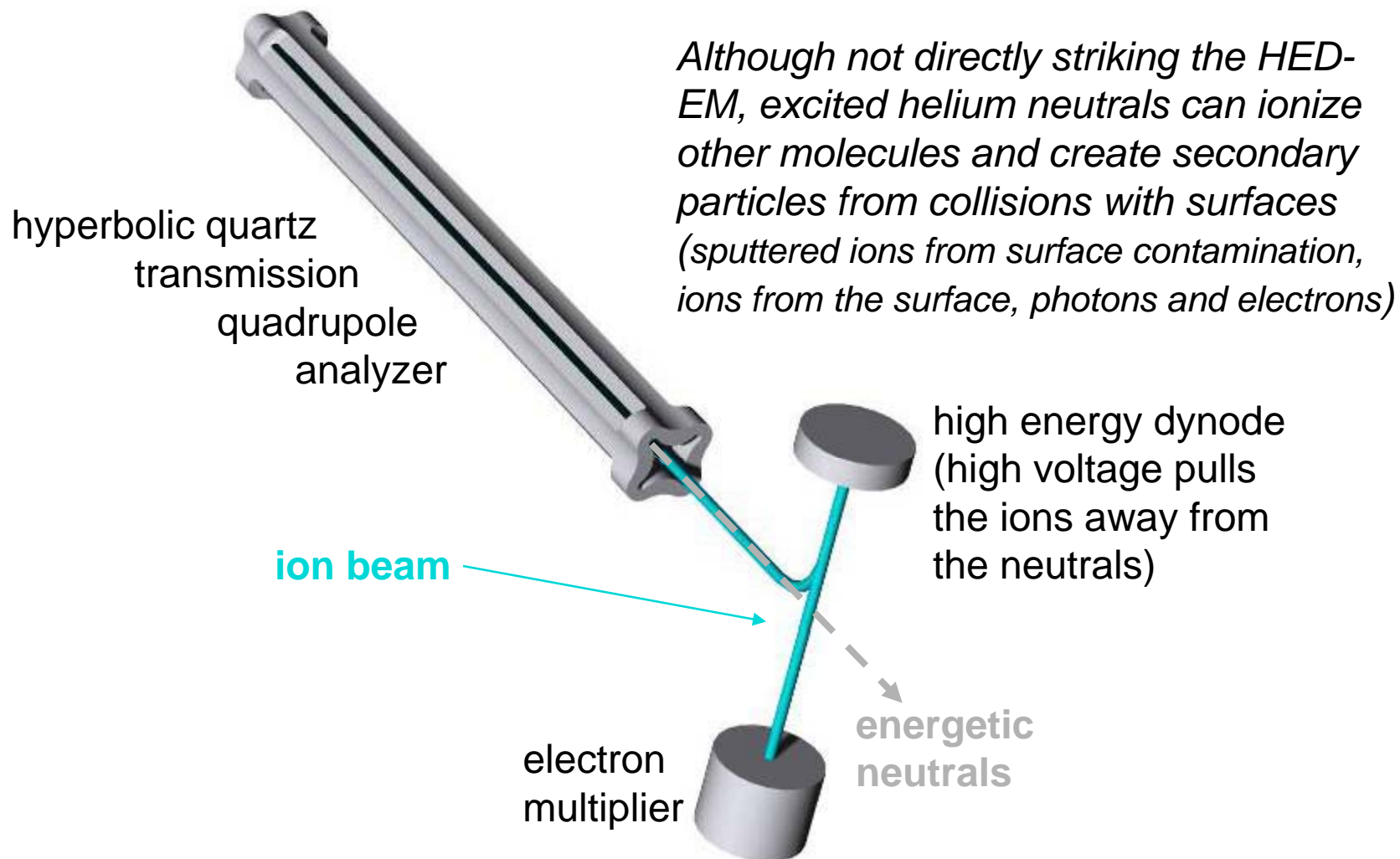
Overlay of three chromatograms of lettuce extract run with 2 min of back flush

# Benefits of Backflushing

- **More samples per day per instrument**
- **Longer column life**
- **Lower operating costs**
- **Less frequent and faster GC & MSD maintenance**
- **Less chemical background**
  - **More consistent retention times**
  - **More consistent baselines**
  - **Higher quality spectra (no increase in noise during analysis sequence)**
  - **Higher quality quantitation (no increase in interfering ions during analysis sequence)**

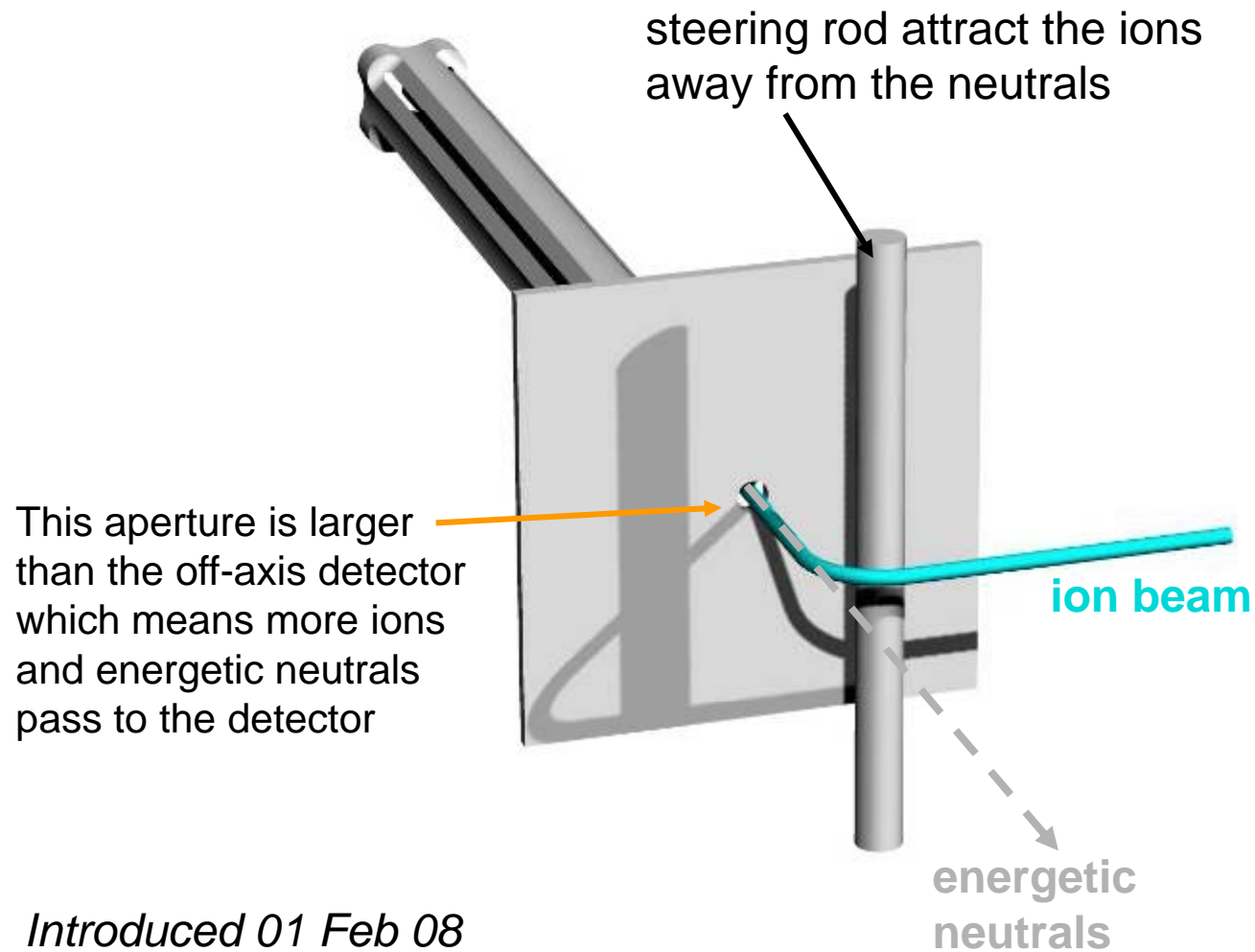


# Conventional Off-Axis Detector



# Triple-Axis Detector

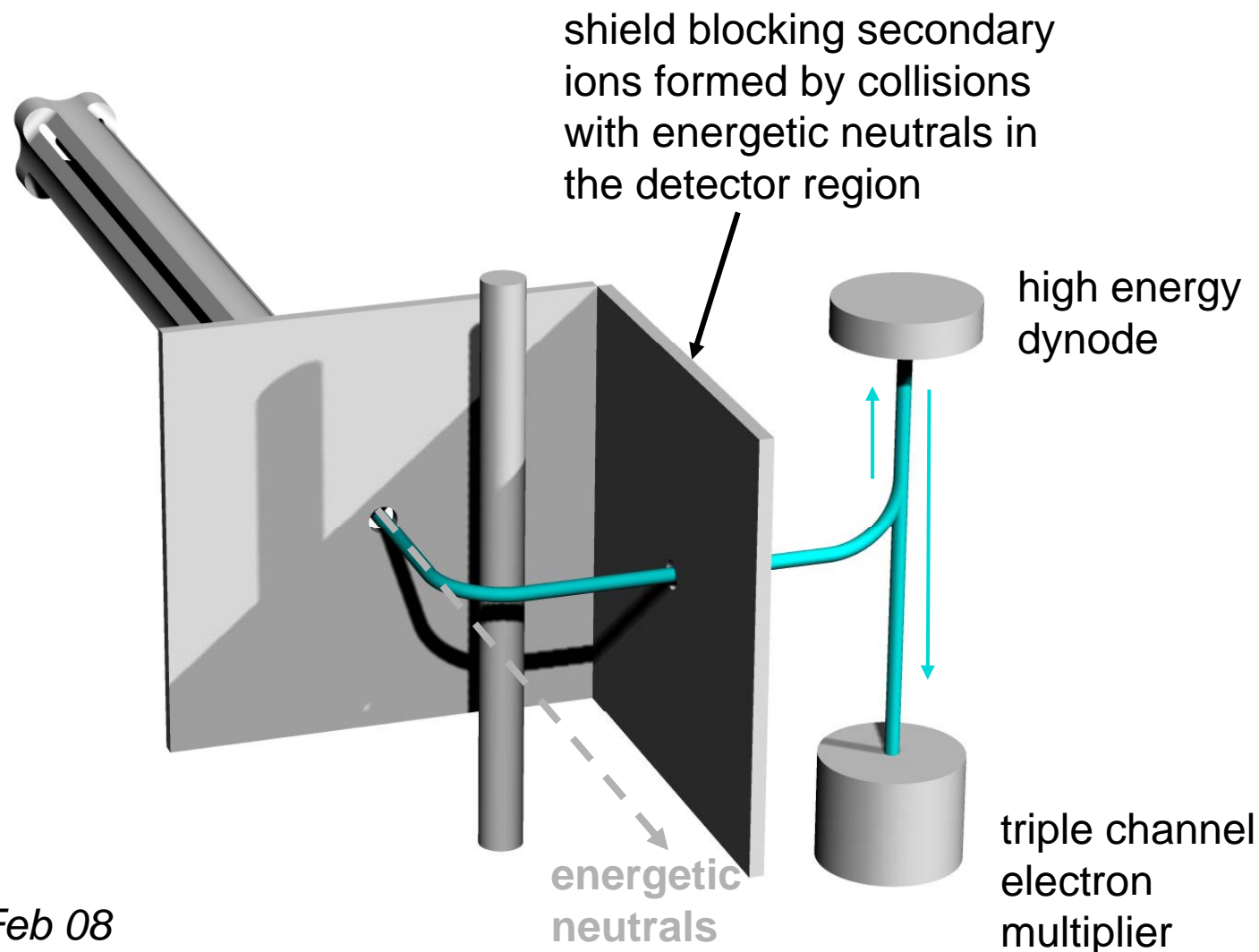
slide 1 of 3



*Introduced 01 Feb 08*

# Triple-Axis Detector

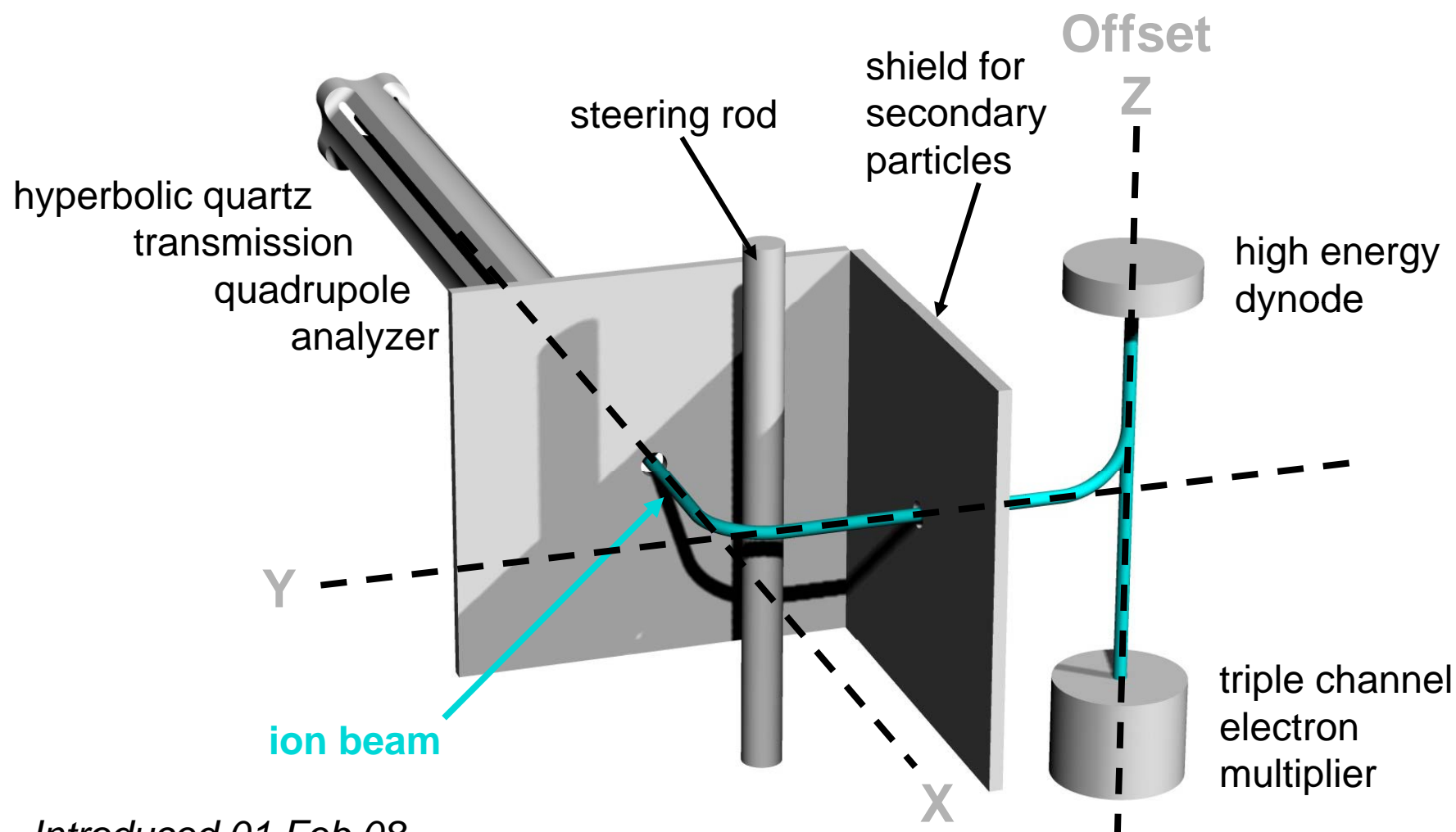
slide 2 of 3



*Introduced 01 Feb 08*

# Triple-Axis Detector

slide 3 of 3



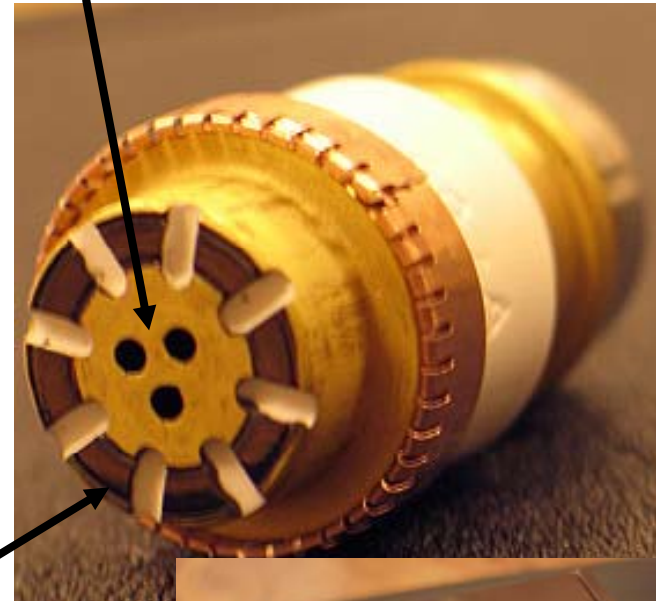
*Introduced 01 Feb 08*

# Triple Channel EM

Triple channels improve signal

Triple channels increase life

*Exit of the triple channels*



*Collector removed to show exit passages*

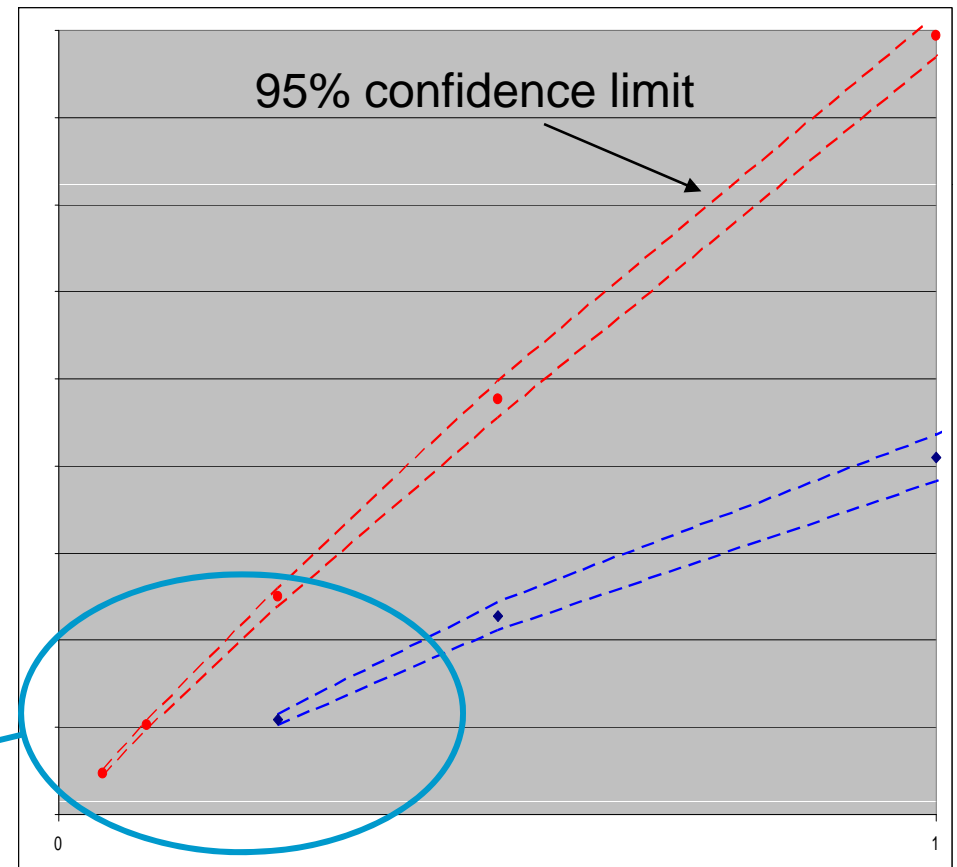
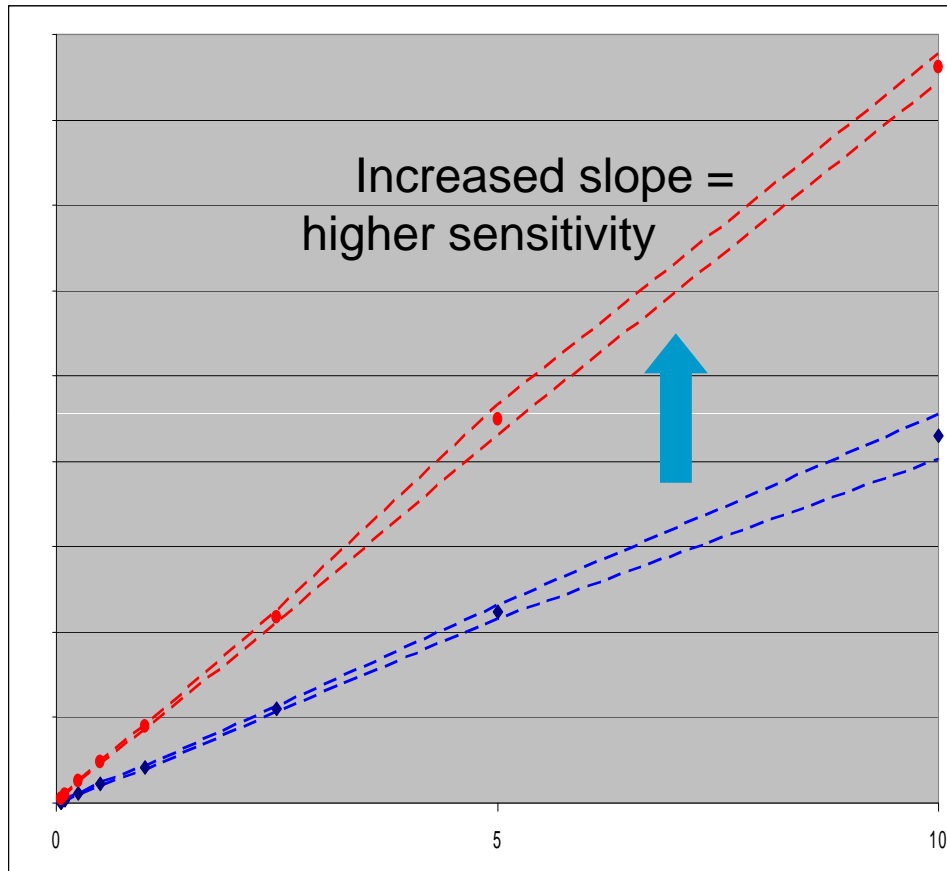


*Collector*

*Introduced 01 Feb 08*



# Triple-Axis Detector: Higher Signal – Lower MDL



# New Detector for Enhanced EI Sensitivity!

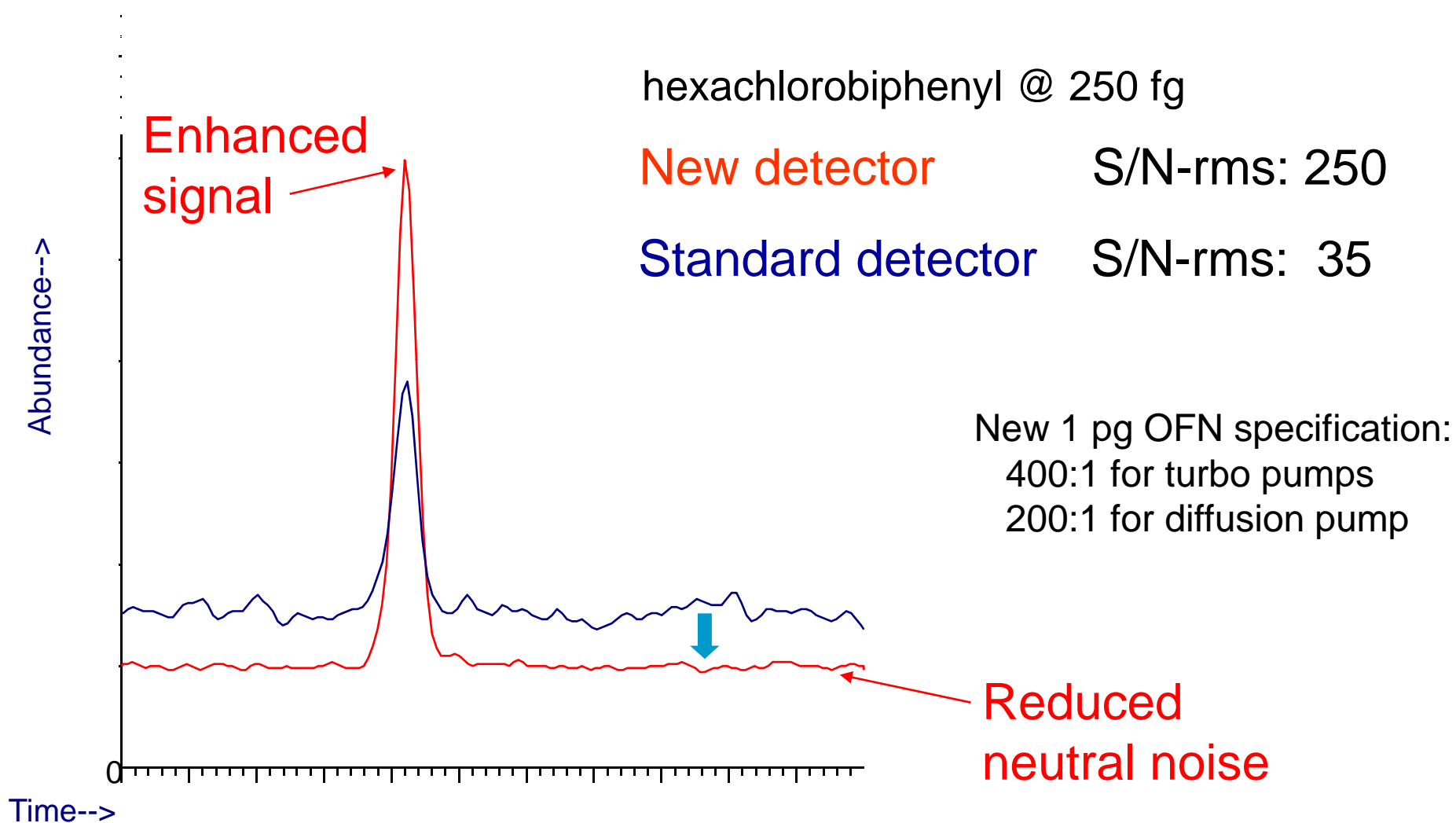
hexachlorobiphenyl @ 250 fg

New detector

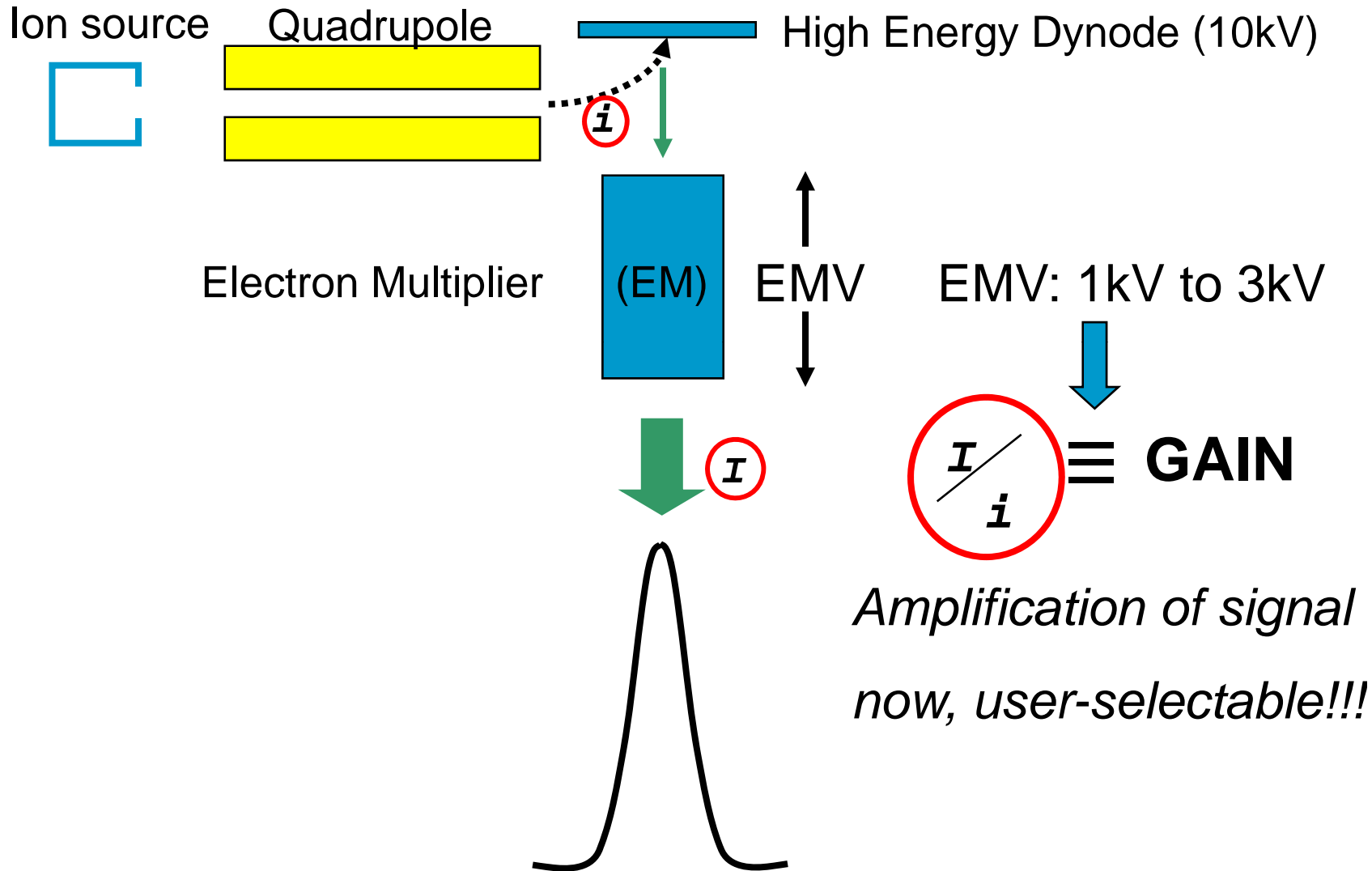
S/N-rms: 250

Standard detector

S/N-rms: 35

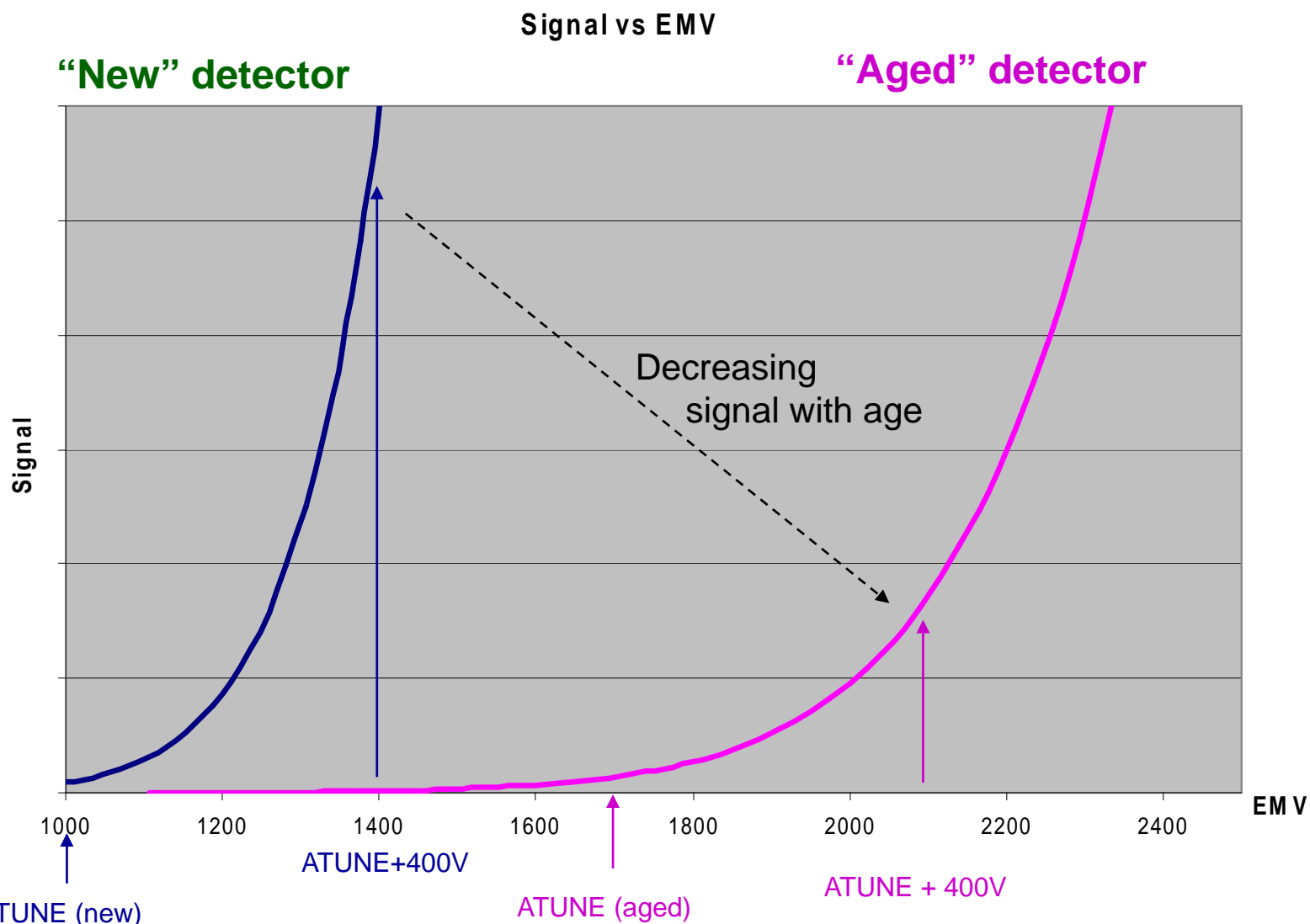


# Gain Normalized Optimization of the EM



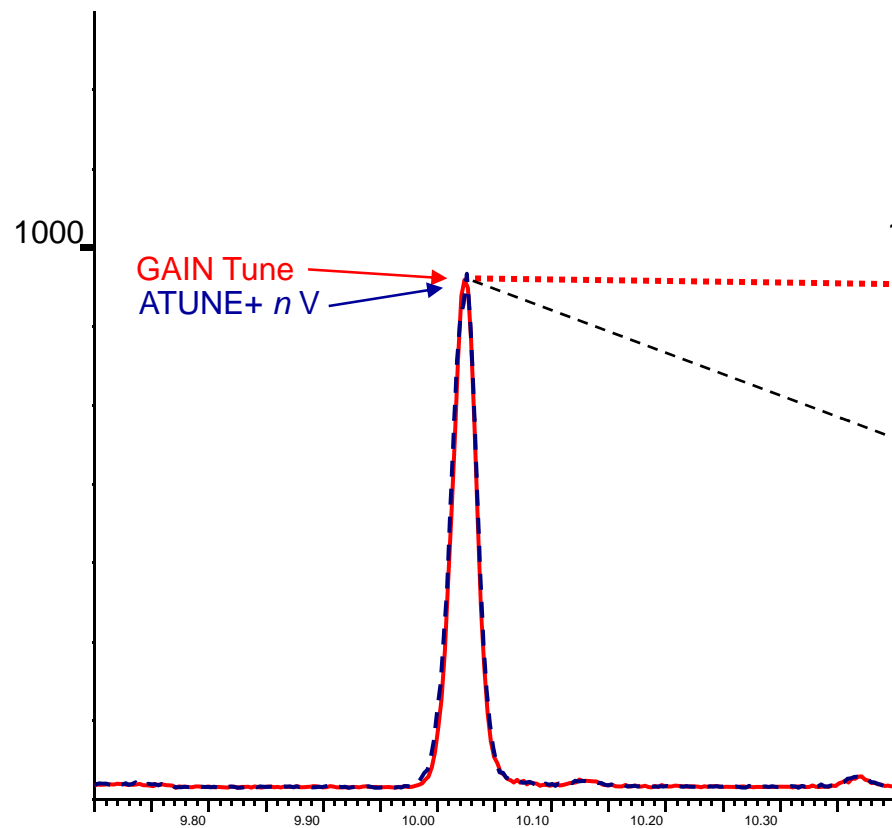
# Disadvantage of *ATUNE + nV*

Detectors “age” over use: the same EMV setting will not give the same signal!

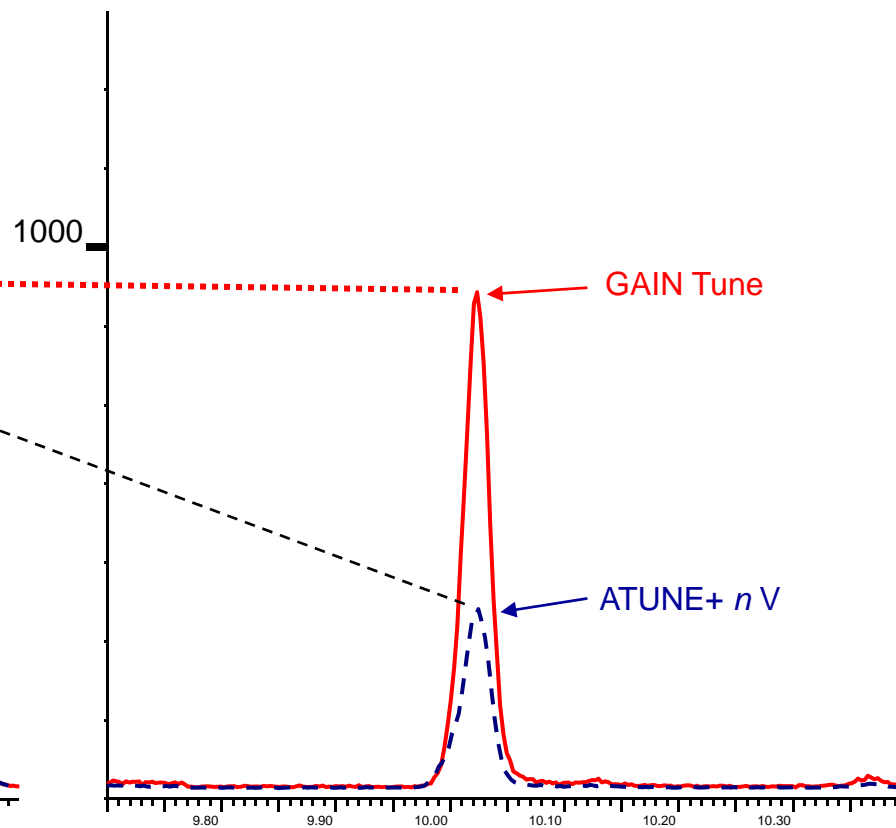


# New Gain Normalized Methods

“New”



“Aged”

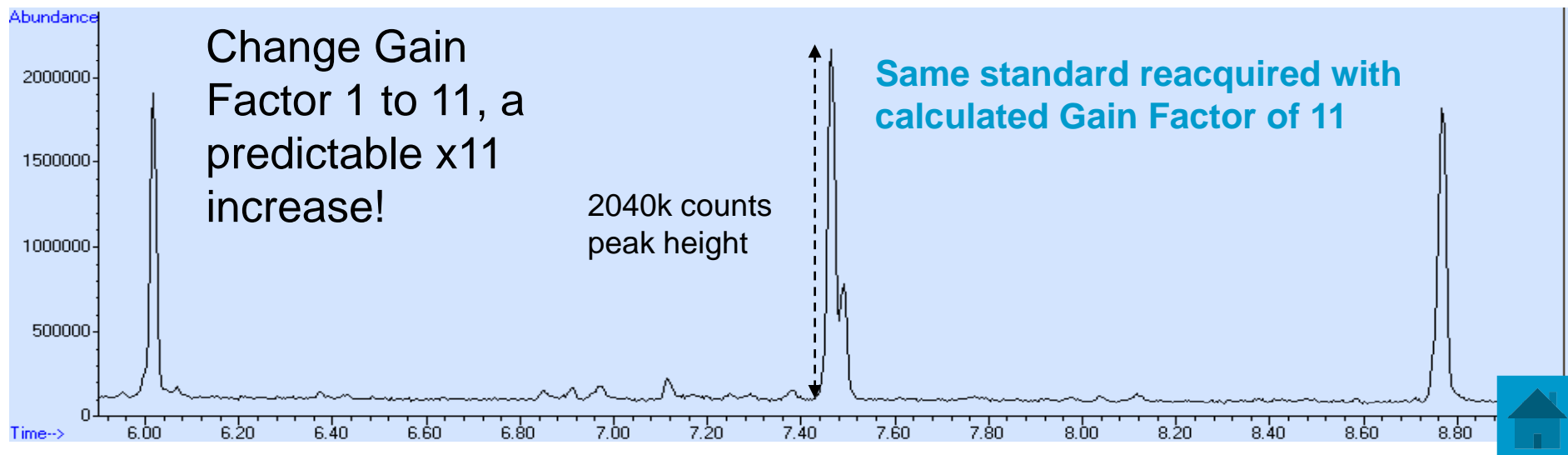
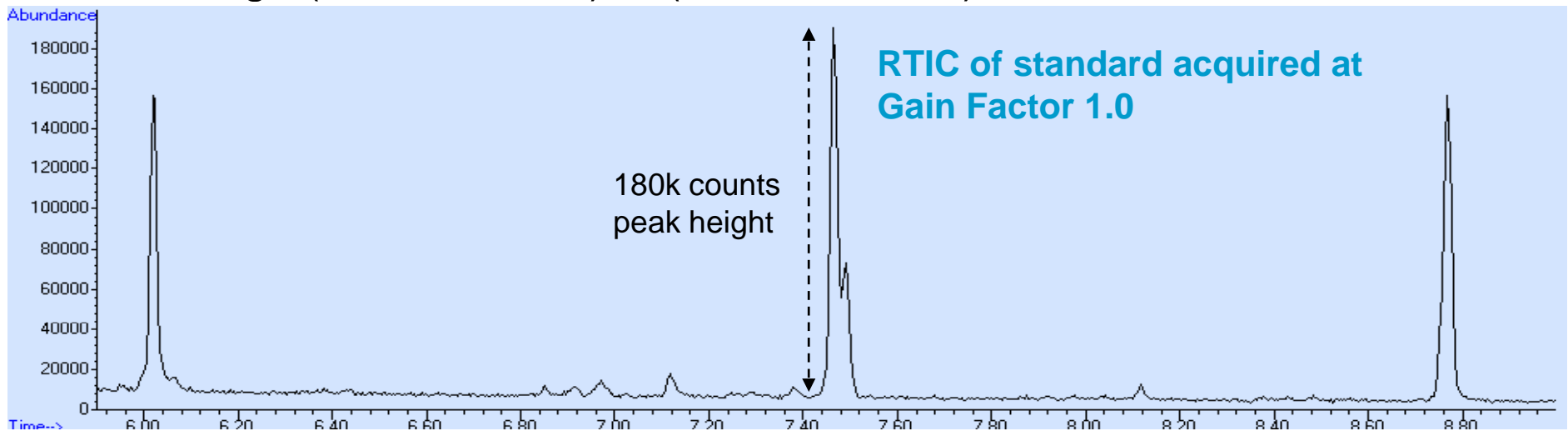


Consistent sensitivity over the life of the electron multiplier!  
Consistent sensitivity from MSD to MSD and lab to lab!



# Using Gain Factor for Method Optimization

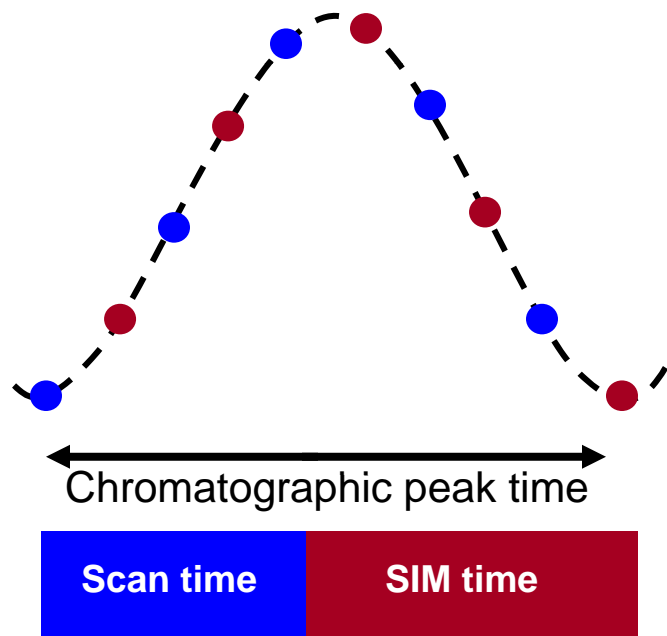
Change (Atune + 200V) to (Atune + 400 V) – How much increase?



# Fast Electronics

Fast electronics allow SIM and Scan data in a single run

- **SIM** = maximum sensitivity for target compounds
- **Scan** = best identification of unknowns

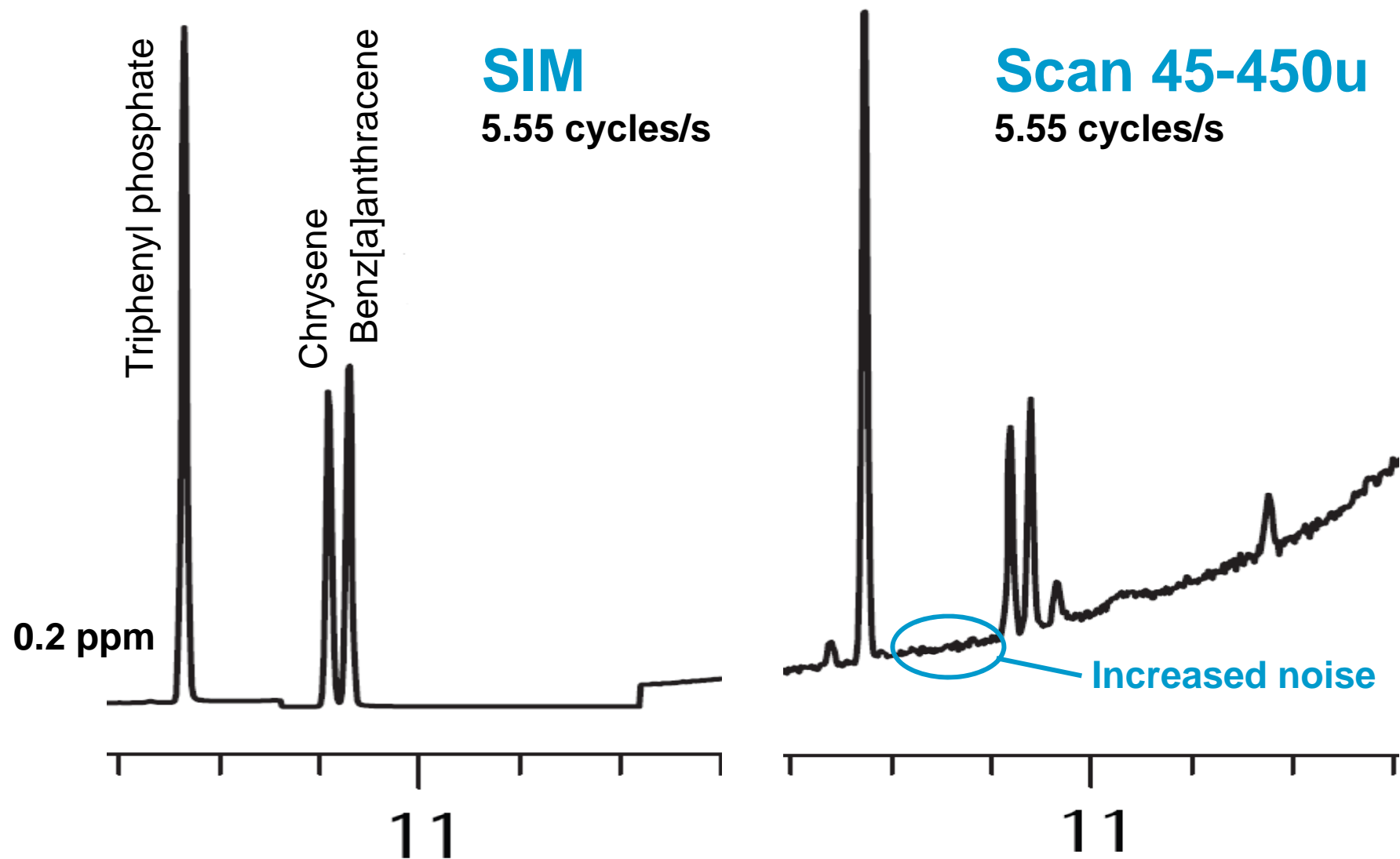


- Scan data points
- SIM data points

... more information from a single run



# Synchronous SIM/Scan Comparison of PAHs



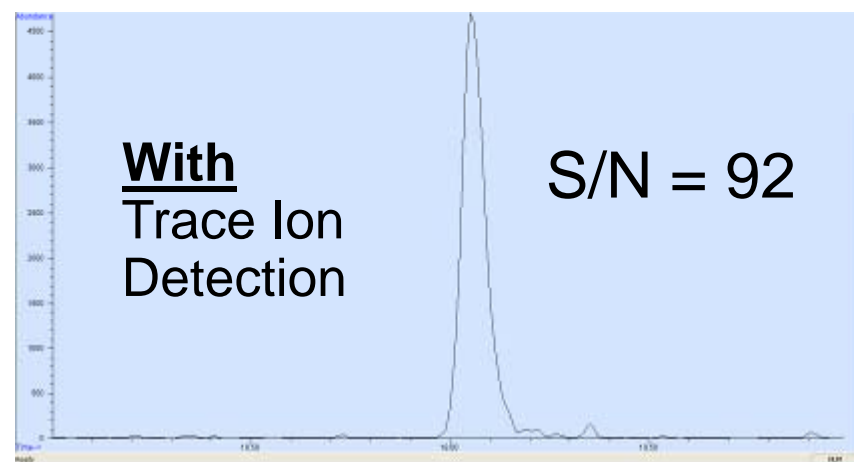
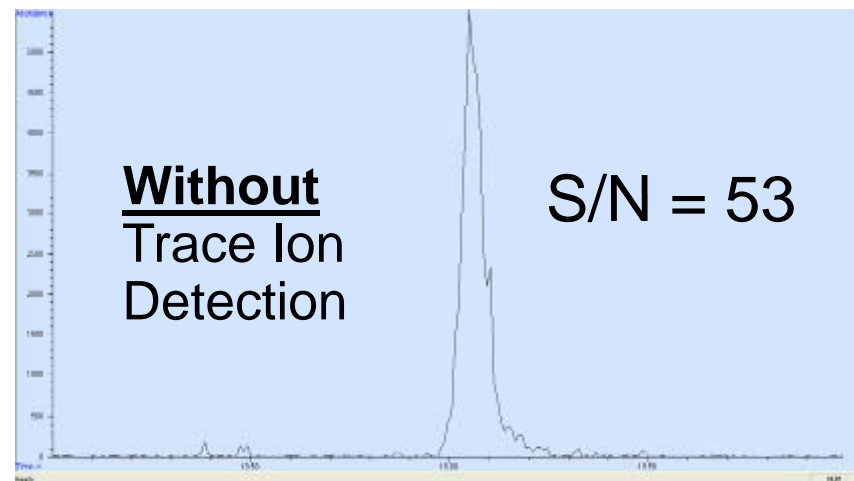


# Trace Ion Detection Technology

## Agilent proprietary algorithm

- Reduced noise level
- Improved peak shape
  - Especially under-sampled peaks
- Improved library match

*Default “OFF” in the ChemStation*

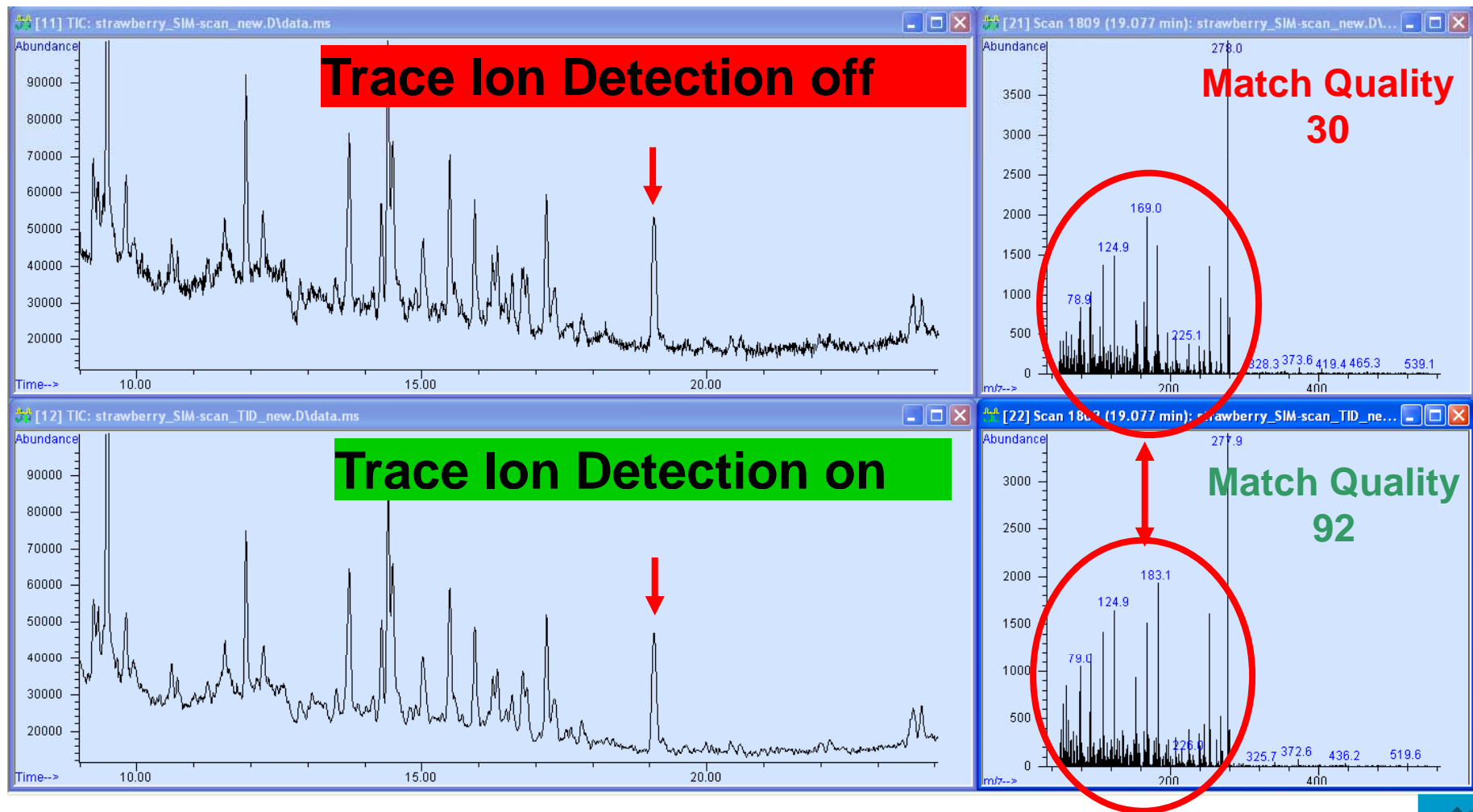


... better detection at trace levels



# Improve Library Match Quality

## Fenthion in strawberry extract



# NIST AMDIS Background

- AMDIS: Automated Mass Spectral Deconvolution and Identification Software
  - G. Mallard, S. Stein, O. Toropov, NIST
- Originally developed for detection of chemical weapons in complex mixtures (environmental samples, process streams)
  - Designed to work without analyst input
- Agilent DRS Revision A.01, March 2004
- AMDIS 2.64 released December 2005 (noise reduction)
- **Agilent DRS Revision A.04, February 2008**
  - Integrated into QEdit for qual, quant, manual integration and reports
  - Truly a new, second generation product for deconvolution reporting

# NIST AMDIS Background

- AMDIS: Automated Mass Spectral Deconvolution and Identification Software

- G.

- Origin  
comp

- De

- Agil

- AMD

- Agilent [DMS Review No. 1, February 2000](#)

**Deconvolution is NOT new technology!**  
**Applied to spectrophotometry**  
**and LC-PDA for years.**

**Deconvolution is especially powerful for**  
**MS due to the spectral orthogonality**  
**(spectral difference; unique m/z ions)**

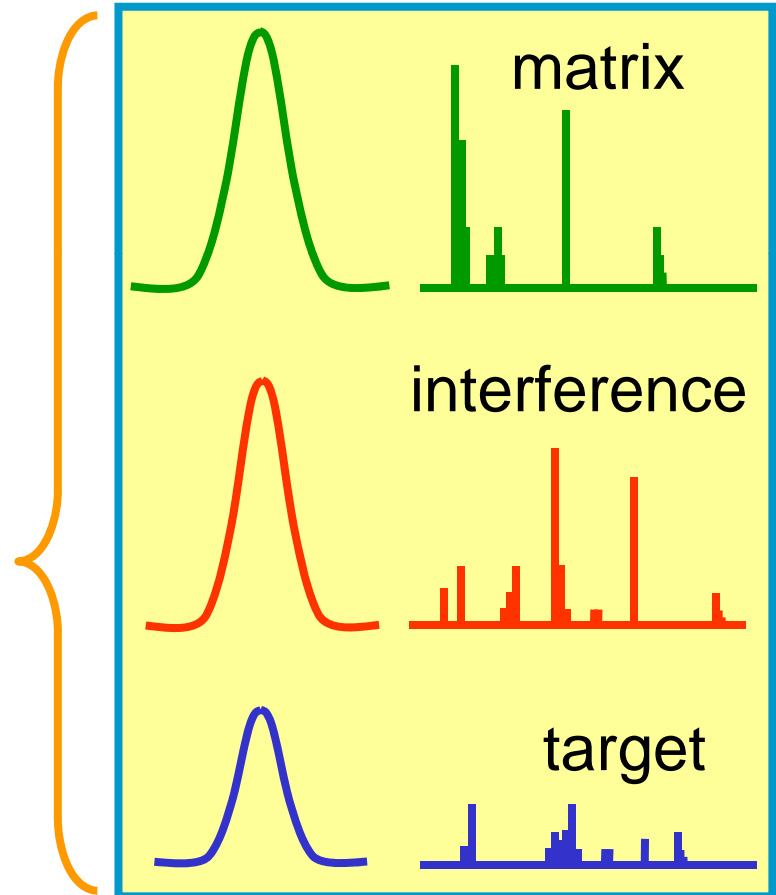
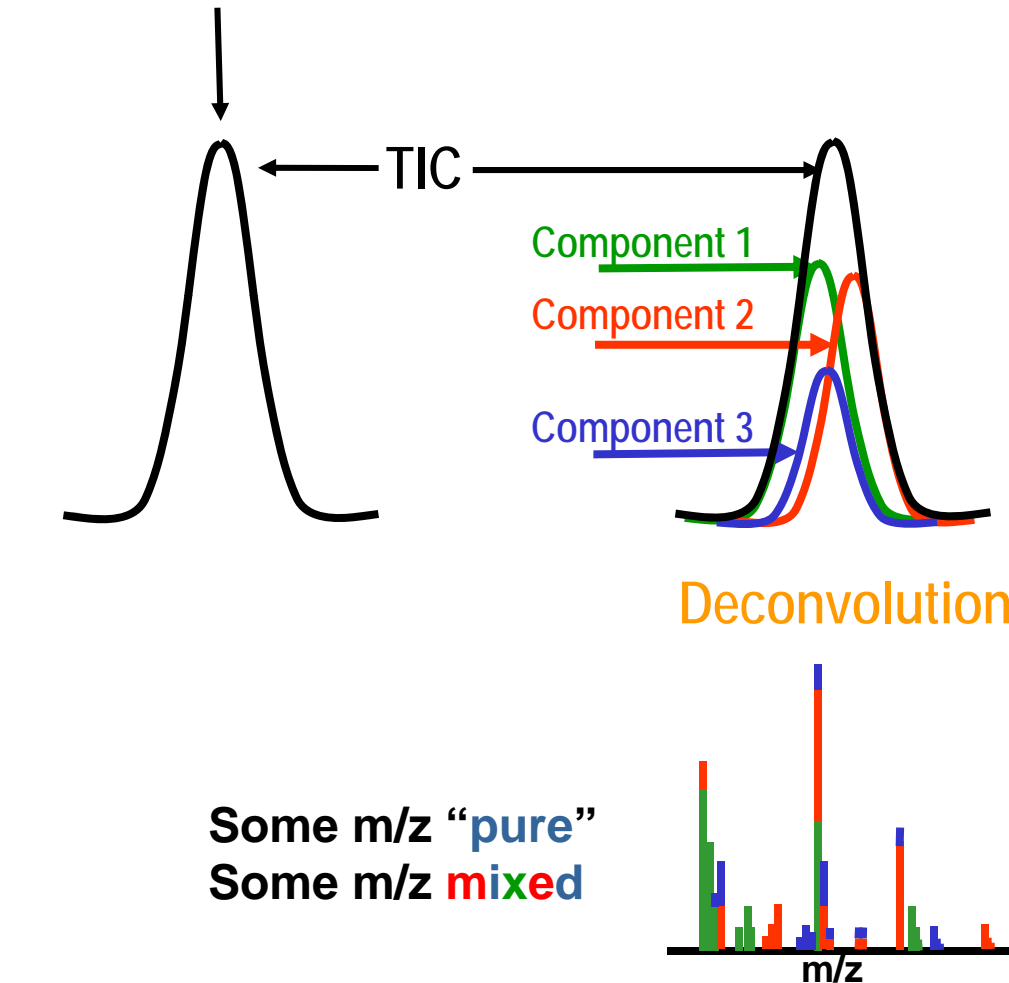
- Integrated into QEdit for qual, quant, manual integration and reports
- Truly a new, second generation product for deconvolution reporting

# Deconvolution: Use Difference in Spectra, Retention Time and Peak Shape to Separate Coeluting Peaks

Peak detected with Trace Ion Detection

TIC & Spectrum

Deconvoluted peaks and spectra  
Mathematical "Separation"

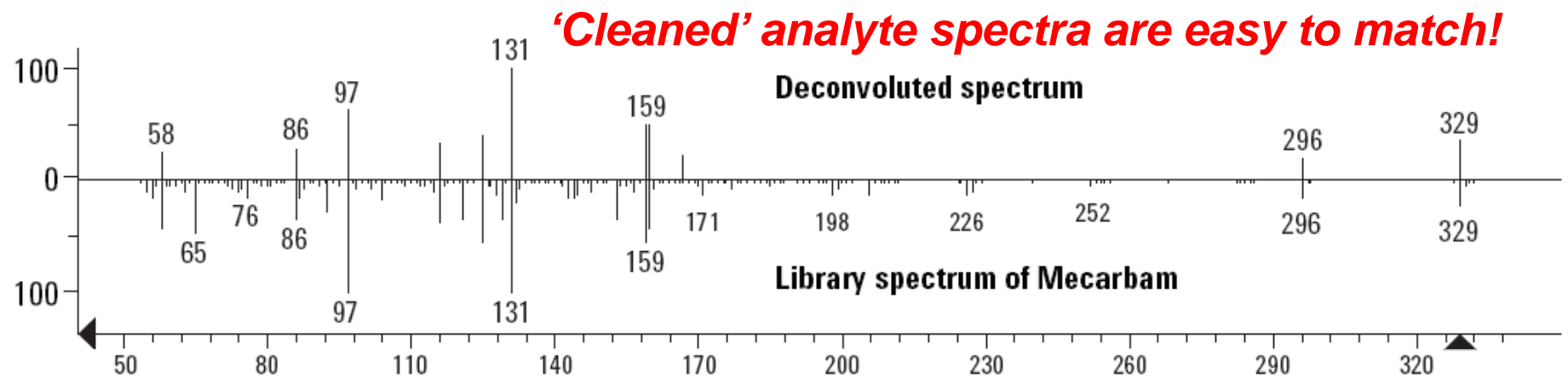
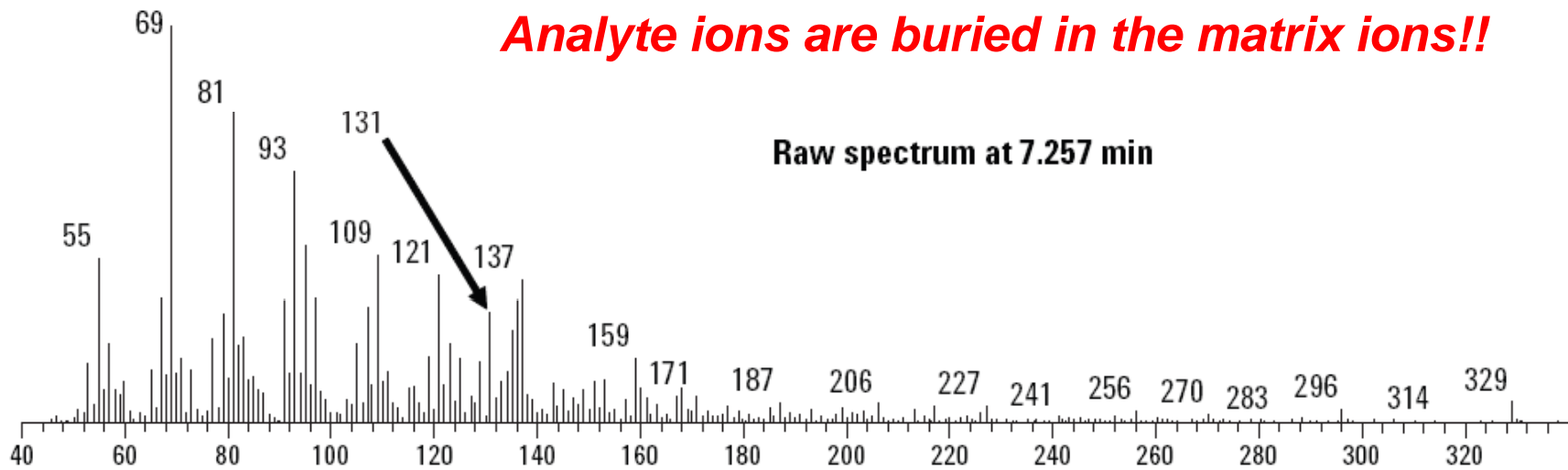


## AMDIS Automatically Purifies Spectra by:

- True deconvolution
  - Even if no available background for subtraction
- Detailed treatment of noise
  - Complete noise analysis; used for component perception
- Correction for baseline drift
  - Flat baselines not required; determines baselines for each m/z
- Corrects for spectral skewing in spectra
  - Distortion generated by concentration change during scan period
- Extracts closely coeluting peaks
  - Separates components that have peak apexes with a single scan

*Power of  
modern PCs  
and matrix  
mathematics*

# AMDIS: Pulling a Useable Spectrum Out of a Mess



# 17 Surface Water Data Files: Pesticide Analysis

	*CDFA	Agilent DRS
Targets Found	37	Same 37 + 99 additional
False Positives	1	0
Processing Time	~ 8 hours	32 minutes

Save about 7.5 hours to do other jobs

\*CDFA is the California Department of Food and Agriculture  
Data files courtesy of Dr. Mark Lee and Steve Siegel



# The Power of DRS: Detect the Undetected

## MSD Deconvolution Report

Sample Name: + 400 ppb ISTDs, 25 µL PTV  
 Data File: C:\MSDCHEM\1\DATA\SPINACH.D  
 Date/Time: 11:23:10 AM Monday, Apr 5 2004

The NIST library was searched for the components that were found in the AMDIS target library.

R.T.	Cas #	Compound Name	Agilent	AMDIS		NIST	
			ChemStation Amount (ng)	Match	R.T. Diff sec.	Reverse Match	Hit Num.
18.445	84742	Di-n-butylphthalate	7.08	86	1.3	92	1
23.966	80057	Bisphenol A		93	7.9	91	1
24.066	72559	p,p'-DDE		79	2.5	77	1
27.928	51036	Piperonyl butoxide	37.83	91	2.2	94	1
29.672	117817	Bis(2-ethylhexyl)phthalate		91	1.9	86	3
31.420	52645531	Permethrin I		67	3.7	74	5
31.616	52645531	Permethrin I		89	15.5	91	3
13.718		Phenanthrene-d10	10				

All of these compounds were missed due to chemical noise, but AMDIS detected and confirmed all five by NIST05.

Hit number of the top 100 hits from 163,000+ compounds

DRS V.03 format

# New DRS V.04: Qual (Spectra) + Quant (Peak Area)

**Overlay of target(s) and Deconvoluted ion plots**

**Spectral review: Before AMDIS After AMDIS AMDIS Library**

**Hits  
X = MSD  
A = AMDIS**

**Target ion plot**

**Deconvoluted ion plot**

**Areas & amounts from target ion and Deconvoluted ion**

Ion	Exp%	Act%
149.00	100	100
91.00	60.00	125.86#
206.00	25.40	14.53#
104.00	16.20	33.38#

# New DRS A.04 Report with Quantitation from both MSD ChemStation and AMDIS results

## MSD Deconvolution Report

Sample Name: + 400 ppb ISTDs, 25 µL PTV  
 Data File: C:\msdchem\1\DATA\Trifecta\SPINACH.D  
 Date/Time: 08:14 AM Thursday, Oct 25 2007

Adjacent Peak Subtraction = 1  
 Resolution = Medium  
 Sensitivity = High  
 Shape Requirements = Medium

GC retention time confirmation

The NIST library was searched for the components that were found in the AMDIS target library.

R.T.	Cas #	Compound Name	Amount (ppm)		AMDIS		NIST	
			Chem station	AMDIS	Match	R.T. Diff sec.	Reverse Match	Hit Num.
18.4431	84742	Di-n-butylphthalate	7.03	6.25	95	1.7	92	1
23.974	80057	Bisphenol A	16.8	7.96	97	8.7	91	1
24.0444	72559	p,p'-DDE	0.65		76	1.4	79	2
25.705	72548	p,p'-DDD	0.16	0.13	52	1.8	65	2
26.9932	50293	p,p'-DDT	0.15	0.09	53	0.7	43	6
27.009	85687	Butyl benzyl phthalate	0.31	0.16	54	0.2	57	25
27.9265	51036	Piperonyl butoxide	37.91	32.31	96	1.6	94	1
29.6685	117817	Bis(2-ethylhexyl)phthalate	3.39	2.69	93	1.2	85	3
31.6131	52645531	Permethrin II	223.78	201.65	90	3.8	91	3
13.718		Phenanthrene-d10	10					

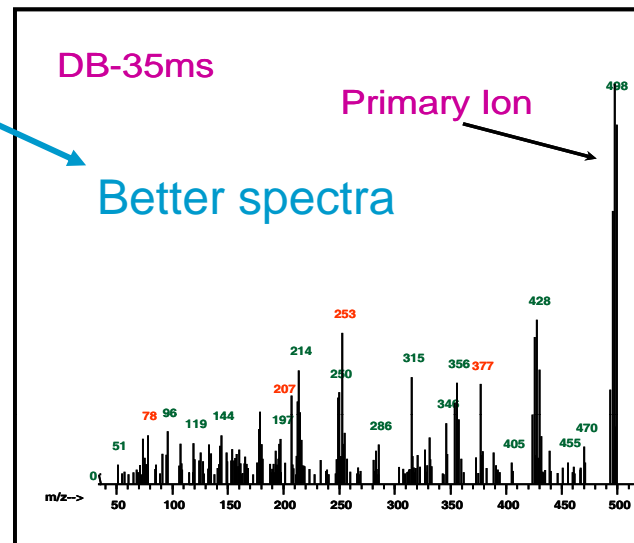
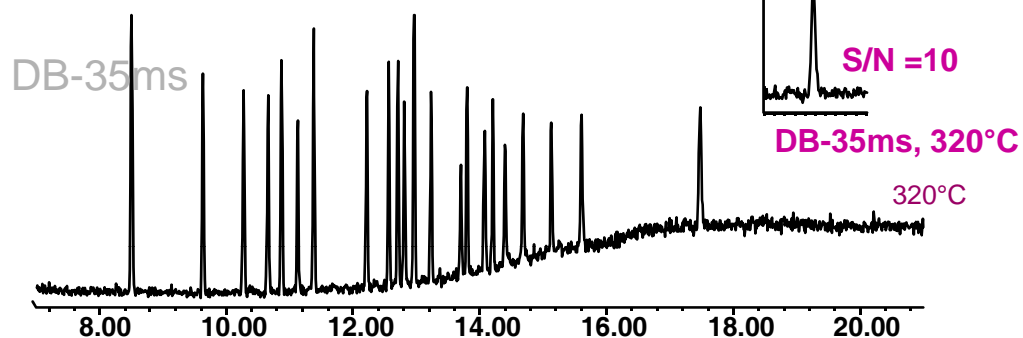
p,p'-DDE target ion mismatch

Lower AMDIS amount due to elimination of interferences

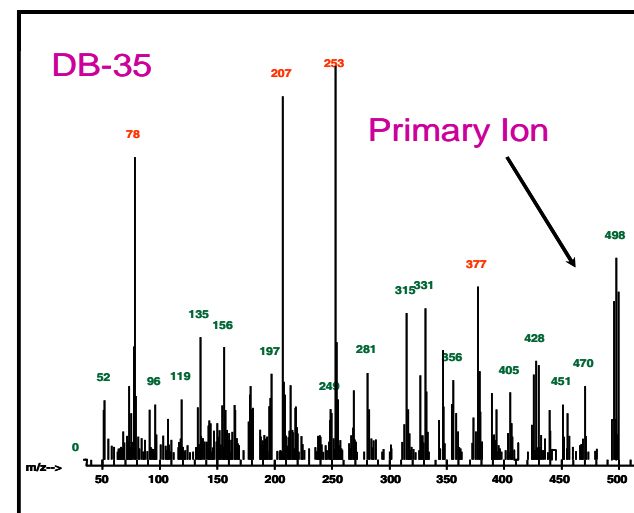
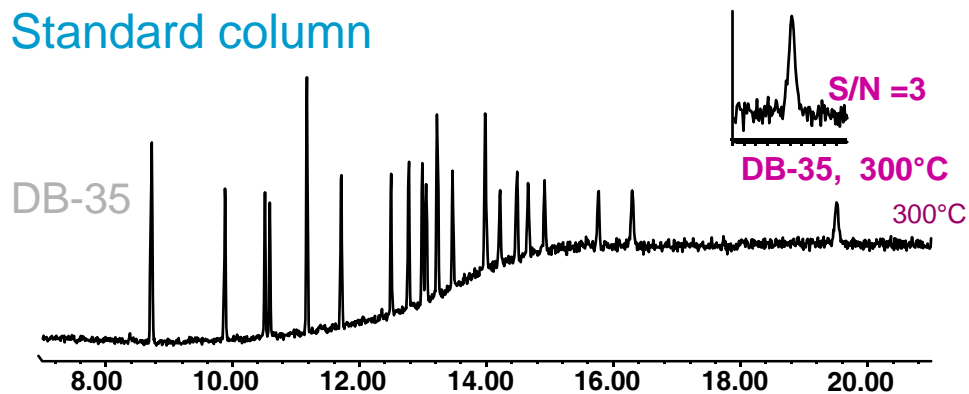
# Industry Standard: Low Bleed Stationary Phases

Better signal to noise, higher upper temp limit, faster run time, improved spectral purity, and greater column inertness

Low bleed column → Better detection limits



Standard column



CLP Pesticides Analysis

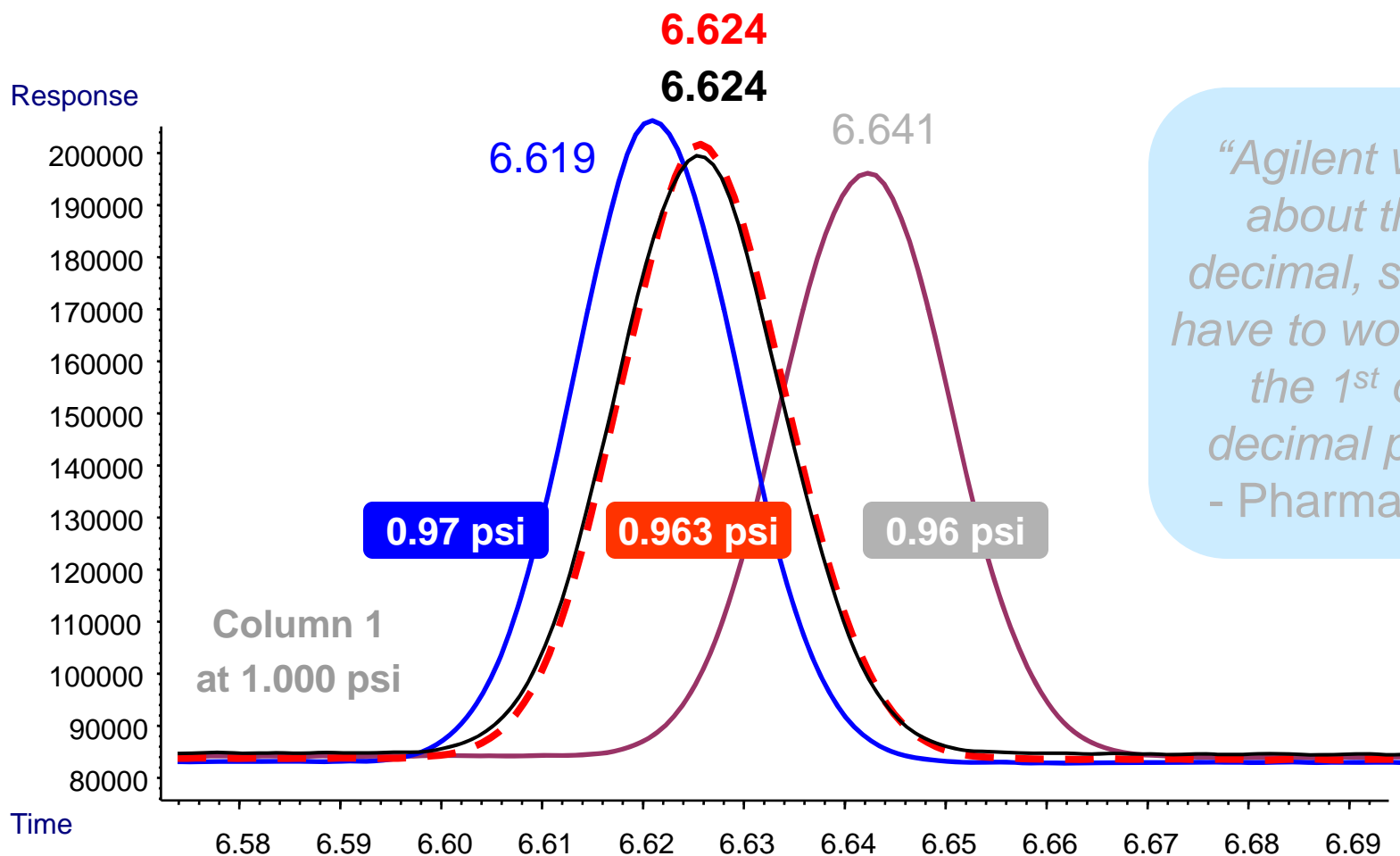


Agilent Technologies

Useful GC/MS Sensitivity  
Agilent eSeminar  
July 2006

# Why 1/1000 psi Matters!

-- Key to even better Retention Time Locking (RTL)

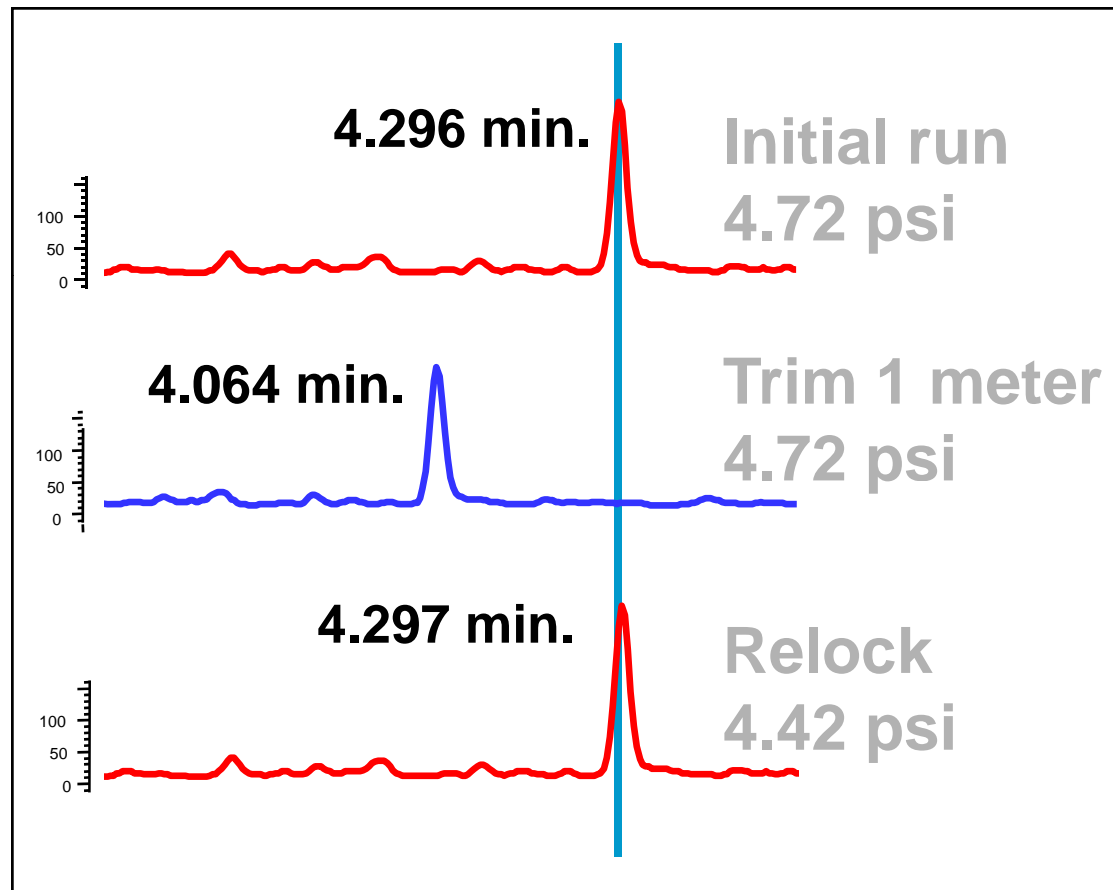


*“Agilent worries about the 3<sup>rd</sup> decimal, so I don’t have to worry about the 1<sup>st</sup> or 2<sup>nd</sup> decimal point...”*  
- Pharma (USA)

# Retention Time Locking

## Improve Confidence with Retention Time Locking

- **Easy**
- **Quick**
- **Repeatable**
  - Run-to-run
  - Operator-to-operator
  - Instrument-to-instrument



# Industry Specific Retention Time Locked Libraries

Part Number	RTL Database/Library	Number of Compounds
G1671AA	Hazardous Chemicals	730
G1672AA	Pesticide	926
G1673AA	Indoor Air Toxics	171
G1674AA	Forensic Toxicology	723
G1675AA	Japanese Positive List Pesticide	431
G1677AA	Environmental Semi-Volatile	one 8270 set of 273 ; two 525 sets of 120

*Library include GC method details, Getting Started manual, application notes, and HELP files*

Part Number	RTL Database/Library	Number of Compounds
Free	Volatile Organic Compounds	65
Free	PCB Congeners	209
Free	Forensic Toxicology	277
Free	Fatty Acid Methyl Ester	37
Free	Flavors	409
Free	Organotin Derivatives	Methyl, Ethyl, Pentyl

**modify a library to your need... or create your own**

# But what if the GC/MS isn't enough?

Why use a GC/QQQ System in place of a GC/single quad ?

Allows for the selective quantitation of target compounds in high chemical background samples

Gives better S/N in complex matrices than can be achieved by single quad approaches

Newer regulations in some applications specify GC/QQQ





# Agilent GC/MS Portfolio Newest Member



The Agilent 5975C Series GC/MSD is built on a solid foundation of industry leadership, reliability and performance.

**Industry leading GC/MS System**  
**5975C with 7890GC**

## 7000A GC/MS/MS

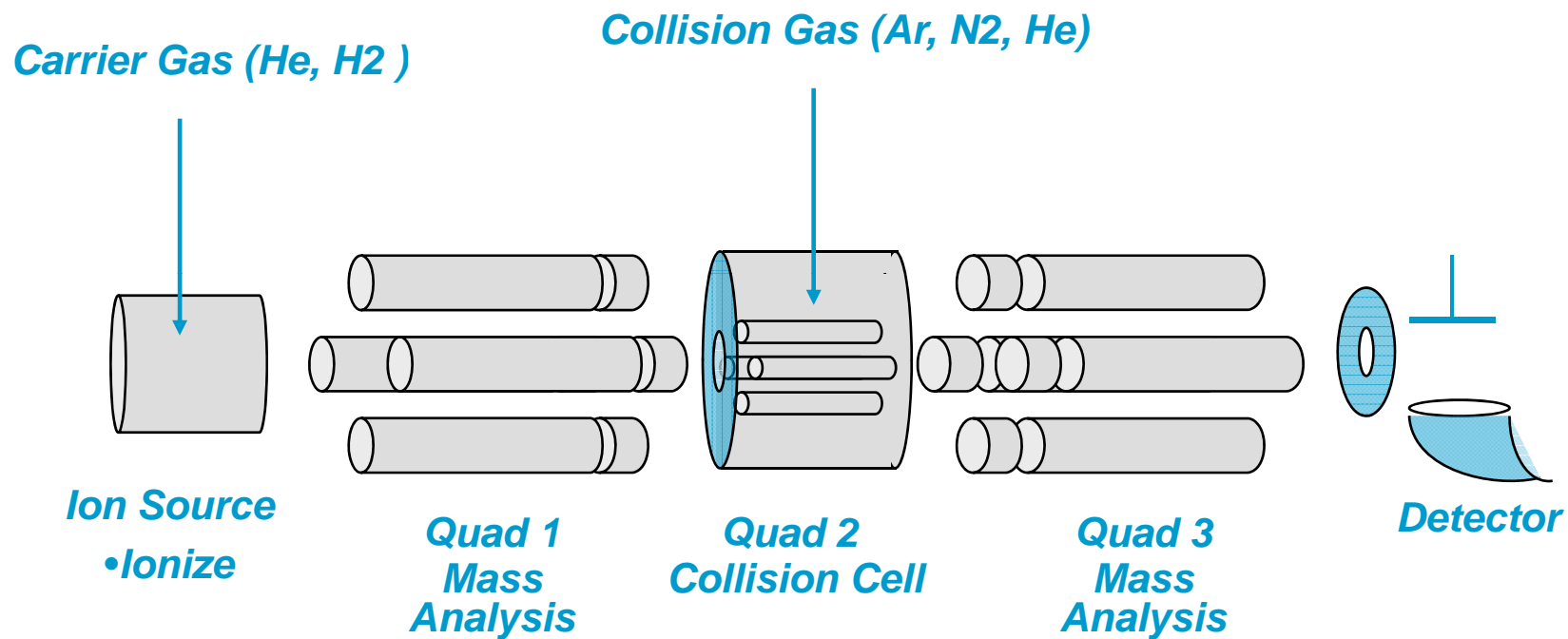


**Power of MS/MS**

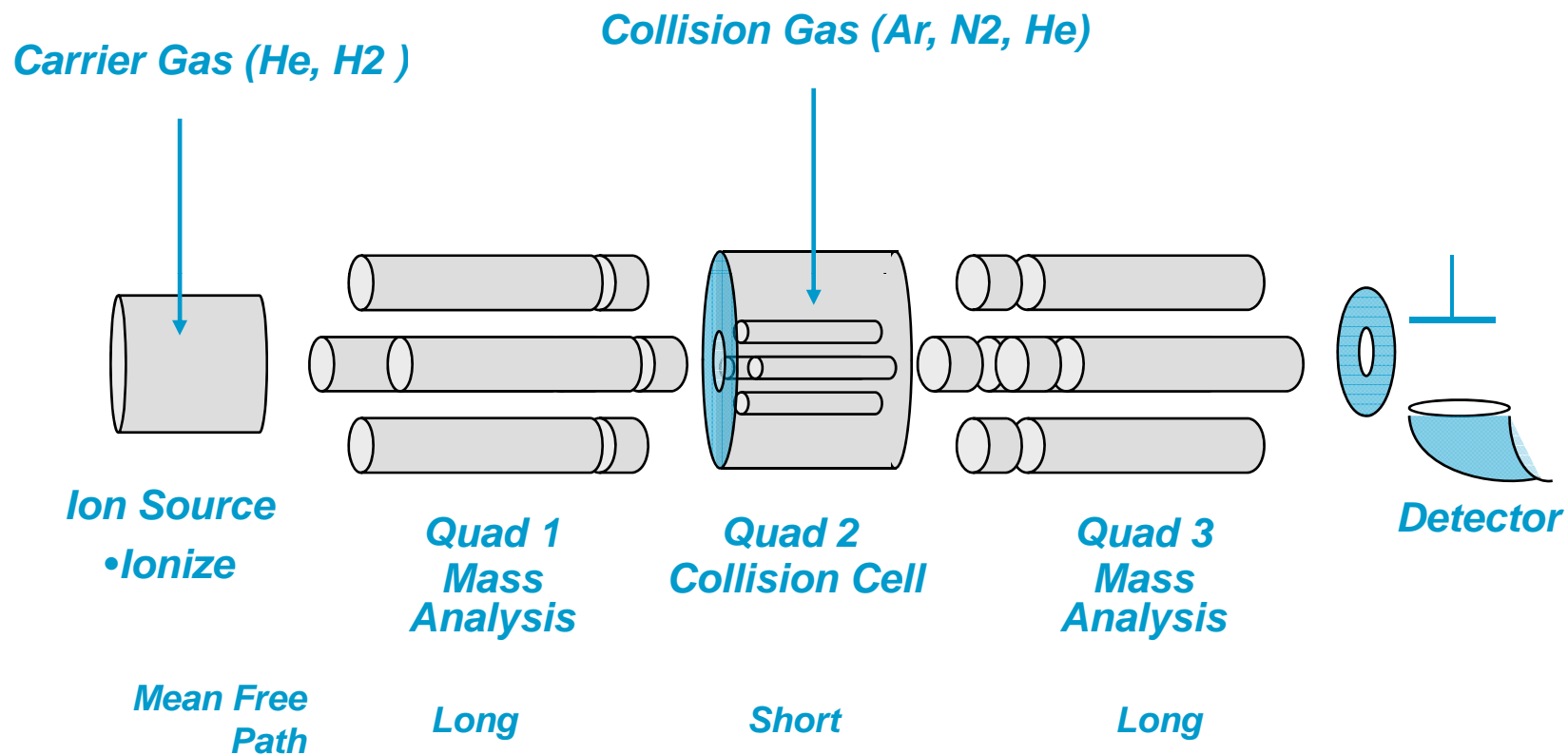
# What is a Triple Quadrupole?



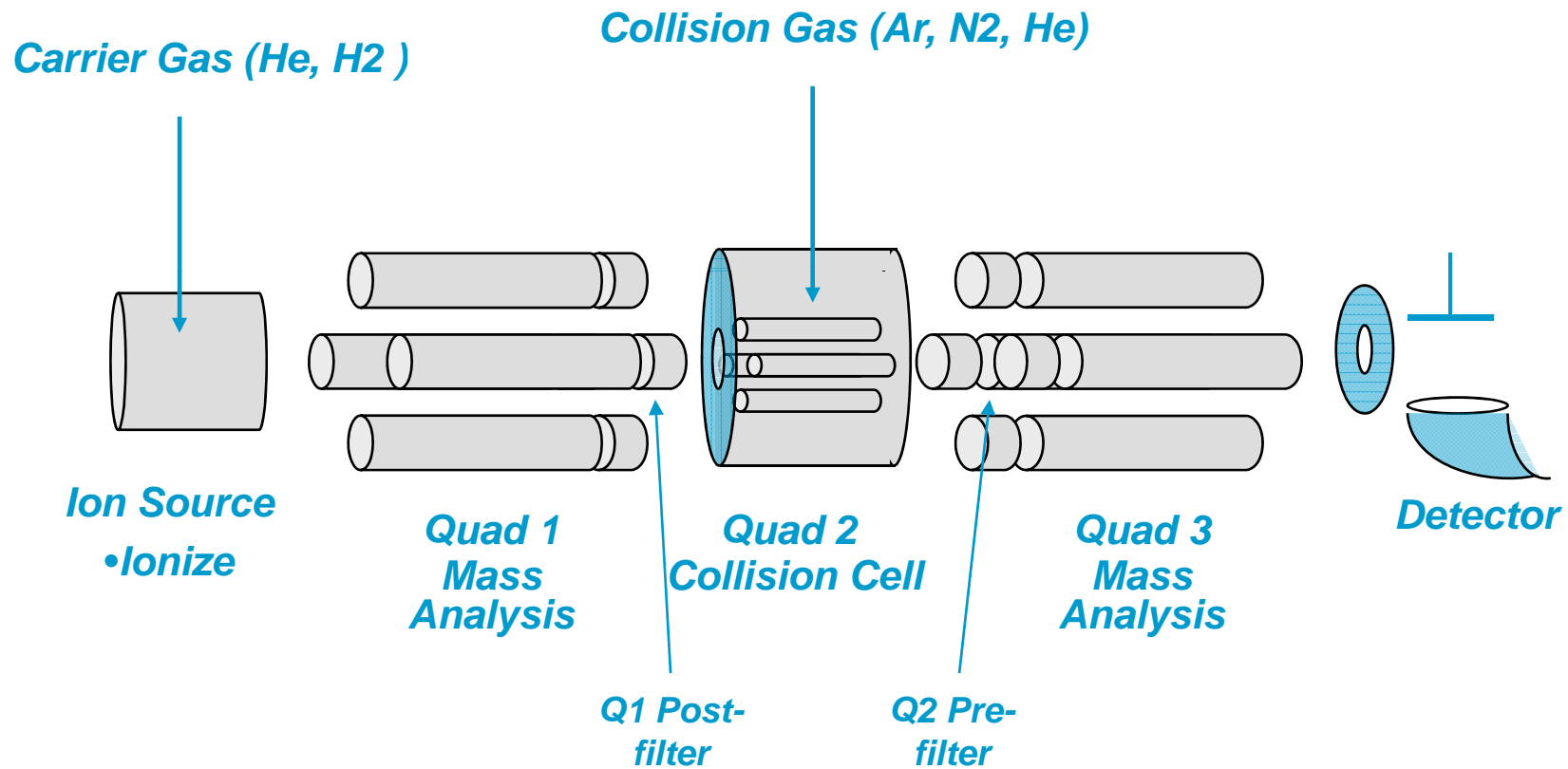
# GC/MS Triple Quad (QQQ)



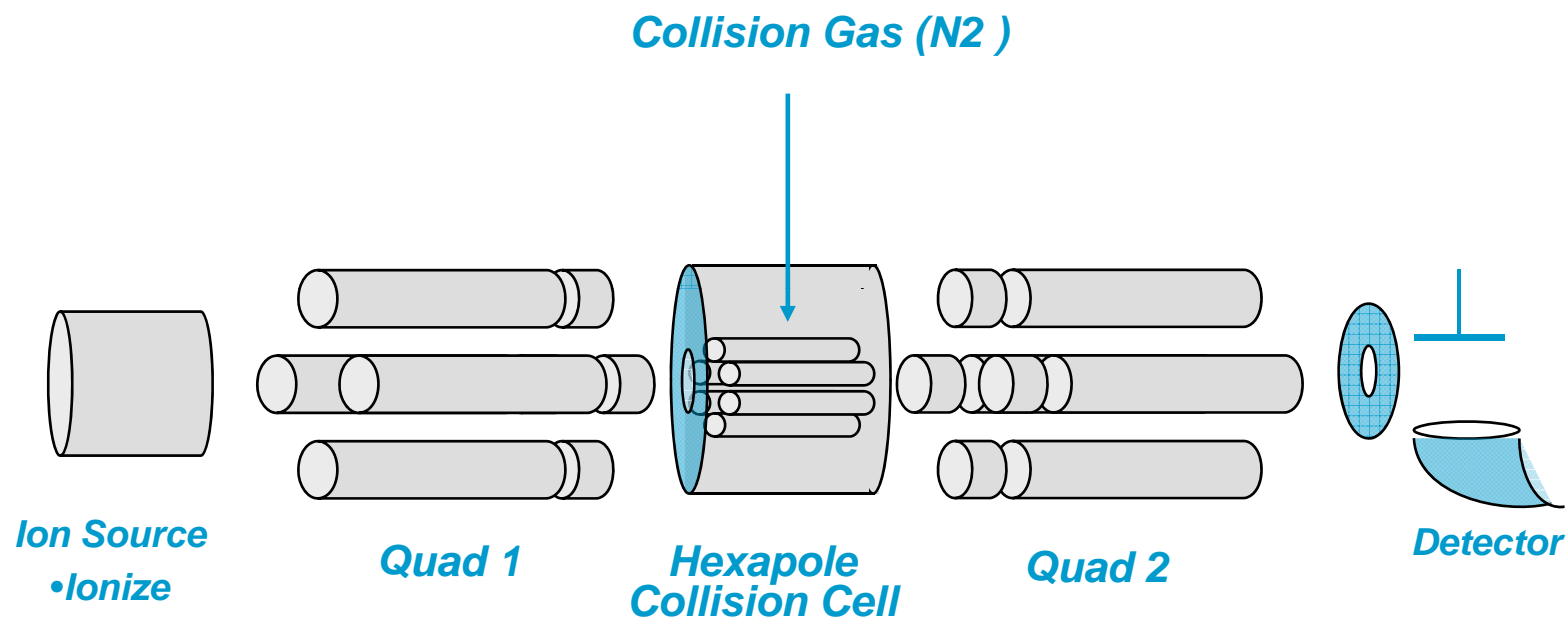
# GC/MS Triple Quad (QQQ)



# GC/MS Triple Quad (QQQ)



# Agilent 7000 GC/MS/MS (QHQ)

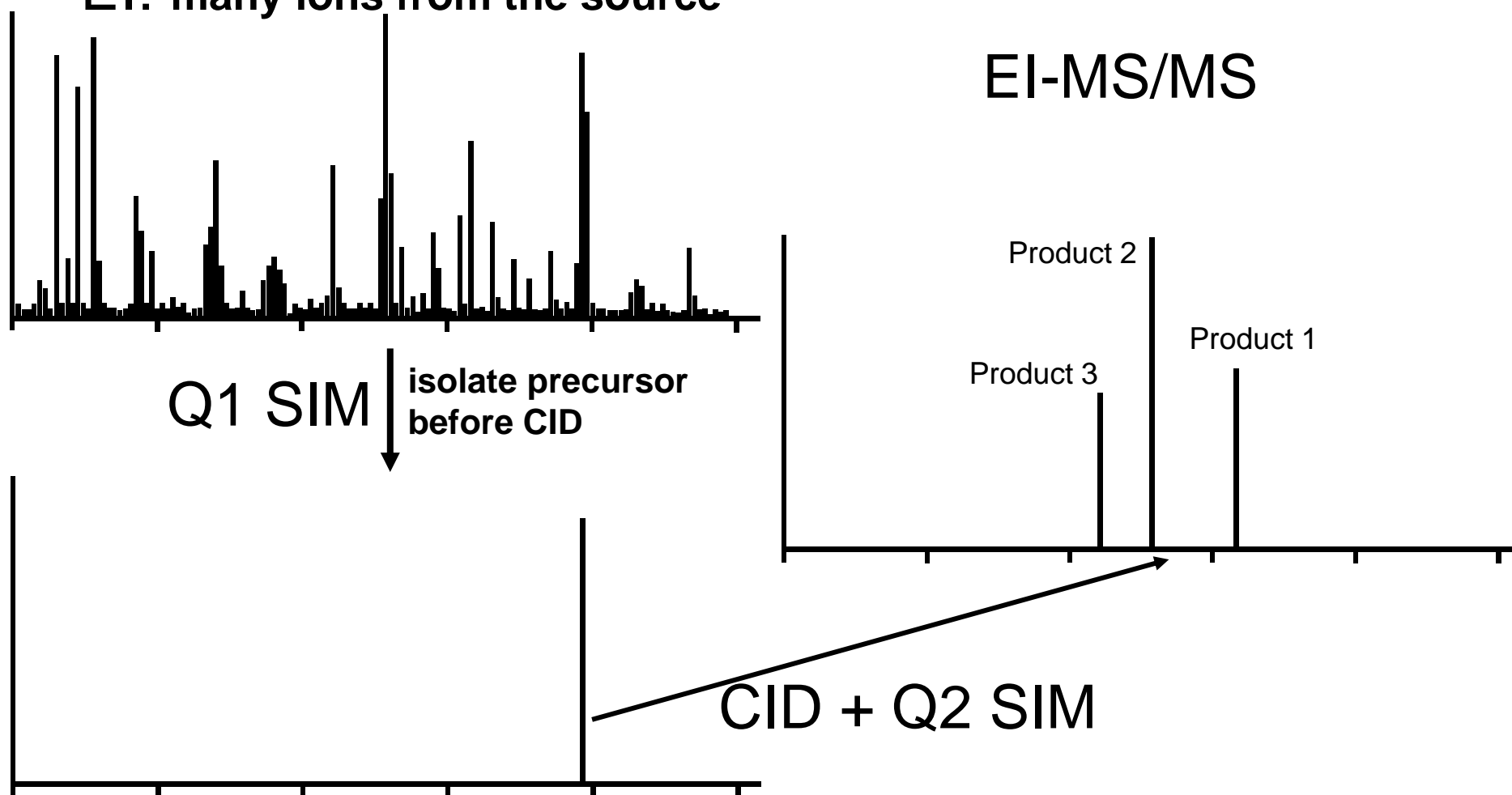


**No mass filtering in the collision cell**  
**The hexapole field has excellent transmission efficiency**  
**for precursor and product ions**

# What is MRM MS/MS?

## Multiple Reaction Monitoring

EI: many ions from the source

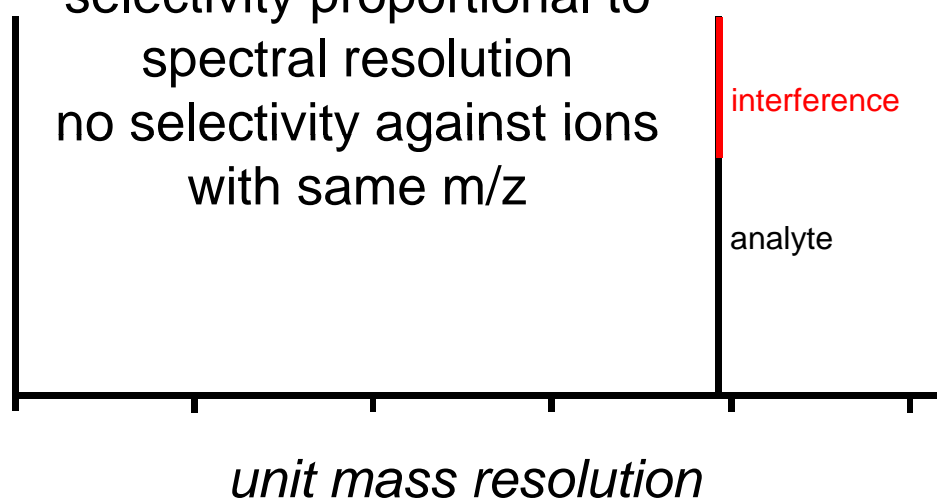


# Why MS/MS?

## Greater Selectivity Than SIM

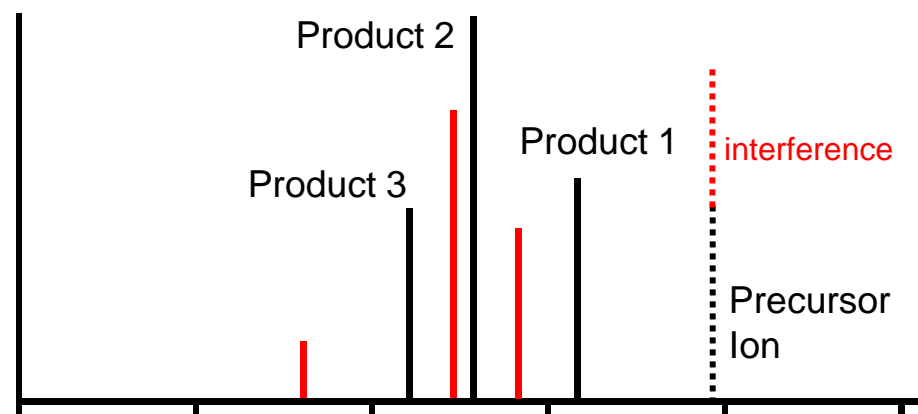
### EI-SIM

selectivity proportional to  
spectral resolution  
no selectivity against ions  
with same  $m/z$



### EI-MS/MS

Precursor selectivity same as SIM  
High probability that at least one product  
ion will be a unique dissociation product  
of the precursor BUT not the interference

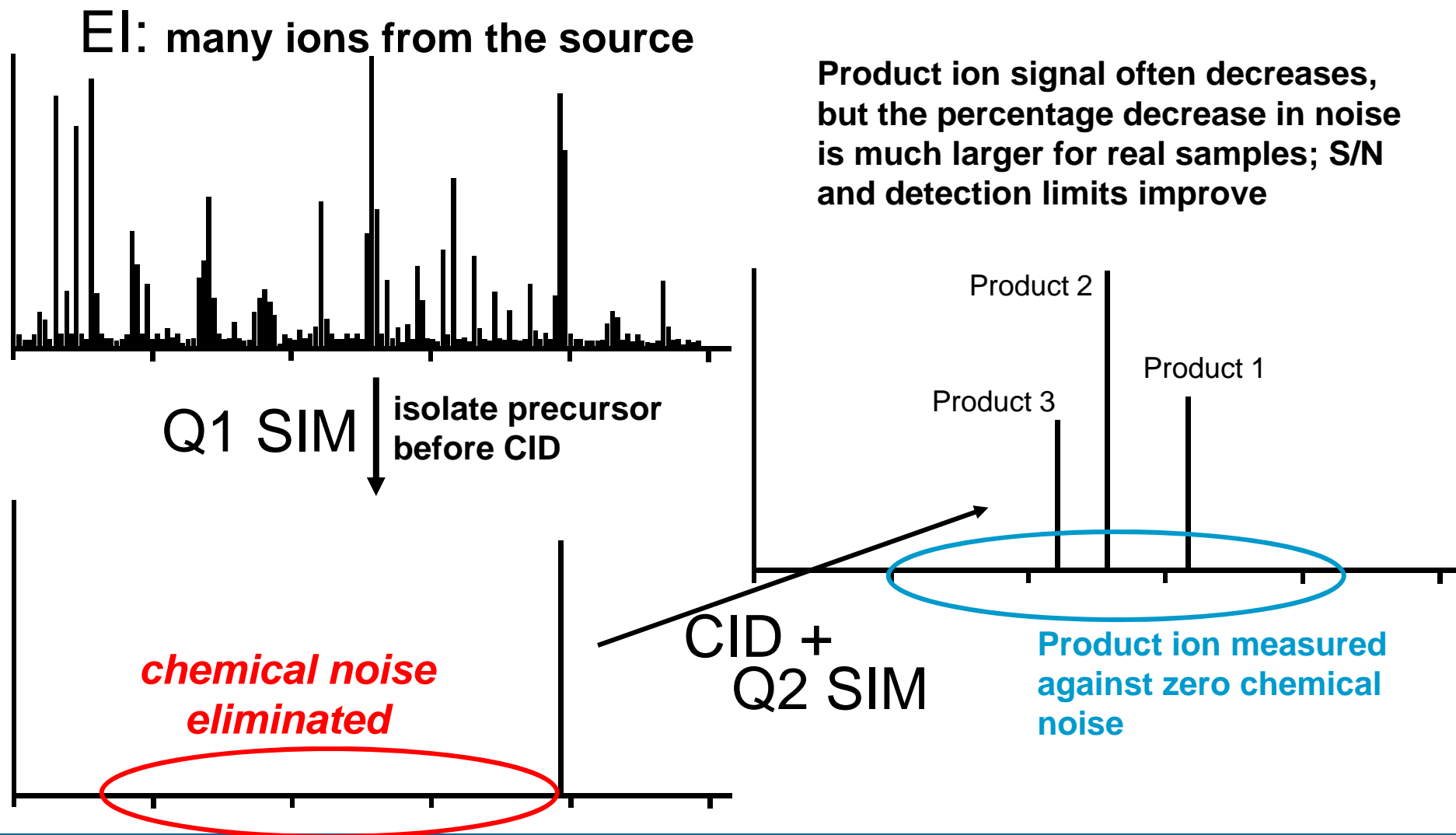


The precursor ion should **NOT** be used for ion ratios or quantitation since the interferences will be the same as the SIM ion



# Why MS/MS?

## Lower detection limits by reducing noise



## Why a GC/MS/MS System?

Allows for the selective quantitation of target compounds in high chemical background samples

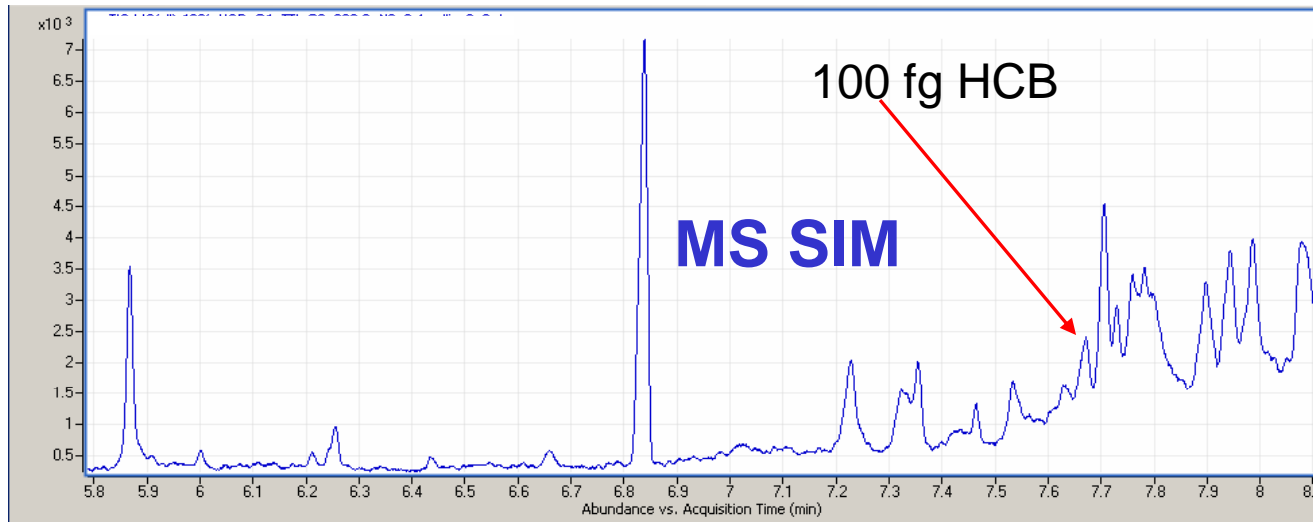
Better S/N in complex matrices than can be achieved by single quadrupole scan or SIM approaches.

Newer regulations in some markets specify analytical power commensurate with GC/MS/MS

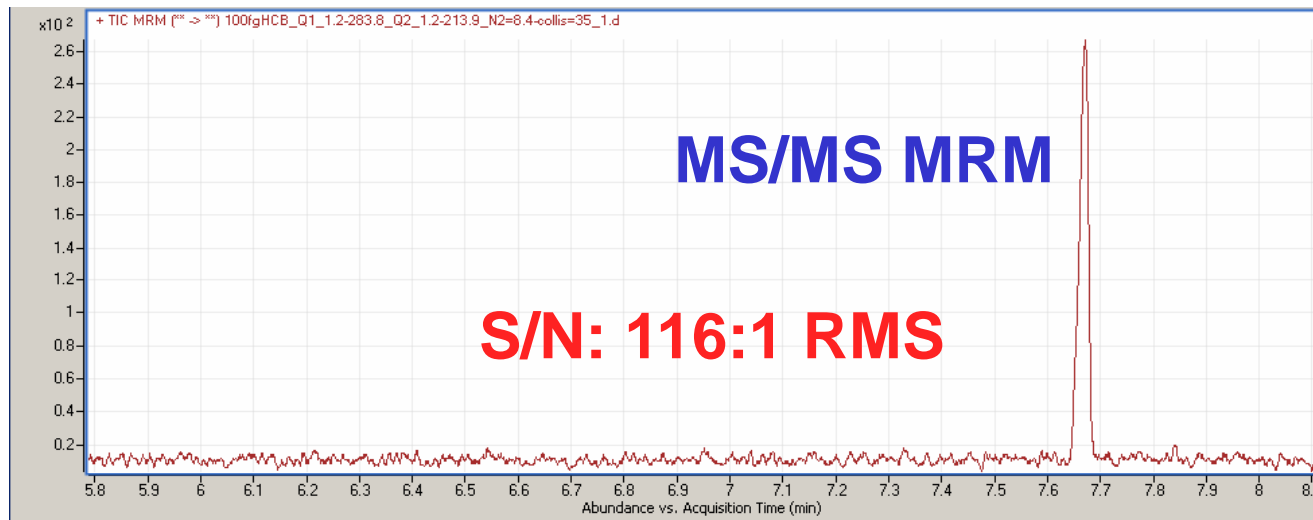


# Why GC/MS/MS?

## A Picture Is Worth a Thousand Words



GC/MS Single Quad SIM



GC/MS/MS QQQ MRM

EI 100fg HCB in "DIRTY" Matrix

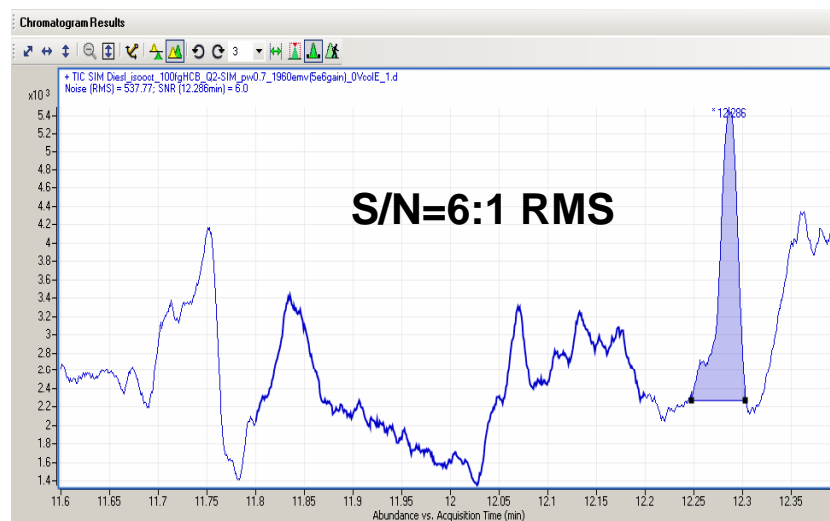
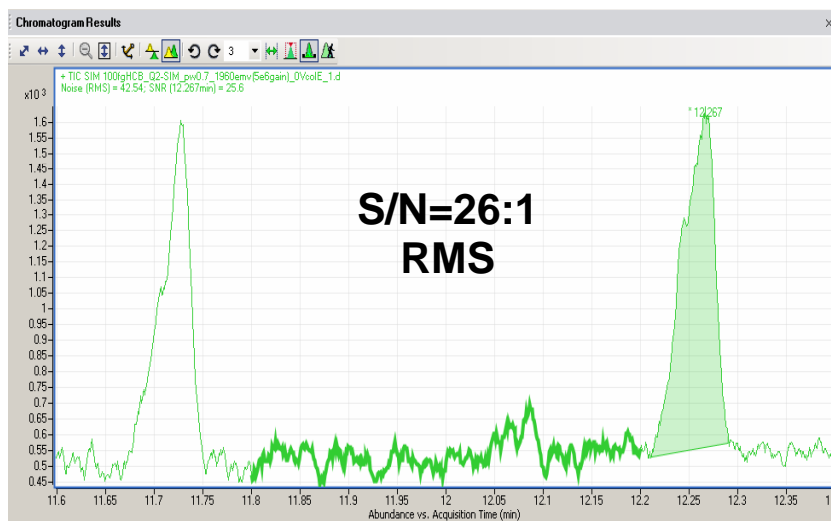
*A chromatographer's dream: single peak on flat baseline*

# SIM vs MRM for HCB

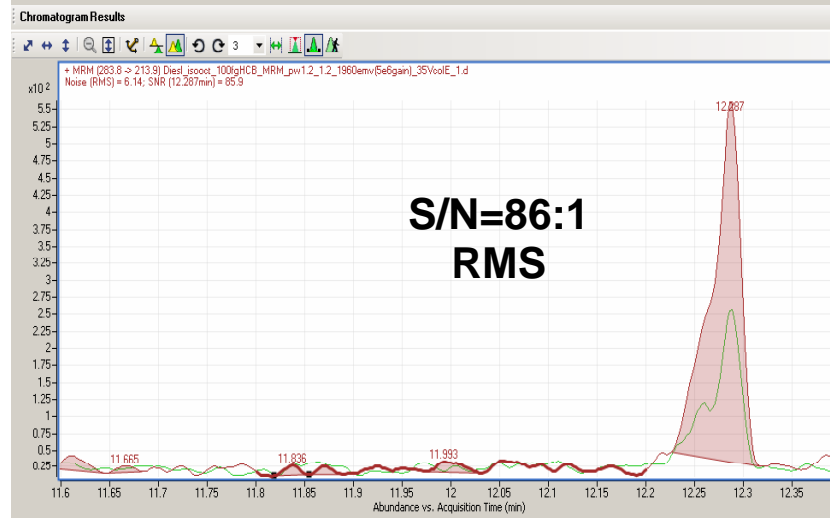
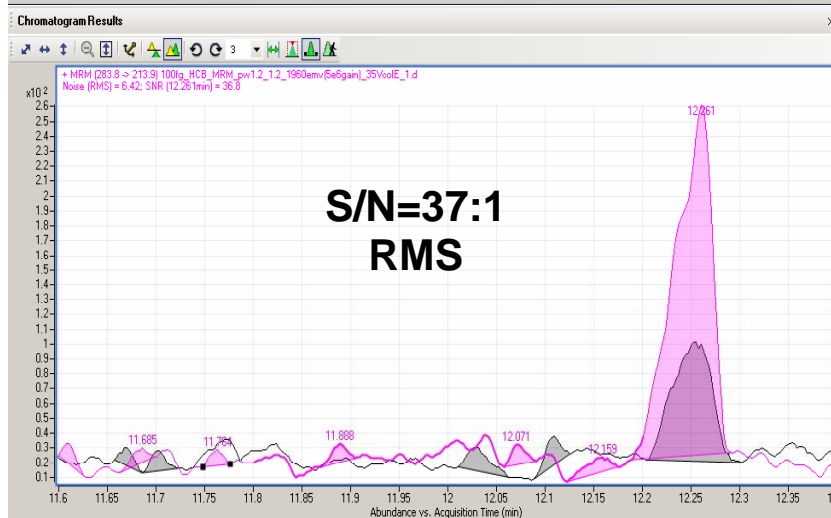
## 100 fg HCB in Clean Matrix

## 300 fg HCB in Diesel

Single MS: SIM 283.8



MS/MS: 283.8:213.9



# Emerging Contaminants Require New Solutions

- Pharmaceutical compounds in water systems
- Per-fluorinated organic compounds in ground water (PFOS/PFOA)

Both of these classes of compounds are at extremely low levels in the environment. They are also very poor candidates for GC/MS analysis, even after derivitization.

The solution: LC/MS!

For accurate low level target compounds: LC/MS/MS

For identifying unknown contaminants: LC/TOF and LC/QTOF

# Emerging Contaminants Require New Solutions

A new and expanded portfolio for applications for environmental problems, from PFOS to pharmaceuticals in water, require combining exceptional performance and reliability to HPLC/MS solutions



LC/MSD  
Single Quad



6410 QQQ



6210 TOF



6510 QTOF



6300 Series Ion Traps

# Relentless Triple Quadrupole Innovation

## *Extending Outstanding Performance*

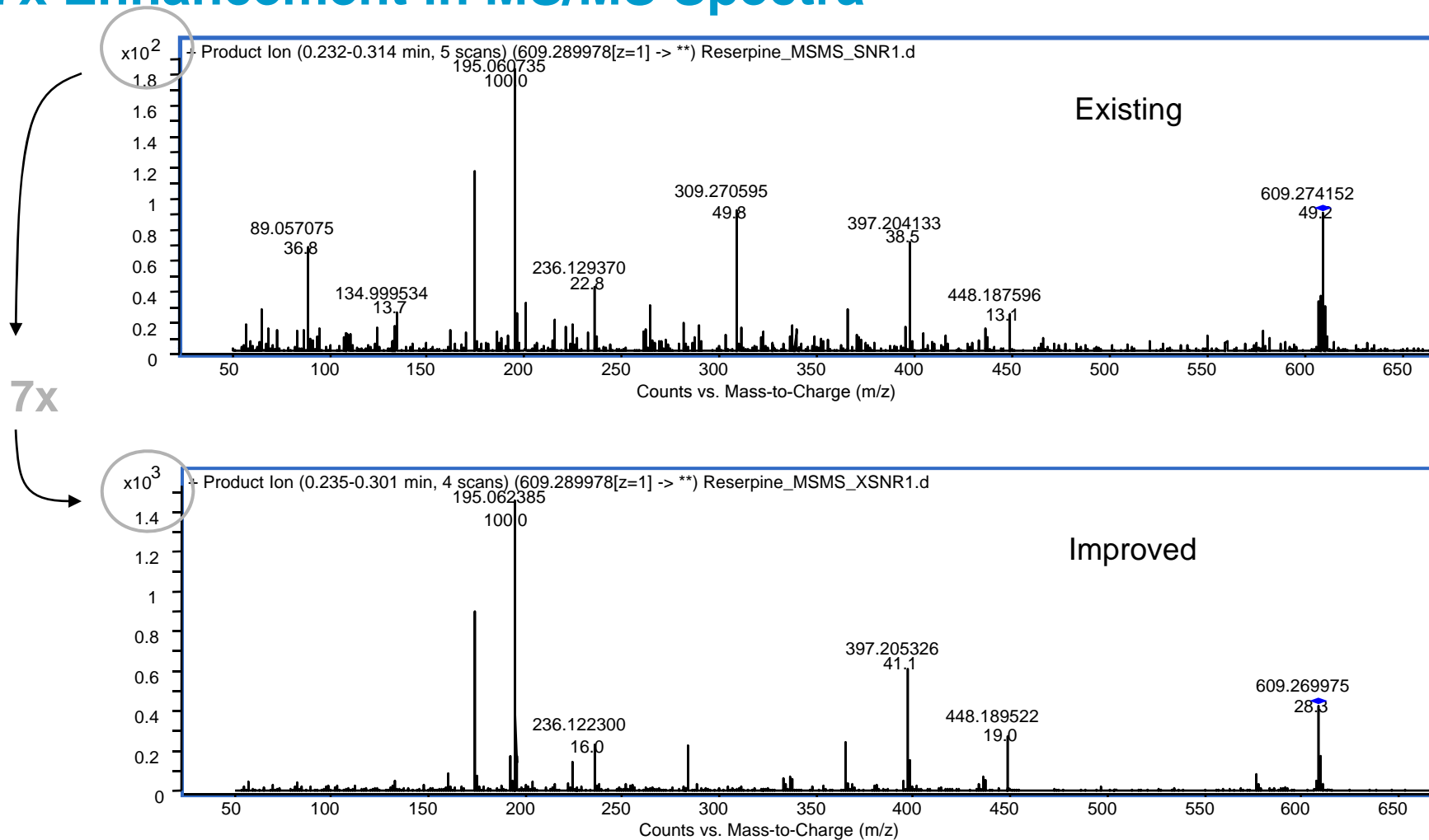
6400 Series Triple Quad for Targeted MS/MS Quantitation

- ✓ Polarity Switching
- ✓ 200 MRM / Time Segment
- ✓ Automated Method Optimization
- ✓ Compliance (21 CFR Part 11 Support)
- ✓ Extended mass range (2000 m/z)
- ✓ Faster Reporting



# New Levels of Sensitivity

## 7x Enhancement in MS/MS Spectra



### Reserpine Sample



# 6500-Series Accurate Mass Q-TOF




The power of  
**Accurate Mass**  
MS and MS/MS

Agilent 6520 Accurate-Mass Q-TOF LC/MS

Our measure is your success.

products | applications | software | services

 **Agilent Technologies**

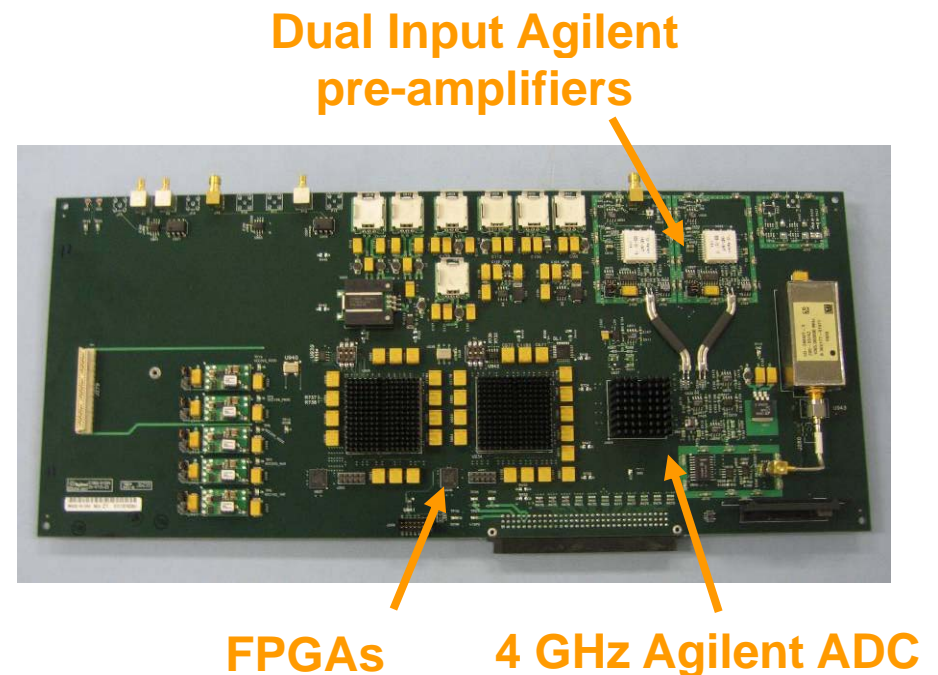
Identification of Unknown Cpds  
Dramatically Outperforms other  
Q-TOFs and Orbitraps

- ✓ 1-2 ppm MS Accuracy
- ✓ 2-4 ppm MS/MS Accuracy
- ✓ R > 20,000
- ✓ Extended Dynamic Range –  
Approaching 5 Decades in-Scan
- ✓ 10 Hz Scan Rate
- ✓ Agilent Robustness/Reliability

# Proprietary New Ultra High Speed Acquisition System

Two New Modes: 4 GHz ADC for Enhanced Resolving Power  
2-Channel x 2 GHz Dual Gain for Extended Dynamic Range

- 4 GHz (8 bit) Analog-Digital-Converter **ADC**
  - Adapted from Agilent’s High Speed Oscilloscope Systems
- Ultra High Speed **FPGA** process and store transients in real time
  - Up to 20,000 m/z depth

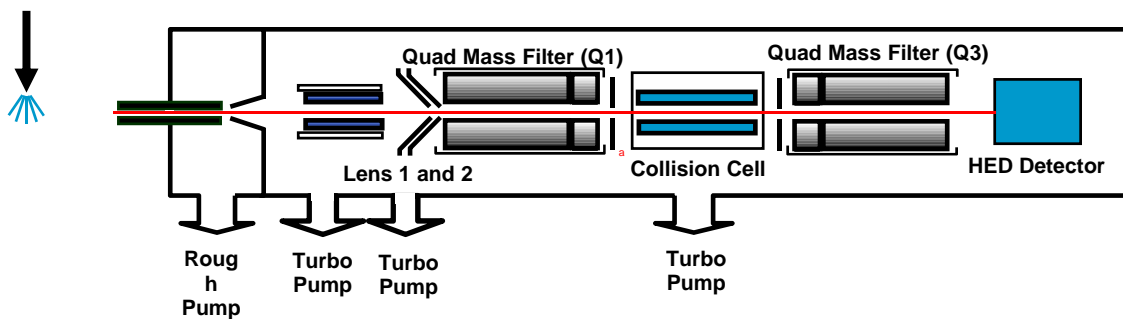
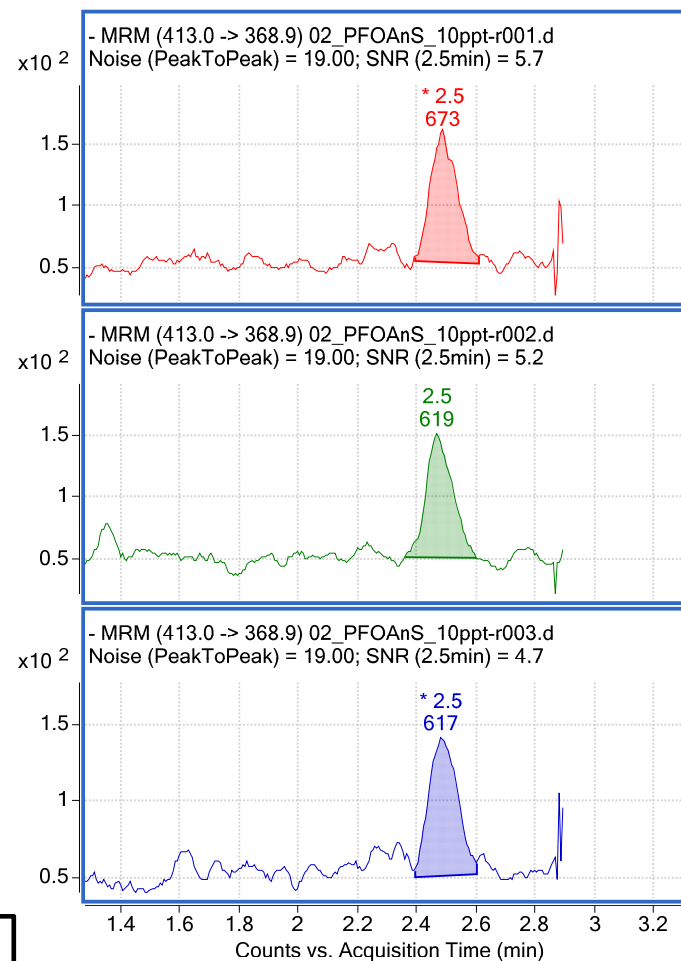


# MassHunter™: Unified Platform for LC/MS Instrument Control and Data Processing



- Easy and intuitive to learn and use**
- Common software for all LC/MS instruments & applications**
- Fast, customizable reporting**
- Rapid generation of high quality quantitative results!**

# Analysis of PFOA and PFOS using the Agilent 6410 Triple Quadrupole LC/MS/MS



# Better Software to Find Answers Faster

Agilent MassHunter Quantitative Analysis - 20071115\_PFOa - PFOAnS\_ESTD\_20071116

File Edit View Analyze Method Update Report Tools Help

Analyze Batch Layout: Restore Default Layout

**Batch Table**

Sample: Sample Type: <All> Compound: 1: PFOA ISTD: Time Segment: <All>

Sample					PFOA M...		PFOA Results					
Name	Type	Level	Data File	Exp. Conc.	RT	Resp.	S/N	MI	Calc. Conc.	Final Conc.	Accuracy	
PFOAnS blank	Blank		01_Blank-r001.d		2.534	127	0.75		0.0000	0.0000		
PFOAnS blank	Blank		01_Blank-r002.d		2.509	170	0.86		0.0000	0.0000		
PFOAnS blank	Blank		01_Blank-r003.d		2.498	145	0.78		0.0000	0.0000		
PFOAnS 10 ppt	Cal	1	02_PFOAnS_10ppt-r001.d	0.0113	2.489	614	1.75		0.0112	0.0112	99.3	
PFOAnS 10 ppt	Cal	1	02_PFOAnS_10ppt-r002.d	0.0113	2.470	619	2.95		0.0115	0.0115	101.5	
PFOAnS 10 ppt	Cal	1	02_PFOAnS_10ppt-r003.d	0.0113	2.483	614	1.51		0.0112	0.0112	99.4	
PFOAnS 10 ppt	Cal	1	02_PFOAnS_10ppt-r004.d	0.0113	2.490	622	3.72		0.0116	0.0116	102.5	
PFOAnS 10 ppt	Cal	1	02_PFOAnS_10ppt-r005.d	0.0113	2.483	649	1.77		0.0128	0.0128	113.0	
PFOAnS 10 ppt	Cal	1	02_PFOAnS_10ppt-r006.d	0.0113	2.503	635	2.96		0.0122	0.0122	107.6	
PFOAnS 50 ppt	Cal	2	03_PFOAnS_50ppt-r001.d	0.0565	2.517	1561	2.57		0.0528	0.0528	93.4	
PFOAnS 50 ppt	Cal	2	03_PFOAnS_50ppt-r002.d	0.0565	2.483	1593	3.52		0.0542	0.0542	95.9	

**Compound Information**

MRM (413.0 -> 368.9) 02\_PFOA 2.503 635.0000

MRM (413.0 -> 368.9)

MRM (2.375-2.618 min, 37 s...)

**Calibration Curve**

Type: Quadratic Origin: Ign Weight: 1/x ISTD QC

PFOA - 7 Levels, 7 Levels Used, 24 Points, 24 Points Used, 0 QCs

$$y = 406.7132 * x^2 + 22778.7217 * x + 358.1030$$

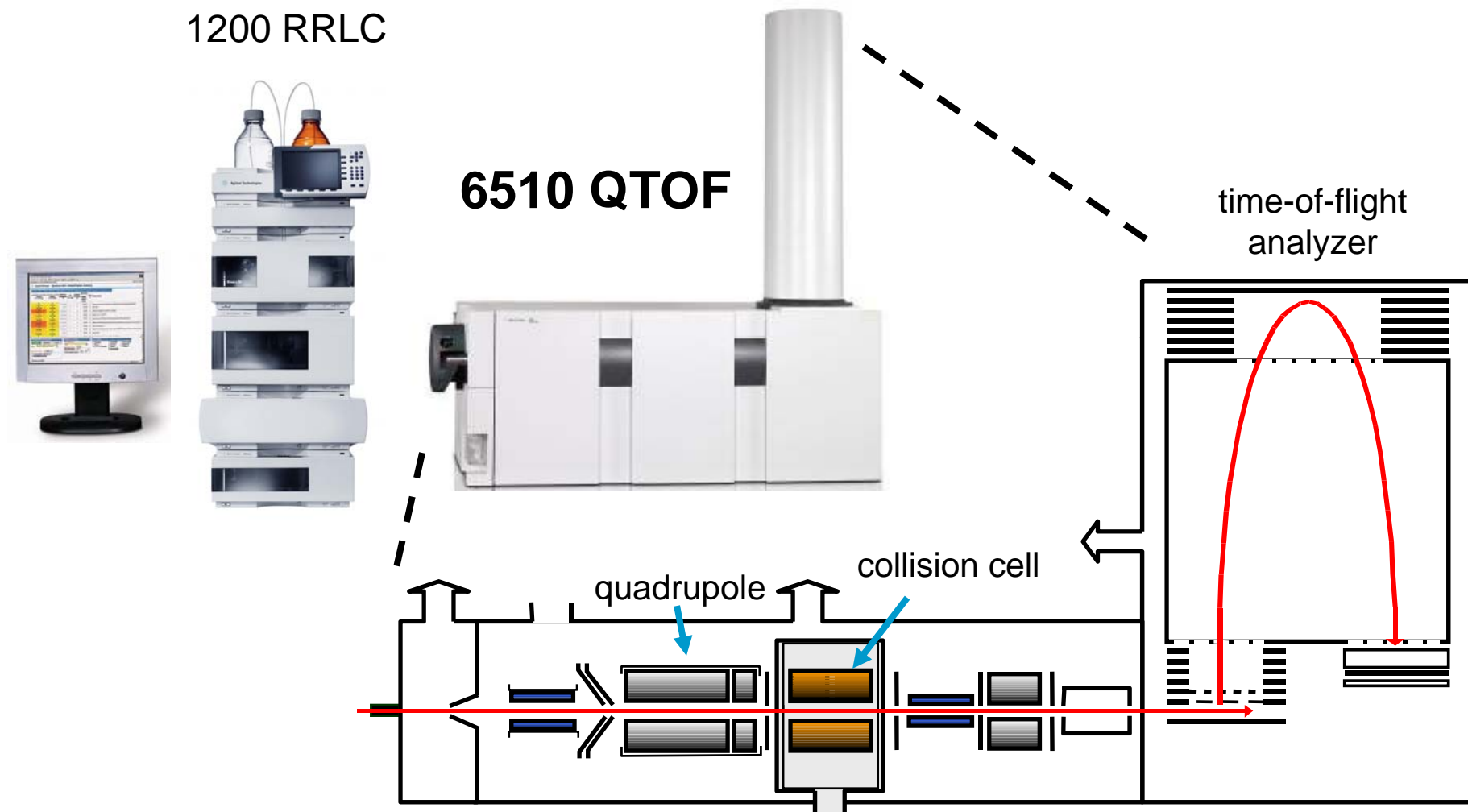
$$R^2 = 0.99955522$$

Responses x10<sup>5</sup>

Concentration (ng/ml)

PFOAnS 10 ppt PFOA 27 Samples (27 total)

# Searching for Unknown Contaminants



# Example: Pharmaceutical Compounds in Ground Water

Various water samples collected by USGS, containing any of the following compounds:

## Neutral Masses of Potential Residues in Water

151.06333	Acetaminophen	254.09429	Ketoprofen	308.10486	Warfarin
176.09496	Cotinine	255.16231	Diphenhydramine	309.13405	Fluoxetine
180.04226	Aspirin	267.12593	Venlafaxine	310.07358	Sulfadimethoxine
180.06473	1,7-dimethylxanthine	270.02452	Sulfamethizole	313.97805	Triclocarban
194.08038	Caffeine	274.14298	Trimethoprim	314.14126	Ranitidine
201.03607	Thiabendazole	278.08375	Sulfamethazine	318.15551	Fluvoxamine
214.03967	Clofibric acid	284.01347	Sulfachloropyridazine	324.16379	Citalopram
230.09429	Naproxen	287.95116	Triclosan	329.14272	Paroxetine
236.09496	Carbamazepine	293.05000	Norsertaline	330.00772	Furosemide
239.10769	Bupropion	295.01668	Diclofenac	344.10084	Dehydronifedipine
239.15214	Albuterol	295.11840	Norfluoxetine	348.16852	Enalaprilat
250.15698	Gemifrozil	296.96447	HCTZ	413.98602	Miconazole
252.11572	Cimetidine	297.11873	Duloxetine	414.16133	Diltiazem
253.05211	Sulfamethoxazole	299.15214	Codeine	418.27192	Simvastatil
		305.07380	Sertraline	573.51210	Erythromycin

# Processing large amount of data with MFE

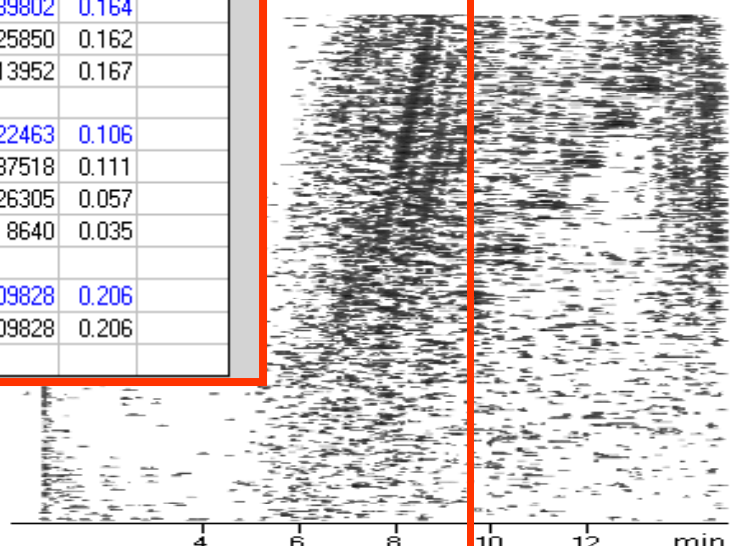
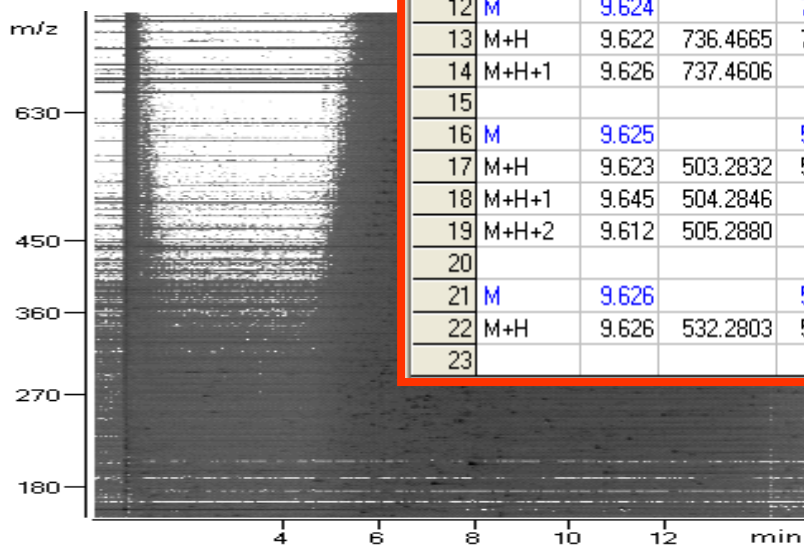
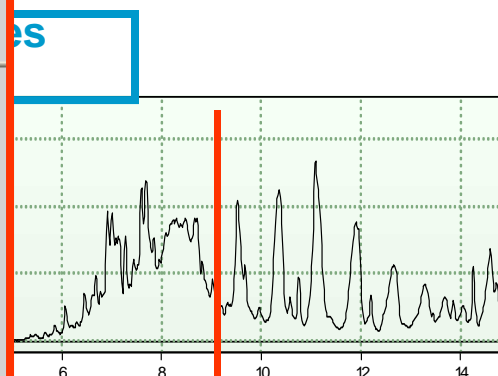
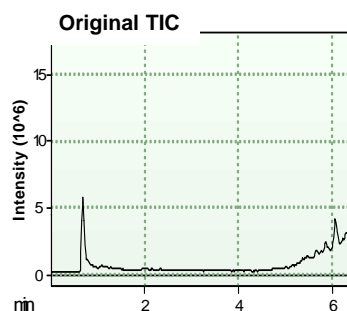
Display filtering:

- S/N > 2
- $m/z$  150 to 800
- [M+Na] and [M+NH<sub>4</sub>]

- At least 2 ions
- Relative intensity > 0.01%

Export Group #229 (RT=9.625) --- 5 Features

	species	RT	m/z	mass	abund.	width	satur.
1	M	9.621		590.3064	1111237	0.193	
2	M+H	9.617	591.3131	590.3058	470077	0.207	
3	M+H+1	9.630	592.3153		243624	0.258	
4							
5	M+Na	9.623	613.2965	590.3072	321761	0.136	
6	M+Na+1	9.623	614.3035		75775	0.145	
7							
8	M	9.629		236.0961	949907	0.049	
9	M+H	9.629	237.1034	236.0961	828746	0.049	
10	M+H+1	9.629	238.1064		121162	0.047	
11							
12	M	9.624		735.4592	339802	0.164	
13	M+H	9.622	736.4665	735.4592	225850	0.162	
14	M+H+1	9.626	737.4606		113952	0.167	
15							
16	M	9.625		502.2759	322463	0.106	
17	M+H	9.623	503.2832	502.2759	287518	0.111	
18	M+H+1	9.645	504.2846		26305	0.057	
19	M+H+2	9.612	505.2880		8640	0.035	
20							
21	M	9.626		531.2730	109828	0.206	
22	M+H	9.626	532.2803	531.2730	109828	0.206	
23							





# Agilent Solutions for Environmental Testing

History of leadership and commitment to environmental testing

A focus on usable sensitivity and productivity

Continuing innovations, from “old technology” to new technical challenges

New LC/MS solutions for “new” environmental targets

