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GC/MS and Forensic Specialist

Novel GC/MS Approaches to Forensic Analyses

Agilent Technologies



Agilent Forensic Solutions

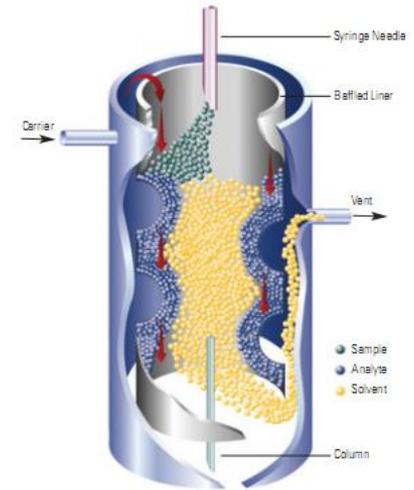
Agilent's GC/MS portfolio

- Single Quad 5975 MSD
- 5975T
- Ion Trap MSn 220 & 240
- 7000B Triple Quad
- GC-APCI QToF



Key Features of Market Leading 7890 GC

- 0.001 PSI accurate gas control
- Capillary Flow Technology
- LTM Column Technology
- Multi Mode Injector
 - Simile On Column
 - Constant Temp Split/Splitless PTV
 - Solvent Venting (LVI)



Agilent's highly versatile Multimode inlet (MMI) combines the capabilities of spit/splitless operation (cold, hot and pulsed), temperature programming and large volume injection with a solvent vent mode. Benefits include higher system sensitivity, ability to analyze thermally labile compounds and more robust handling of dirty samples. (10)

Improved Performance with Cold

1 Hot Splitless

2 Pulsed Hot Splitless

3 Pulsed Hot Splitless with SPC

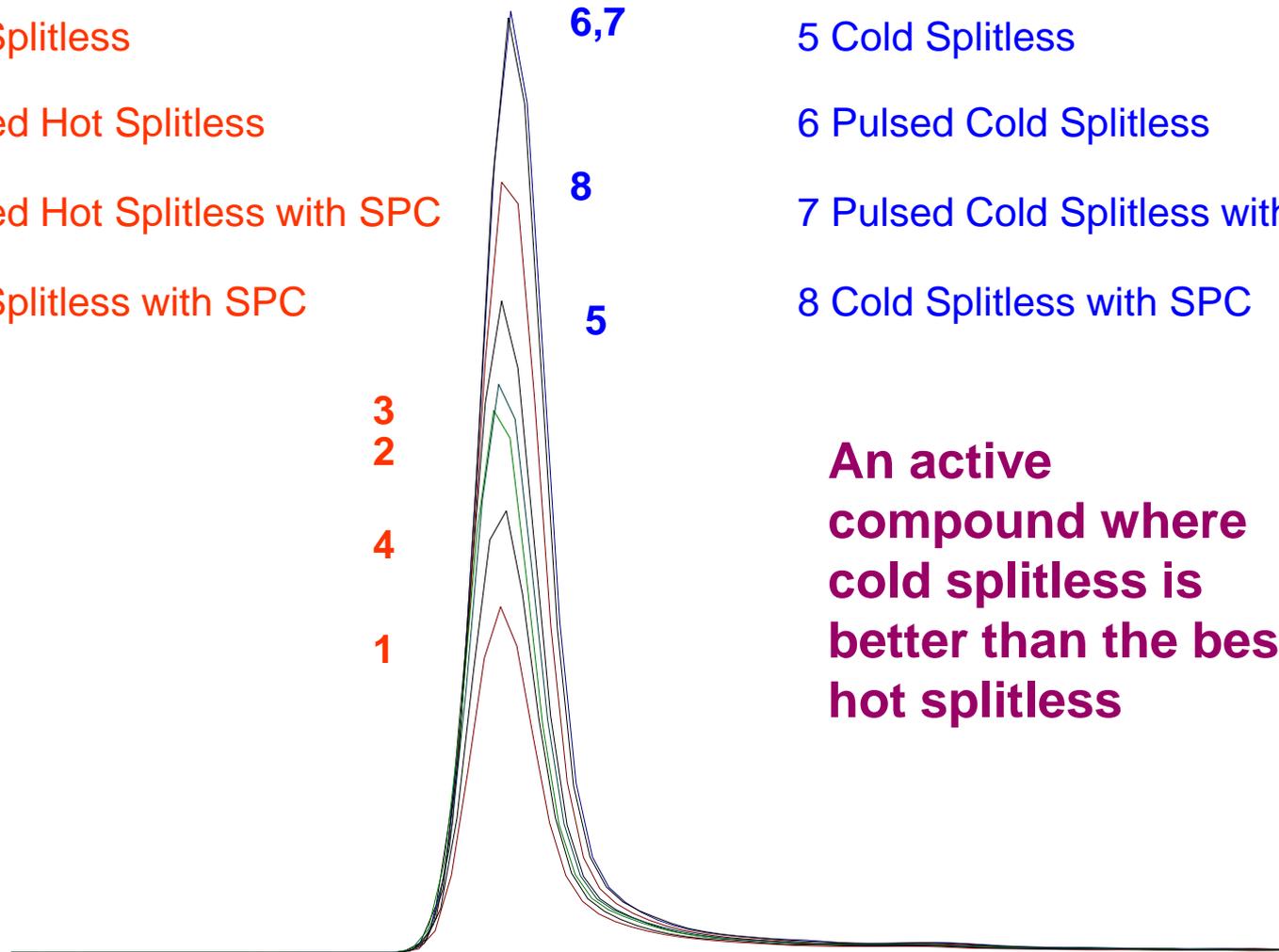
4 Hot Splitless with SPC

5 Cold Splitless

6 Pulsed Cold Splitless

7 Pulsed Cold Splitless with SPC

8 Cold Splitless with SPC



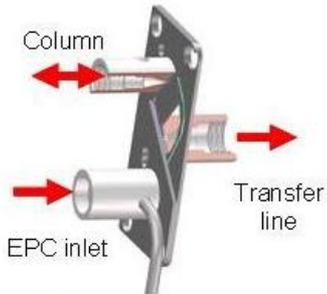
**An active
compound where
cold splitless is
better than the best
hot splitless**

I want to Improve Versatility...

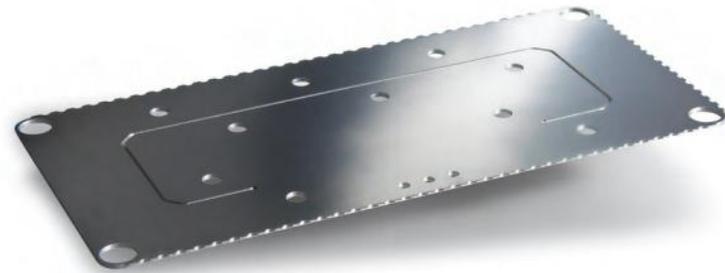
Capillary Flow Technology



- Low Thermal Mass
- Inert Surfaces
- Low Dead Volume
- Absolute Volume known
- 0.001PSI accurate pressure Control



*QuickSwap — Capillary Flow Technology
module for removing columns without
venting MSD*



Purged Ultimate Union, Quickswap, Splitters, Dean Switches, GCxGC Modulators

Ion Traps

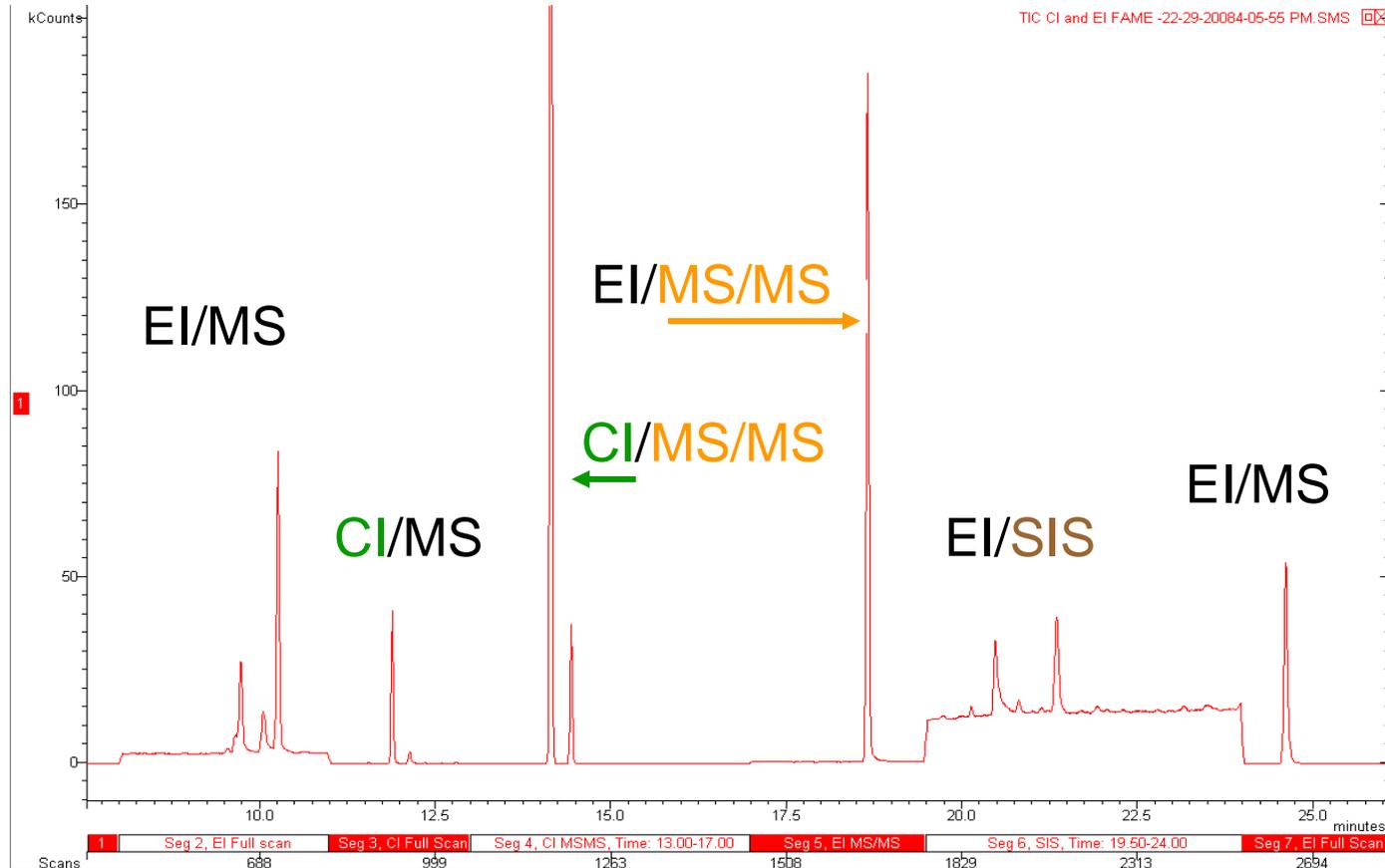
A Versatile MS for routine trace analysis



Unique Points

- High EI full scan sensitivity
 - High CI Sensitivity
 - High Versatility with
 - EI/CI/MSMS
 - Full scan /SIM/ MS/MS
- All possible in same run

Flexibility- Highly Sensitive CI, EI, MS/MS All in One Run



Different ionization (EI and CI) and scanning options (Full scan, MS/MS and SIS) can be utilized even in the same run to enhance both the qualitative and quantitative information content of the results.

7693 Sample Prep Capabilities

Examples of Simple Liquid Manipulation

- Liquid Addition (standards/reagents/etc)
- Aliquoting / Dilutions
- Mixing - Vortex
- Heating
- Barcode Reader
- In Vial L/L Extraction
- Easy Sample Prep SW
- Sample Tray Heating or Cooling



*Ambient
Headspace*



*In-vial
Extraction*



*Small-Volume
Sampling*



Derivatization



Dilution



*Internal Standard
Addition*



*Heating/Mixing
Bar Code*



7696A Sample Prep WorkBench

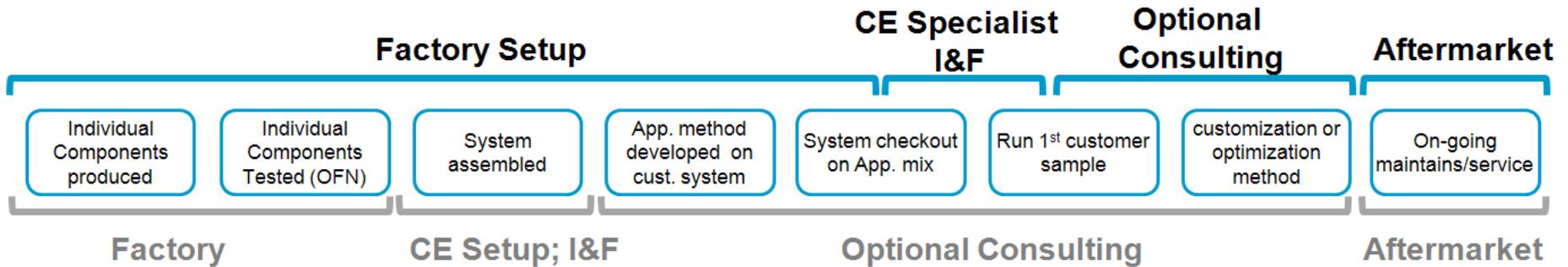
A new standalone instrument for the automation of analytical sample prep

- LC
- GC
- LC/MS
- GC/MS
- other



Fast Track Analyzers

- Factory Installed & Tested
- “Out of the box” analyzer
- Acquisition & Data Process Methods Loaded & Tested



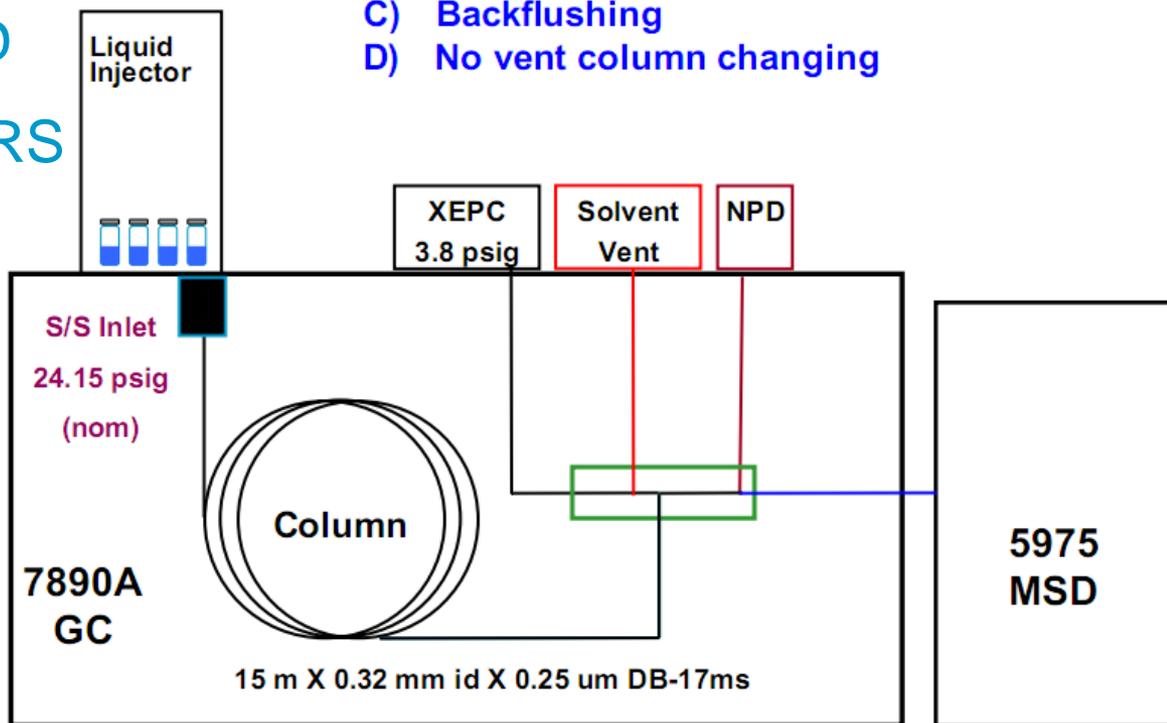
Forensic Toxicology Analyzer

- 7890 GC
- 5975C MSD
- CFT Splitter to NPD
- All drugs detected by NPD
- Retention Time Locked DRS Database Confirms
- SIM Data Quantifies
- Backflushed Column Post Analysis



Improved Forensic Toxicology Screening Using A GC/MS/NPD System with a 725-Compound DRS Database

- A) 1.4:1 MSD:NPD effluent split
- B) Solvent venting
- C) Backflushing
- D) No vent column changing



Chromatograms From Screen of Whole Blood Sample

Scan-TIC

Heavies past end of acquisition are backflushed

NPD

SIM-ion 245

(Fentanyl Target Ion)

1 2 3 4 5 6 7 8

COTININE
MEPROBAMATE
CARISOPRODOL
CAFFEINE
THEOBROMINE
ISTD
DOXEPIN (TRANS)
SERTRALINE
DIAZEPAM
HYDROCODONE
NORDIAZEPAM
FENTANYL

?

THC/THC Acid Oral fluid Analyzer

Confirmation of THC in Oral Fluids Using High-Resolution 2-D GC/MS

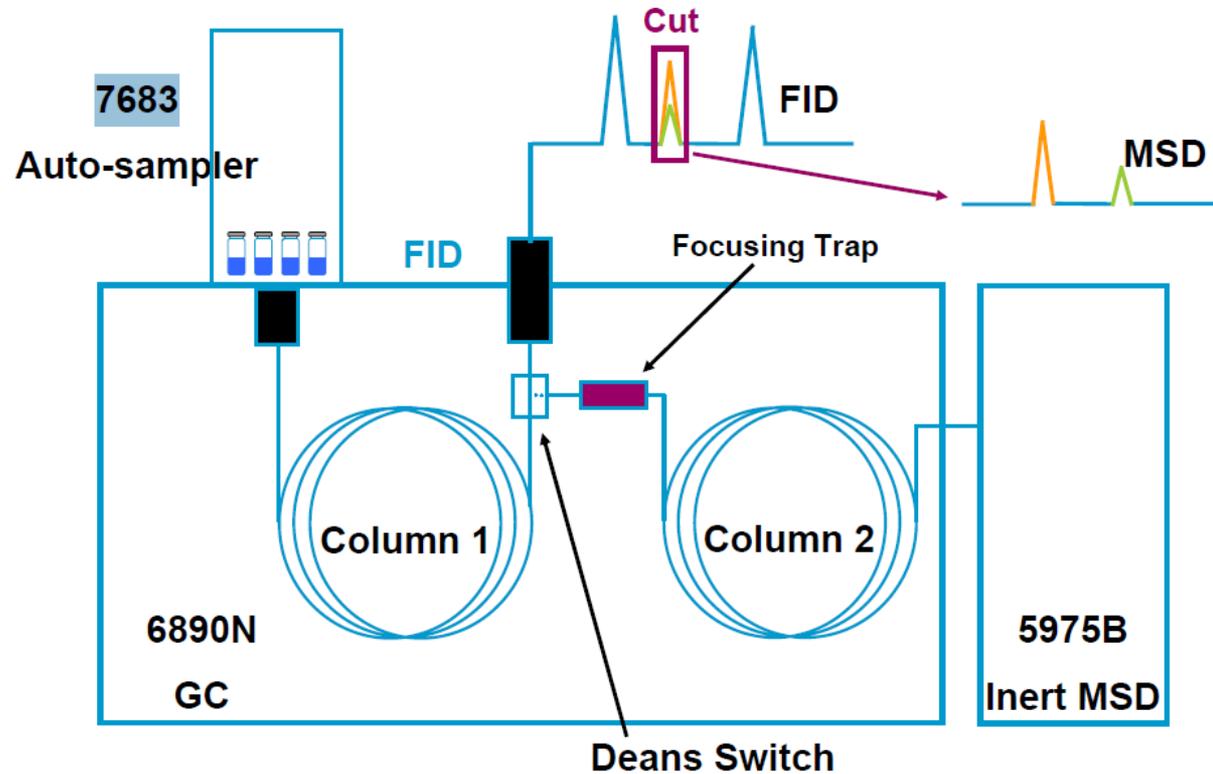
Application

Dean's Switched 2-D GC/MS Solution

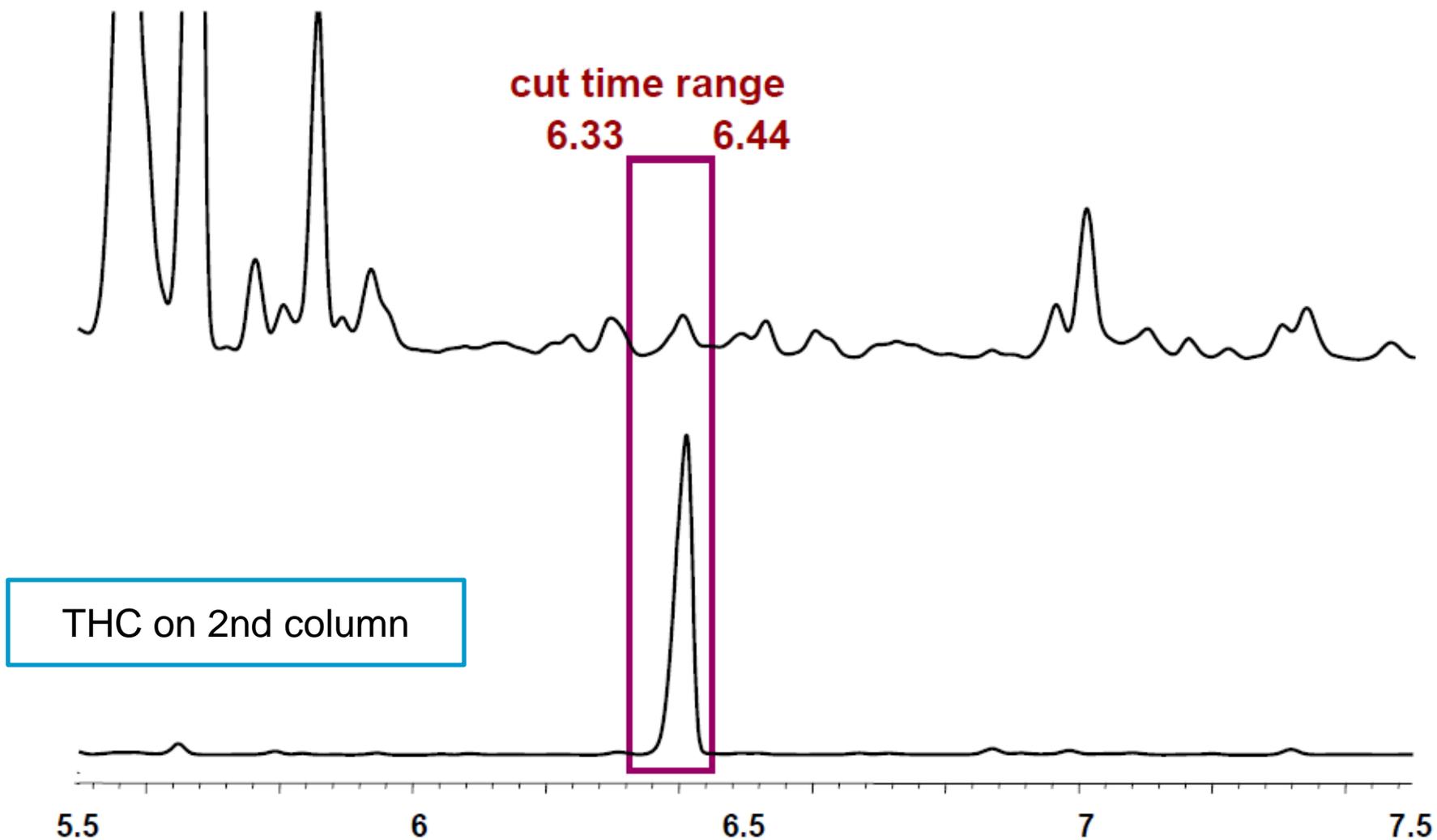
Forensics

Ammonia NCI

- Allows Absolute
- Separation
- Sensitivity
- Confidence!

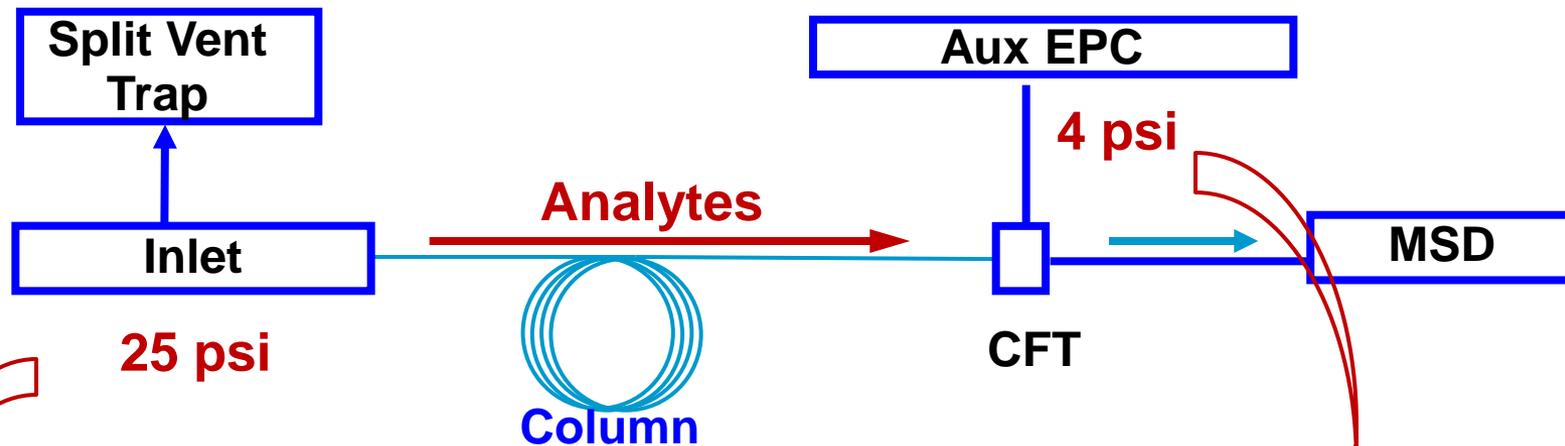


Patient Sample Matrix

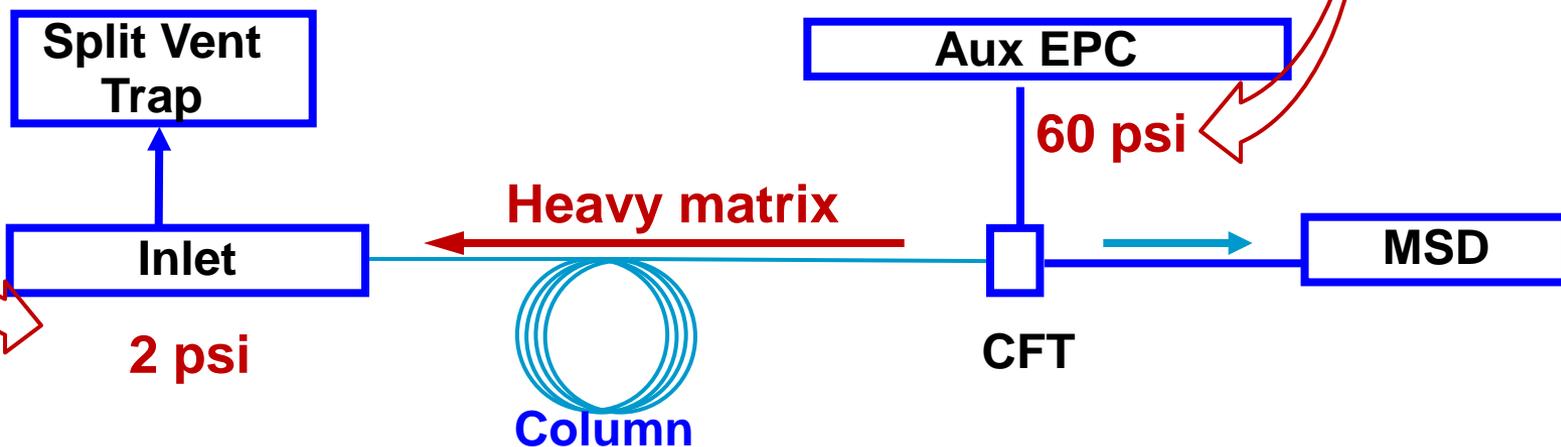


How does Backflush work??

During GC Run



After GC Run



Why Backflush?

- With MS/MS **cannot see “dirty matrix”**
- Large Injections mean more analyte & more dirt
- Non-volatiles contaminate head of column, move slowly through to source
- Heavy matrix contaminates the source faster --- **sensitivity is LOST!**

Ensure the highest sensitivity with GC/MS/MS !

Without Backflush: A Serious Problem

Abundance

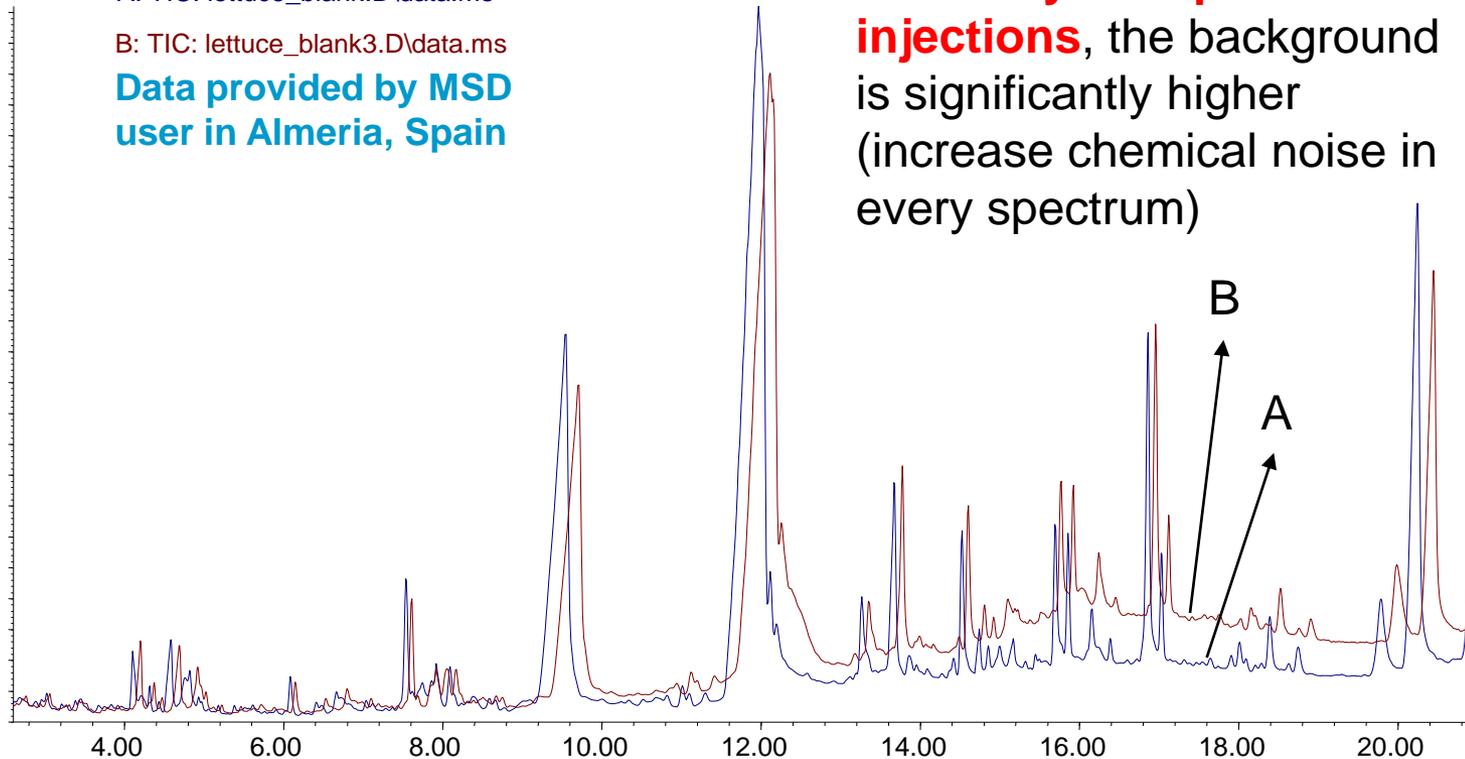
4.6e+07
4.4e+07
4.2e+07
4e+07
3.8e+07
3.6e+07
3.4e+07
3.2e+07
3e+07
2.8e+07
2.6e+07
2.4e+07
2.2e+07
2e+07
1.8e+07
1.6e+07
1.4e+07
1.2e+07
1e+07
800000
600000
400000
200000
0

A: TIC: lettuce_blank.D\data.ms

B: TIC: lettuce_blank3.D\data.ms

Data provided by MSD
user in Almeria, Spain

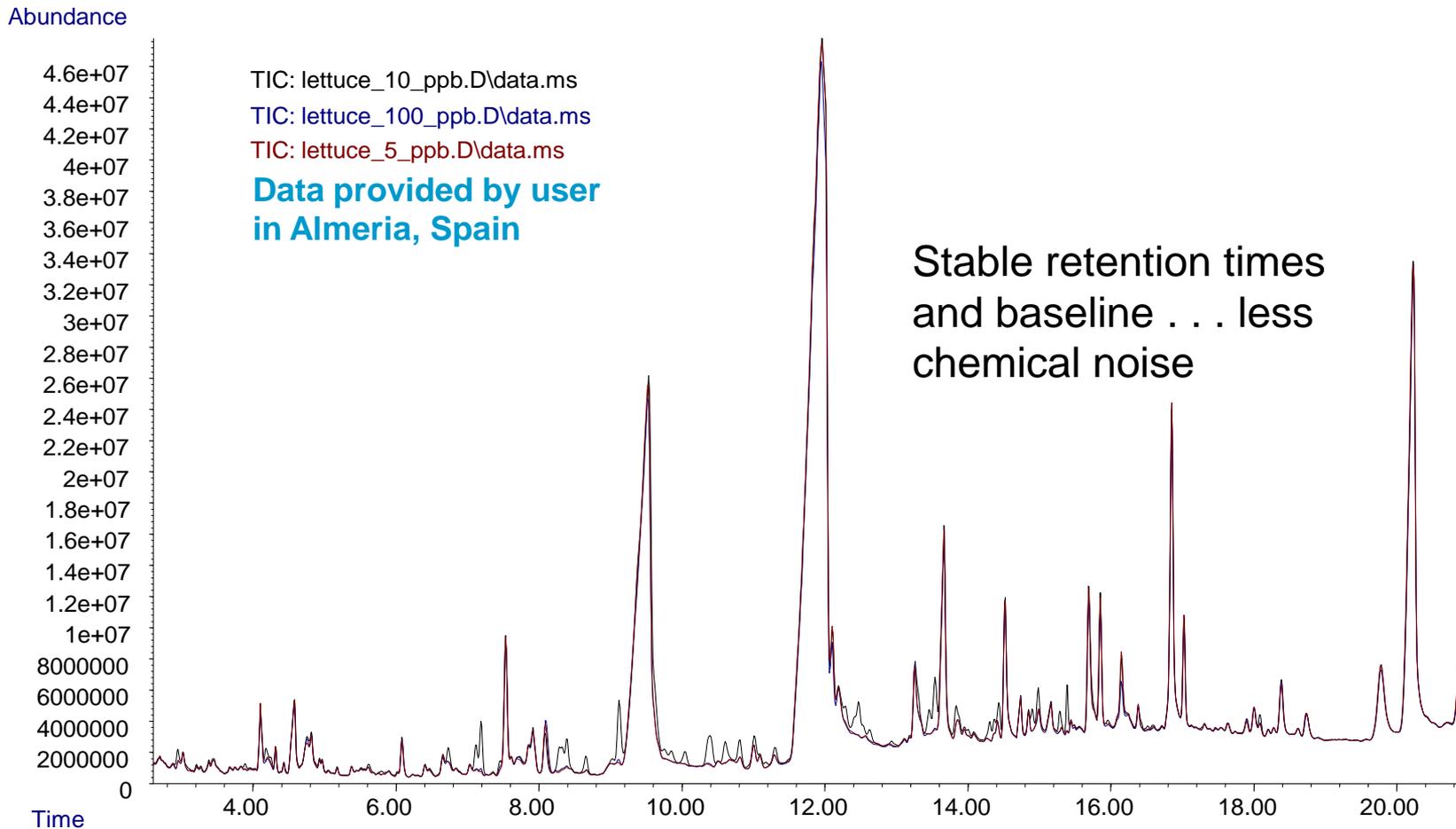
Time



After **only 3 10- μ L injections**, the background is significantly higher (increase chemical noise in every spectrum)

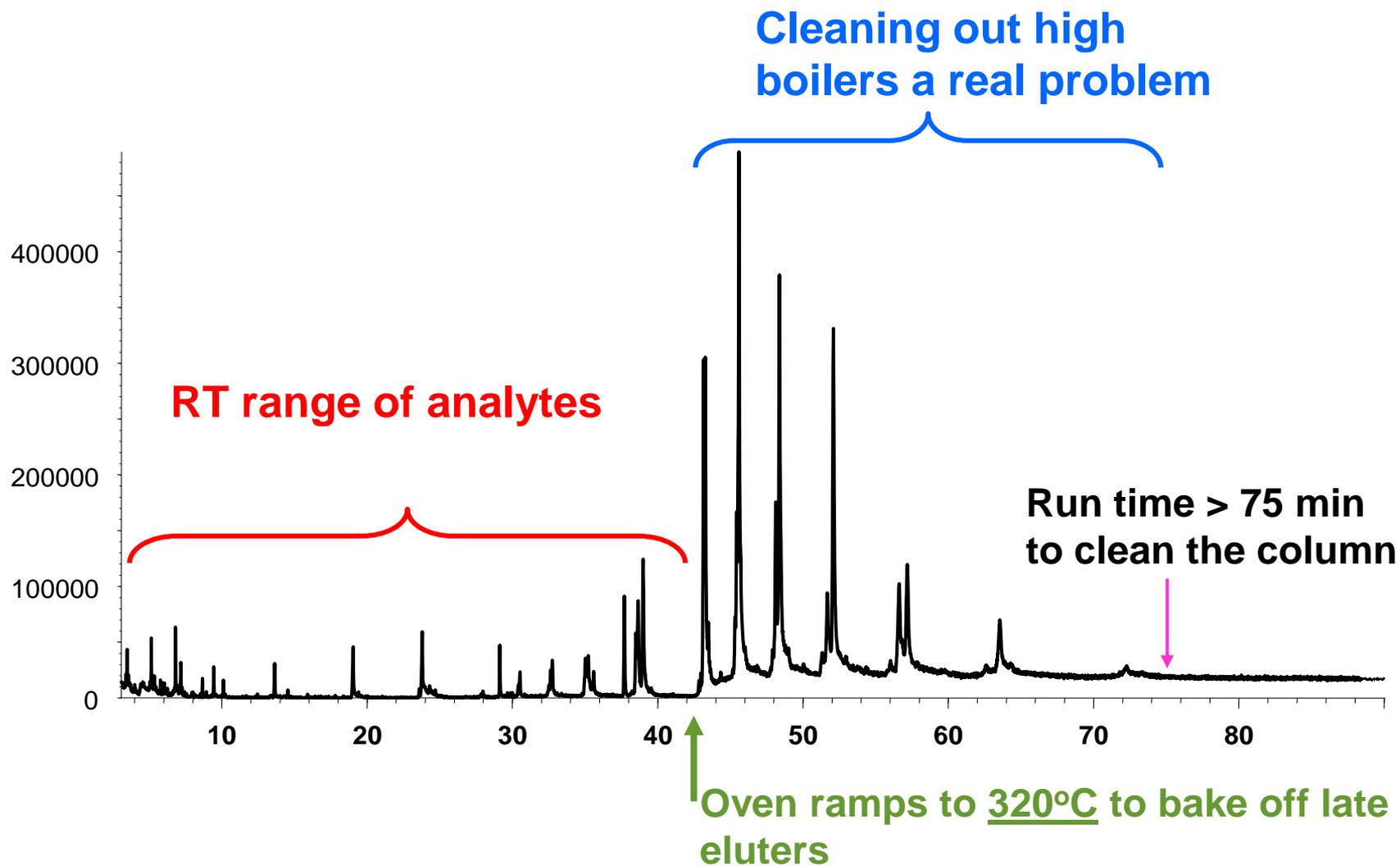
Overlay of two chromatograms of a blank extract injected BEFORE (A) and AFTER (B) three injections without backflush

With Backflush: Clean Background (Less Spectral Noise) and Consistent Retention Times



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

Backflush Reduces Maintenance Need



Improving Detection Limits & Confidence

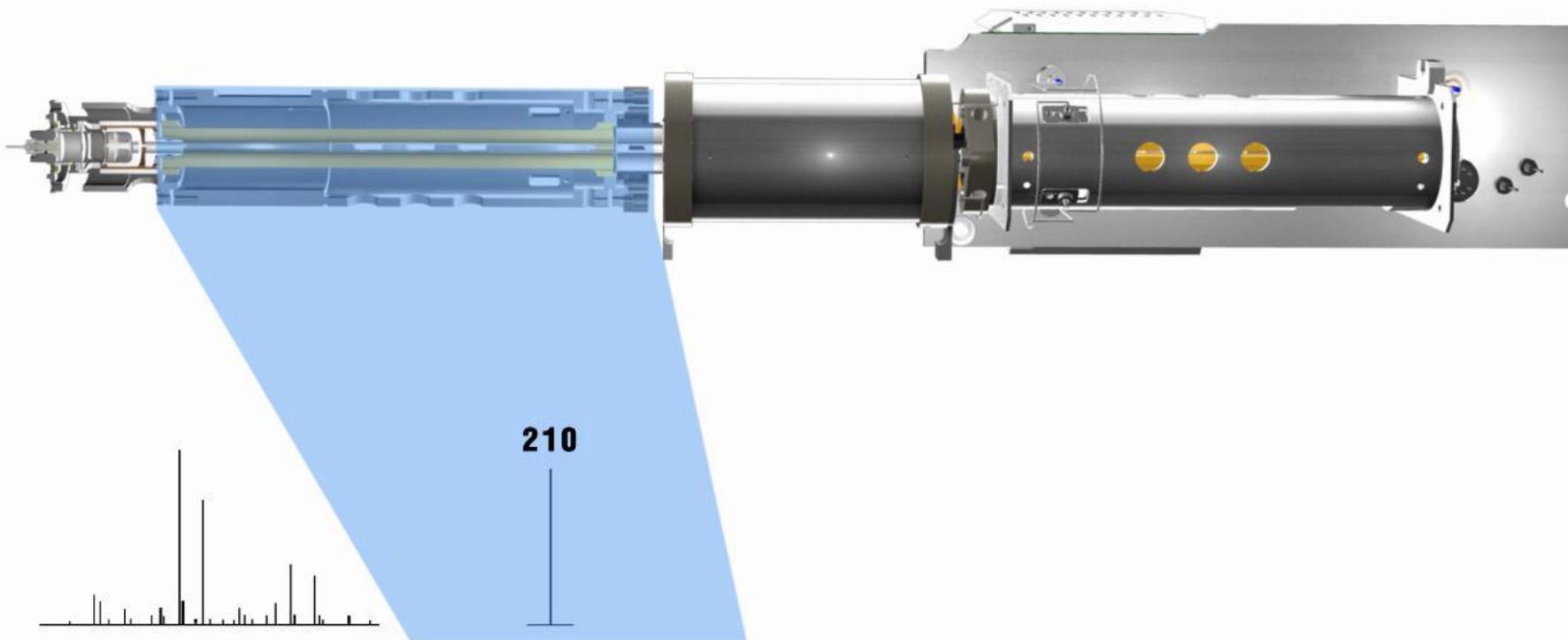
Solvent Venting to increase Injection Volume

Do you want to load more of this?
What about the Chemical Noise?

Now we have a new problem to deal with...



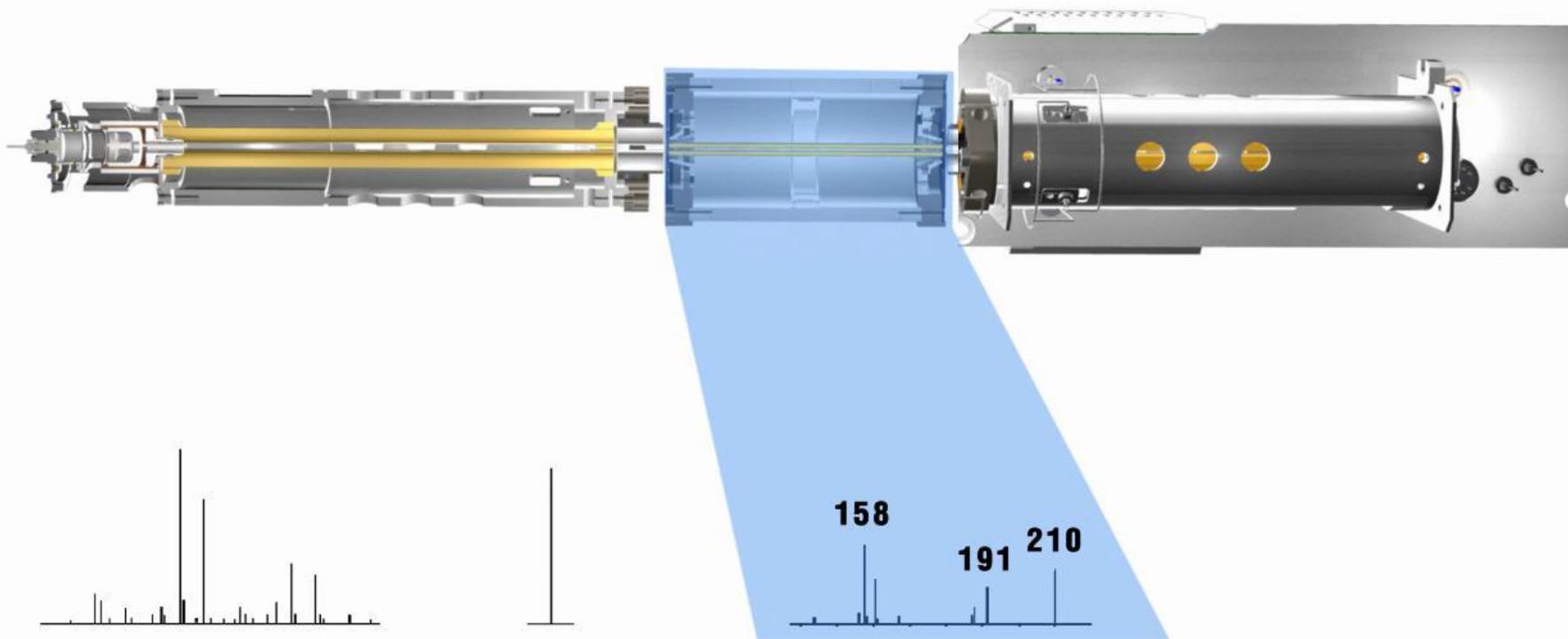
7000 Series Quadrupole MS/MS *Optimized for Gas Chromatography*



Q1 mass filters all ions other than the precursor; **only** target ion 210 pass through

7000 Series Quadrupole MS/MS

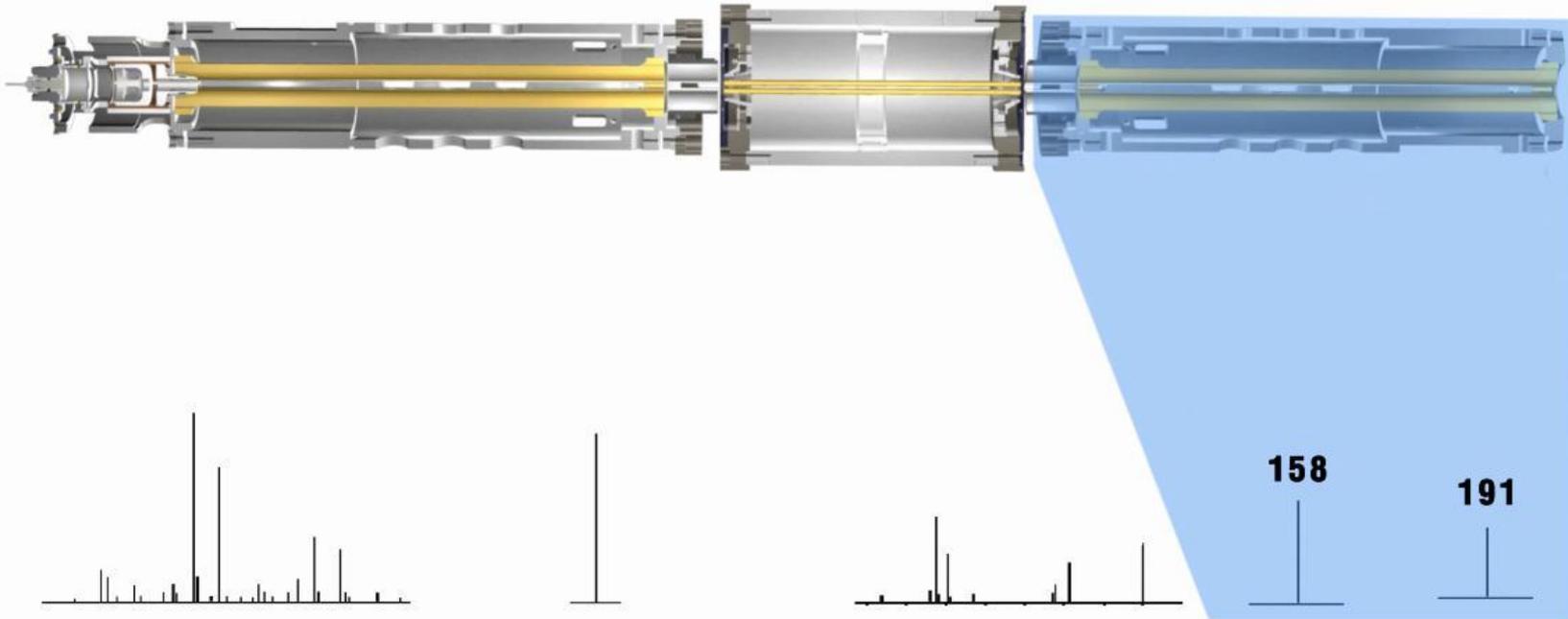
Optimized for Gas Chromatography



Collision cell
dissociates m/z 210
into product ions

7000 Series Quadrupole MS/MS

Optimized for Gas Chromatography



Q2 monitors **only**
characteristic fragments
158 and 191 from m/z
210 for quant and qual

New THC Analyzer.....

- Based on Existing Dean Switched Analyzer
- 2nd Column uses LTM Technology for Accurate & Isolated Temperature Control
- Ammonia NCI
- 7000B GCQQQ Detection
- Large Volume Injection Using MMI
- Target LoD 0.002pg/mg hair



5975T

- Transportable
- LTM Column Technology
 - Fast Analysis
 - Low Power Consumption
- Inert Source
- Anti Vibration Base
- 60% Bench size of 5975



Take high-performance into the field with the most full-featured transportable GC/MS system available:

- Designed for quick response in the field
- 1.8 to 1050u mass range
- Split/splitless inlet with full Electronic Pneumatics Control (EPC)
- Liquid auto injector option
- Vibration-dampening base
- Oil-free mechanical pump
- 2 strong, field-ready cases – one for the 5975T and one to hold consumables and accessories kits

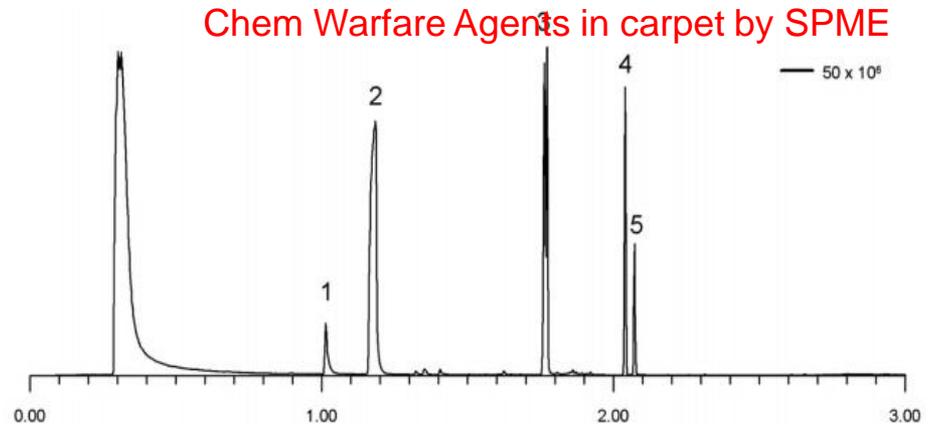
Enviro Forensics

- PAH & Pesticide Fast Track Analyzers
 - Mexico Gulf 2010
- Fast Mobile Response Using 5975T



Detection of Chemical Warfare Agents by Transportable GC/MS

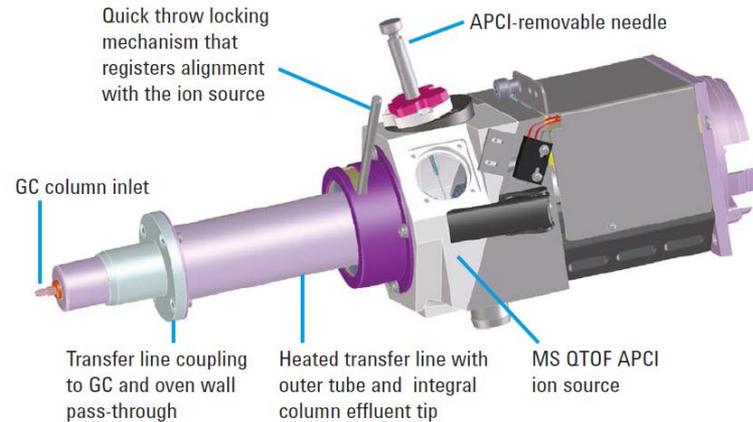
Application Note



Improve Confidence

For confidence in your results, Would you like....

- MS/MS Confirmation?
- Accurate Mass, High Resolution Confirmation?
- The New 7890 to 6540 QToF GC/APCI Interface



GC-APCI interface for the Agilent 6500 Series QTOF and 6200 Series TOF LC/MS systems

Coming Soon....

Would you also like EI data to compare to existing Libraries?
A True High resolution TOF with MS/MS capabilities

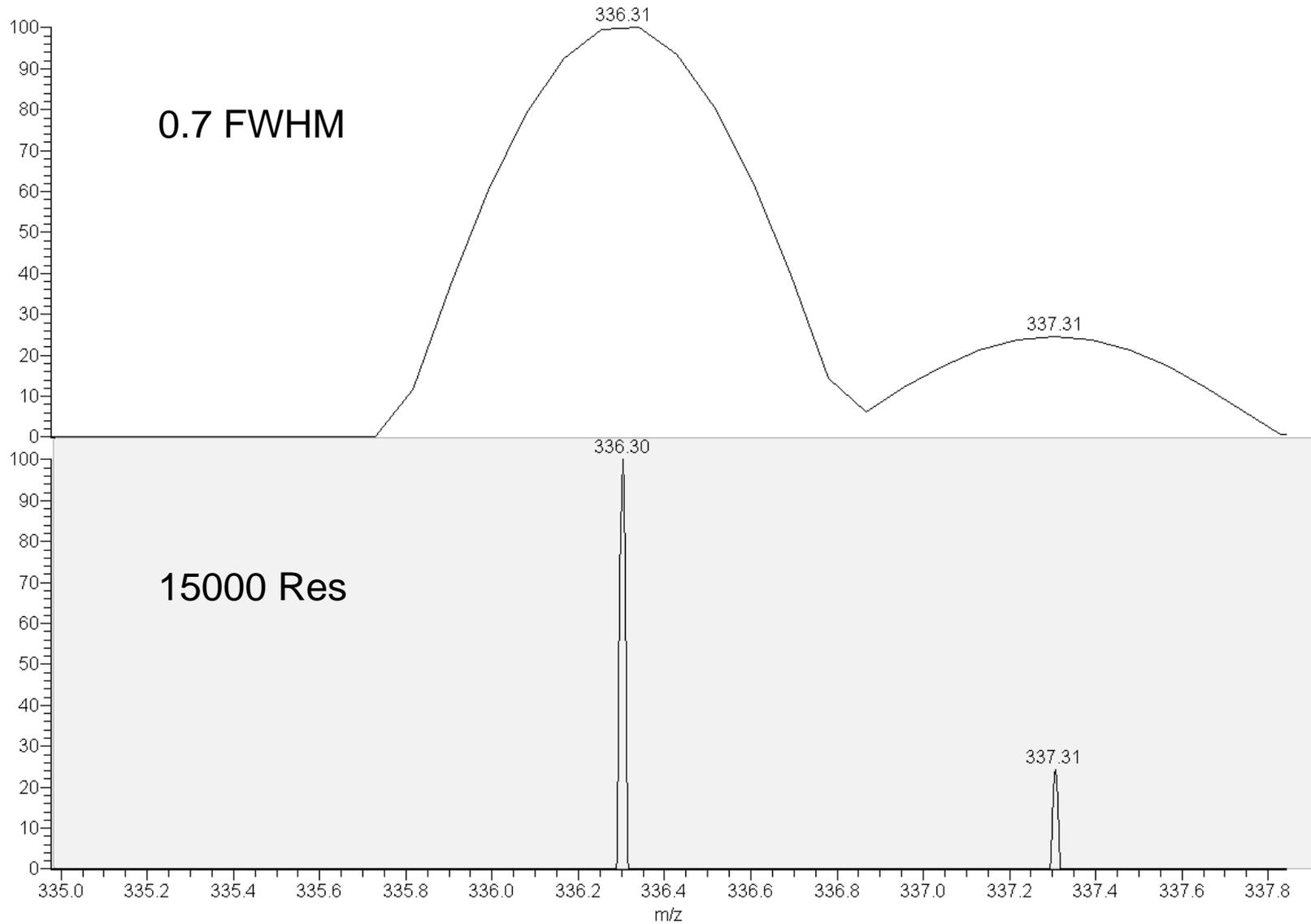
EI/CI GC/QToF MS/MS

Switch from EI to CI without Venting
Solids probe for powders

Full 7890 GC capability with automated
Sample Prep on the 7693 Sampler



So Far...



Summary

Agilent have a myriad of solutions to answer your Forensic Challenges including performance and data confidence:

- Factory Tested GC/MS and GCQQQ Fast Track Analyzers
- Single Quad GC/MS
- Ion Trap GC/MSⁿ
- GCQQQ for ultimate quantitative work
- Soon a QToF for specialized screening applications