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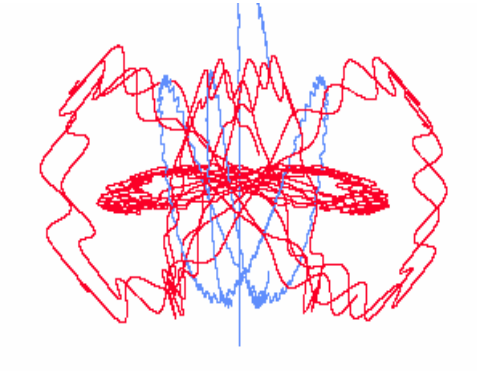
Characterization of a Multi-Port Inlet on a Rugged Mass Spectrometer

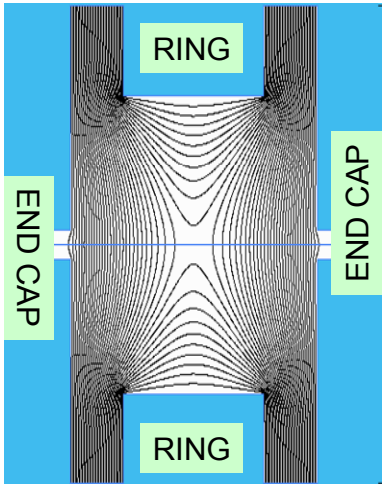
Garth Patterson – Chief Technology Officer

September, 2007

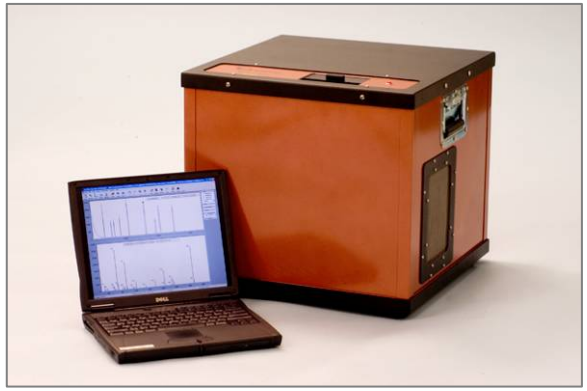
NEW THREATS.
NEW THINKING.

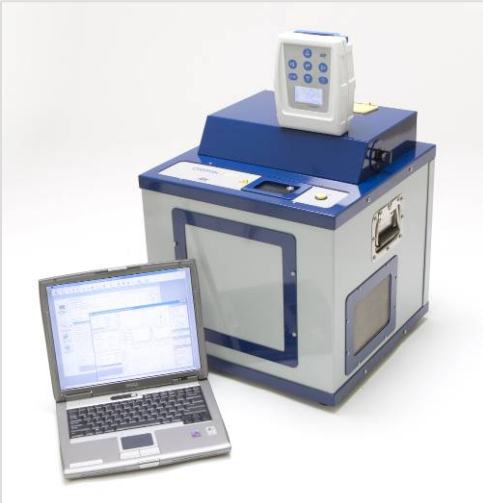
My HEMS history



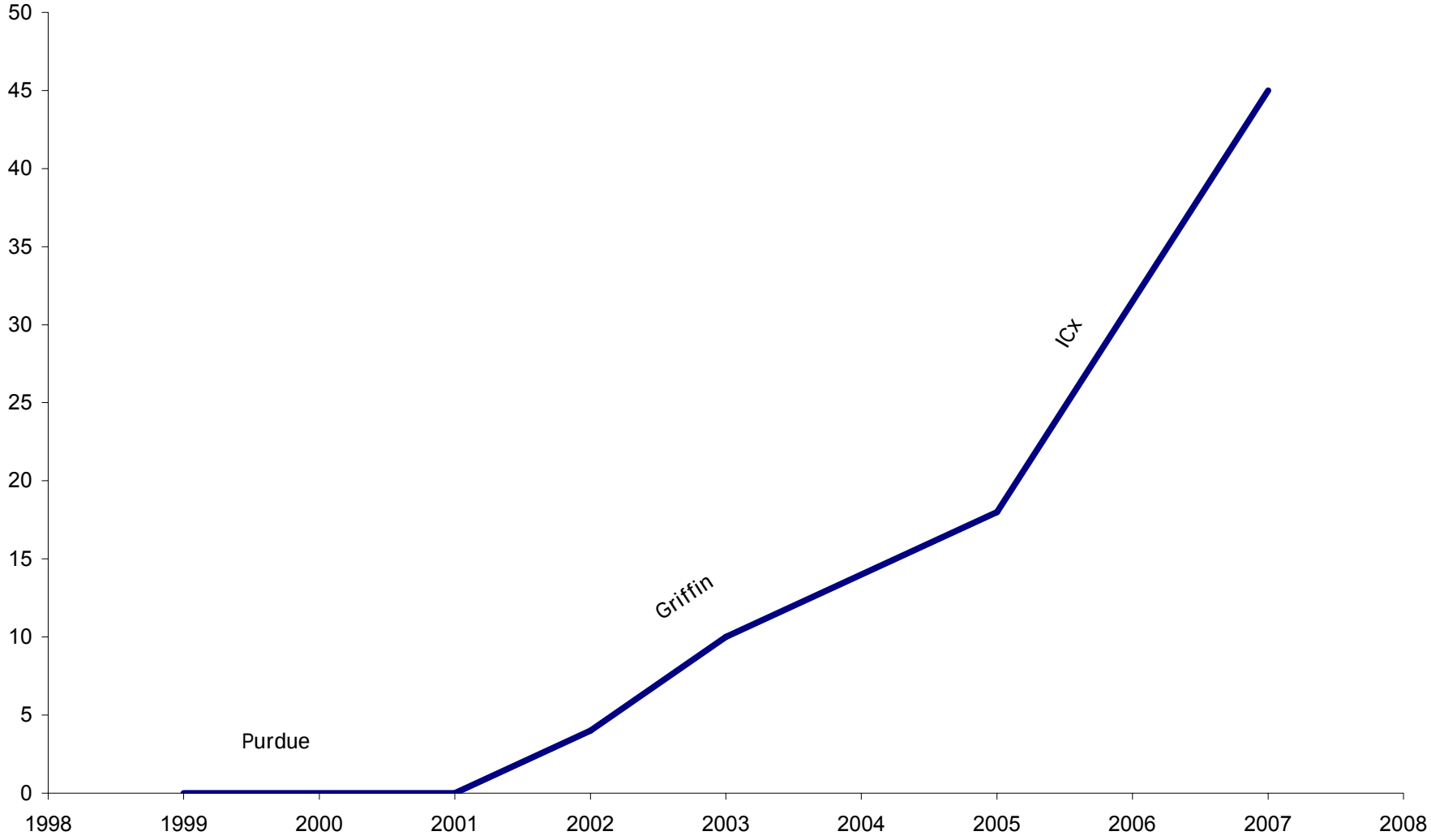


My HEMS history





Griffin Employees



Where is ICx? A company with global impact.

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Griffin Analytical is located in the Purdue Research Park in West Lafayette, IN

ICx Corporate HQ

1 1350 I Street, Washington, D.C.
2 411 West Putnam Avenue, Greenwich CT

Subsidiary	Location
1 360 Surveillance	Victoria, British Columbia, Canada
2 Agentase	2240 William Pitt Way, Pittsburgh, PA
3 Amphitech	3440 Francis-Hughes, #120, 130, Laval (Québec)
4 DAQ	262B Old New Brunswick Rd., Piscataway, NJ
5 Digital Infrared Imaging	Cooper Commerce Center One, 515 Cooper Commerce Dr., Apopka, FL
6 Griffin Analytical	3000 Kent Avenue West Lafayette, IN
7 Harbinger	611 Pennsylvania Ave. SE, #301, Washington, DC 20003
8 Ion Optics	411 Waverley Oaks Road, Suite 144 Waltham, MA
9 MesoSystems	1001 Menaul Blvd. NE, #A, Albuquerque, NM
10 NHM	1640 Powers Ferry Rd, Bldg. 16, Suite 350, Marietta, GA
11 NHM	4624 US 19 S., Ellaville, GA

Subsidiary	Location
12 Nomadics	800 Research Pkwy, #100, Oklahoma City, OK
13 Nomadics	9020 Junction Dr., Annapolis Junction, MD
14 Nomadics	Cambridge, MA
15 Nomadics	Stillwater, OK
16 Nuvonyx	3753 Pennridge Dr., Bridgeton MO
17 Nuvonyx Europe SA	Route départementale 128, BP 46 - 91401 Orsay Cedex - France
18 PBA Engineering	1100-200 Granville St., Vancouver, BC, V6C 2R3, Canada
19 STS	8900E. Chaparral Rd., Scottsdale, AZ
20 Target Instruments	100 Midland Road, Oak Ridge, TN
21 Target Instruments	Kölner straße 99 • 42651 Solingen Germany

Advantages of CIT

Cylindrical Ion Trap Mass Analyzer

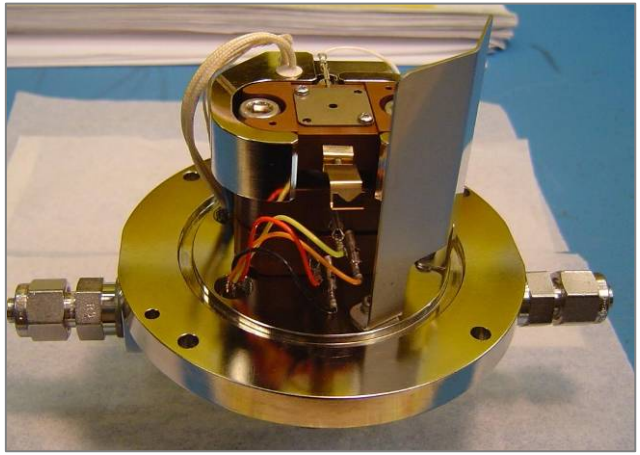
- Simplified geometry
- Ease of fabrication
- Reduced voltage requirements

~1 cm^3

CIT

$$(m/z)_{max} = \frac{8V_{max}}{q_{eject}\Omega^2(r_0^2 + 2z_0^2)}$$

Size (r_0 and z_0)	Voltage (V_{max})	Power
$\frac{1}{2}$	$\left(\frac{1}{2}\right)^2$	$\left(\frac{1}{2}\right)^4$



GRIFFIN | 400 – Mobile GC/MS/MS

griffin analytical

Overview and Specifications

- Gas Chromatograph/Mass Spectrometer
- Detects, Identifies, and Confirms ppt concentrations of CWA's, TICS/TIMS, explosives, and pesticides
- Ruggedized and shock mounted for mobile platform use
- Flexible sample inlets for varying end-user applications
- MS/MS capability

- Size ……..…….. 19.2" x 19.2" x 18.0"
- Weight ……....75 lbs
- Mass Range……425 amu / Unit Mass Resolution
- Power Requirement……115-220 VAC, 50/60 Hz

Griffin 400

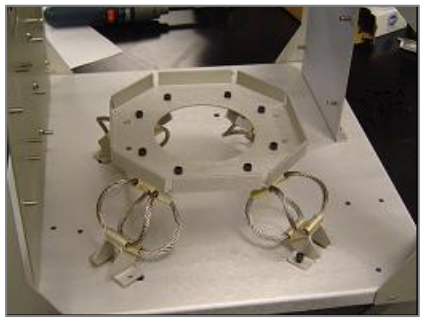
Benefits

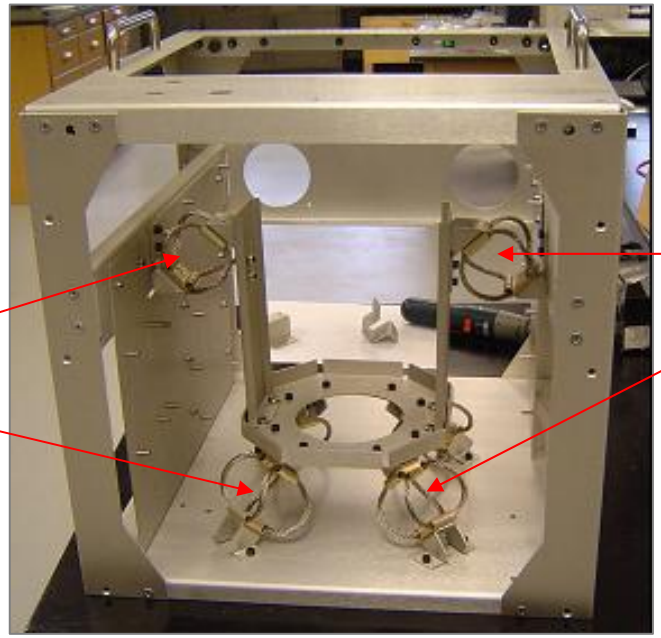
- Ease of Use
- Extended Analytical Flexibility
- Rapid Response Time
- Positive Identification of Known and Unknown Chemical Threats
- Low Operational/Sustainment Costs
- Minimal Training Required

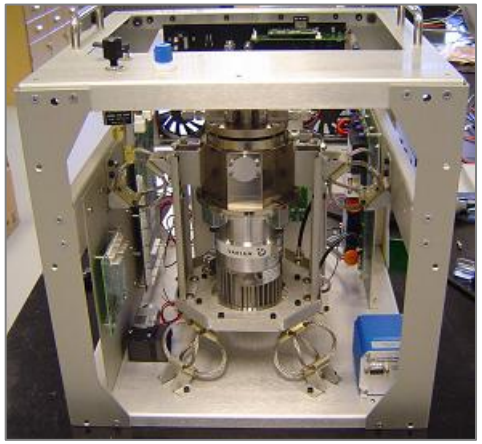
Key Customers

- DoD Operations
- Public Transportation Facilities
- International Governments Labs
- Mobile Laboratory Applications
- Demil Facilities

Rugged for Field Use – Wire rope Isolators







GRIFFIN | 450 – Mobile/Field-Ready GC/MS/MS

griffin analytical

Overview and Specifications

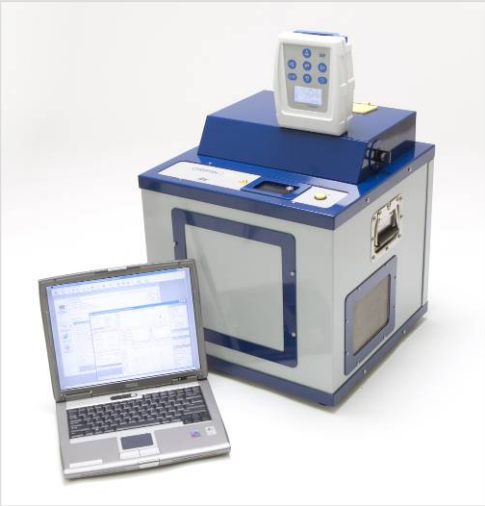
- Gas Chromatograph/Mass Spectrometer
- Detects, Identifies, and **Confirms** ppt concentrations of CWA's, TICS/TIMS, **explosives, and pesticides**
- Ruggedized and shock mounted for mobile platform use
- Flexible sample inlets for varying end-user applications
- MS/MS **capability**

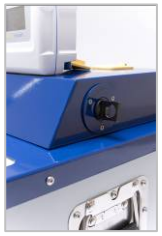
- Size ……..…….. 19.2" x 19.2" x 21.1"
- Weight ……....85 lbs
- Mass Range……425 amu / Unit Mass Resolution
- Power Requirement……115-220 VAC, 50/60 Hz

Benefits

- DIRECT AIR ANALYSIS
  - Sample Loop and Pre-concentration
  - Compatible with Griffin X-Sorber
- Ease of Use
- **Extended Analytical Flexibility**
- Rapid Response Time
- Positive Identification of Known and Unknown Chemical Threats
- Low Operational/Sustainment Costs
- Minimal Training Required

Griffin 450





Key Customers

- DoD Operations
- Public Transportation Facilities
- International Governments Labs
- Mobile Laboratory Applications
- Demil Facilities

GRIFFIN | X-Sorber – Handheld Sampler & Desorber

griffin analytical

Overview and Specifications

- **Battery-operated** single-person portable air sampling system – **rechargeable** at host instrument
- Ideal for safer and efficient downrange sampling– **programmable sample collection methods**
- **Integrated GPS** sample tagging
- On-board control and data management
- Unattended, autonomous operation for long-term (hours) sampling in specific locations
- Ability to archive samples for subsequent analysis and further confirmation (**dual tube sampling**)

- Size* …….…….. Est. 9” x 7” x 2.65”
- Weight* ……..Est. 3 lbs

Griffin Handheld Sampler

Benefits

- Trusted sample integrity
- Simplified automation
- Integrated GPS capability
- Confirmatory results
- **De-contaminable**
- Pre-concentration tubes are compatible with other commercially available thermal desorption systems
- **Easy to use**, requiring minimal training

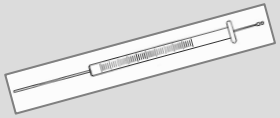
Key Customers

- Force protection
- Security personnel
- International security
- Intelligence community
- Container & Cargo Screening
- Venue protection

Sample Introduction (Inlets)

What is Mass Spectrometry?

Direct Liquid Injection



SPME

Autosampler

Direct Air

X-Sorber

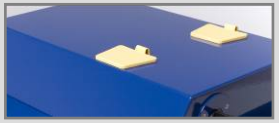
Transfer Line

Split/Splitless Liquid Injector

Griffin 300
Griffin 400
Griffin 450

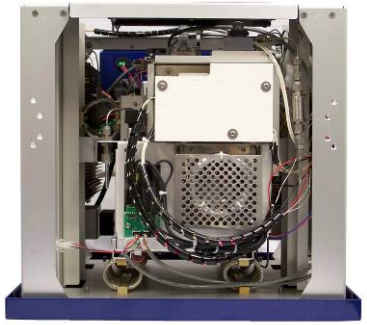
Universal Sampling Port

Griffin 450



Pre-Concentration or Sample Loop

LTM-GC



GSS 3.2 - Multi-Level User Software

ICx Griffin Product Families

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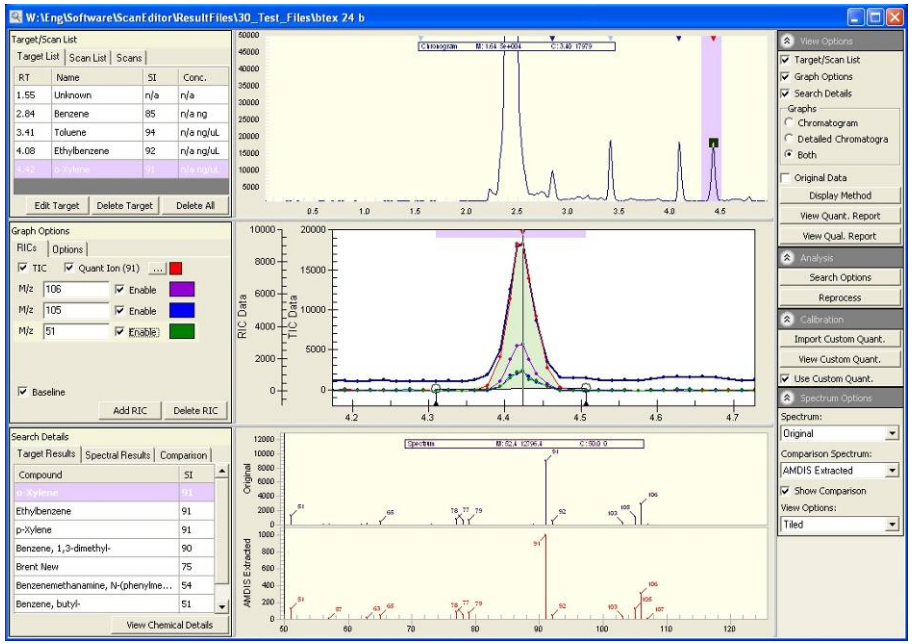
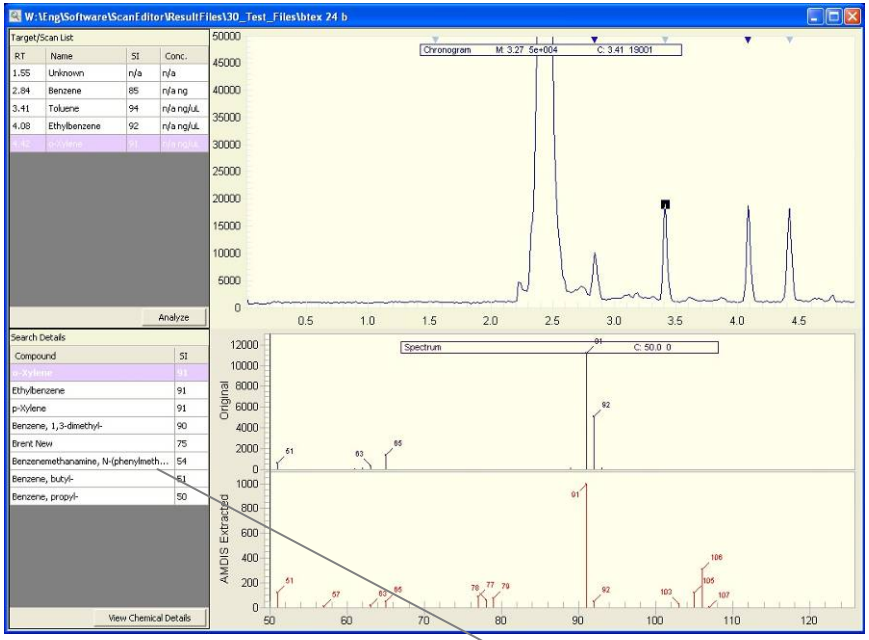
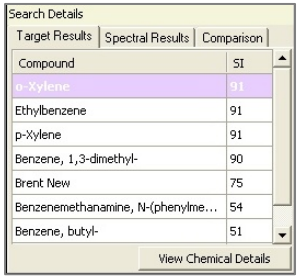
Developer View – *Data Review AND Analysis*

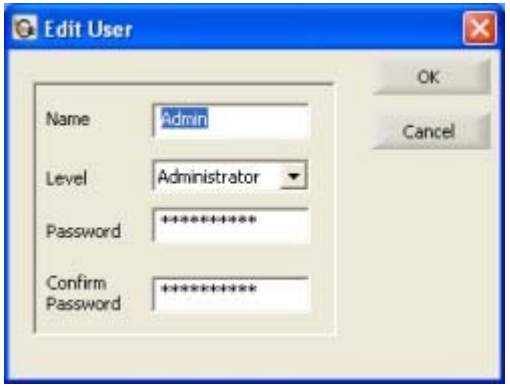


Operator View – *Data Review Only*





Developer View – *Set-up Users for Log-in*



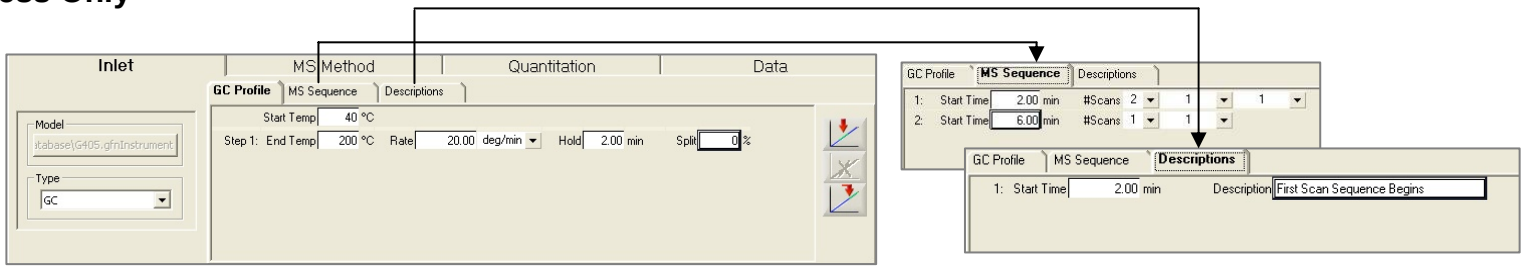
Operator View – *Log-in Only*

GSS 3.2 - Method Development – Griffin GC/MS

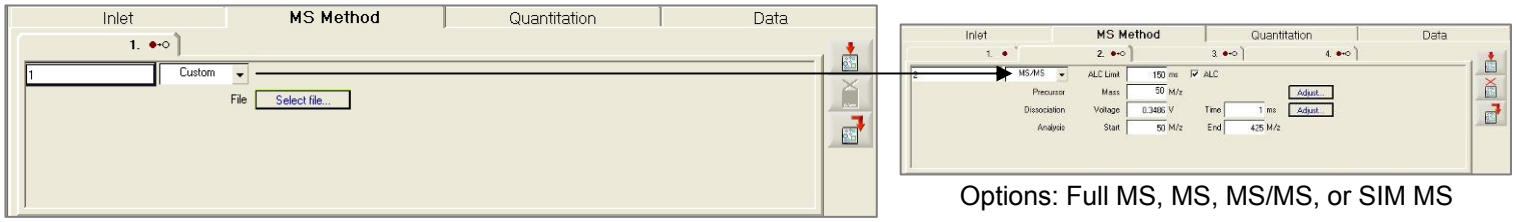
ICx Griffin Product Families

Developer Level Access Only

1. **Inlet Optimization**

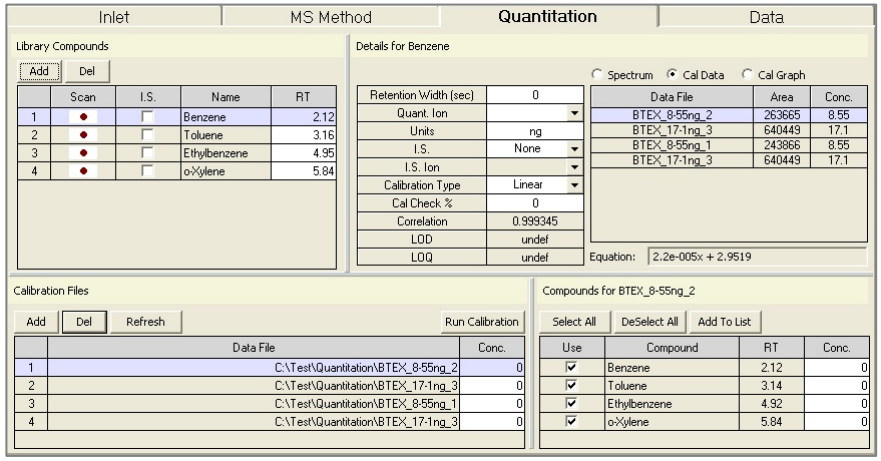


2. **MS Detail Optimization**

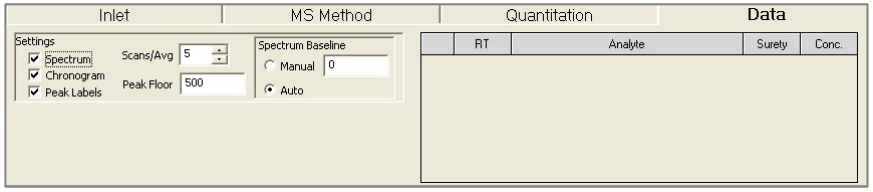


Options: Full MS, MS, MS/MS, or SIM MS

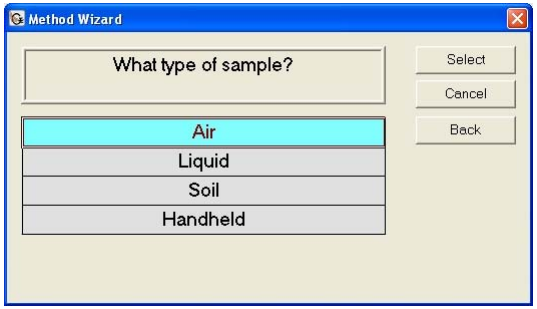
3. **Quantitation Optimization**



4. **Data Optimization**



Operator Level – Method Wizard

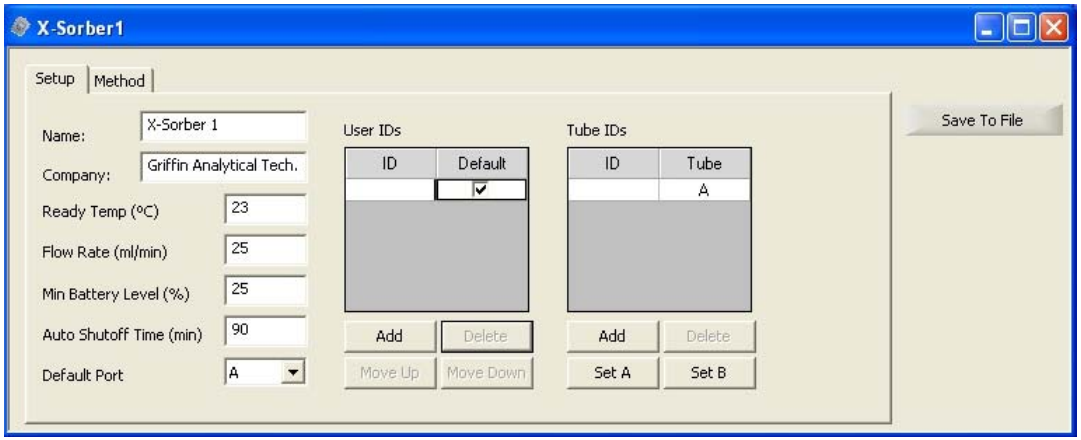


Method WIZARD!

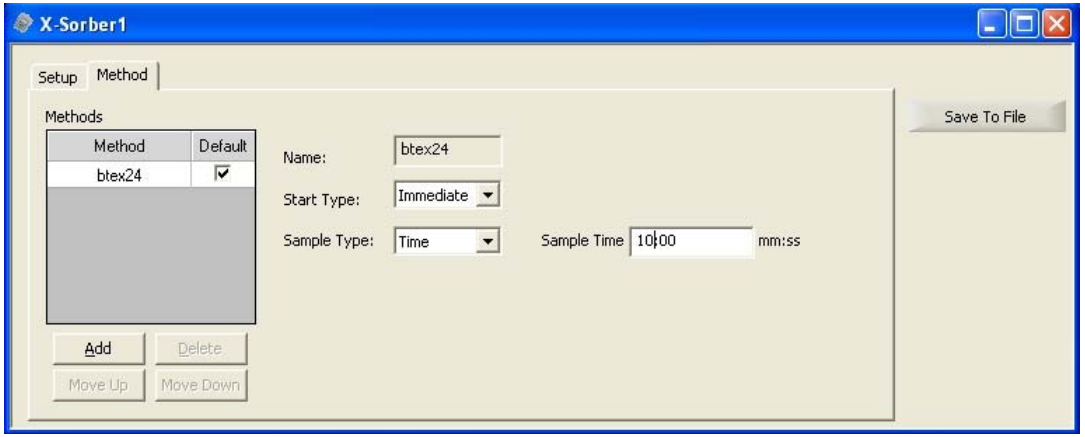
Intuitive step-by-step process.

GSS 3.2 - Method Development – Griffin X-Sorber

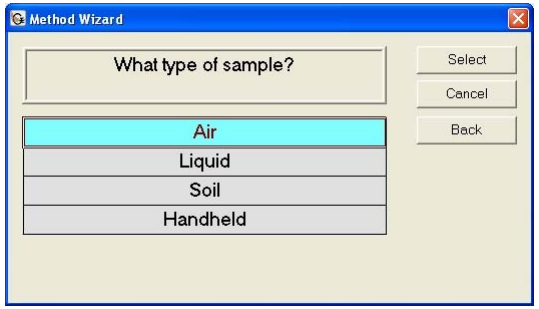
Developer Level Access Only



These methods can be added to the Operator Level user list and can be selected through the Method Wizard guide OR manually from a list.



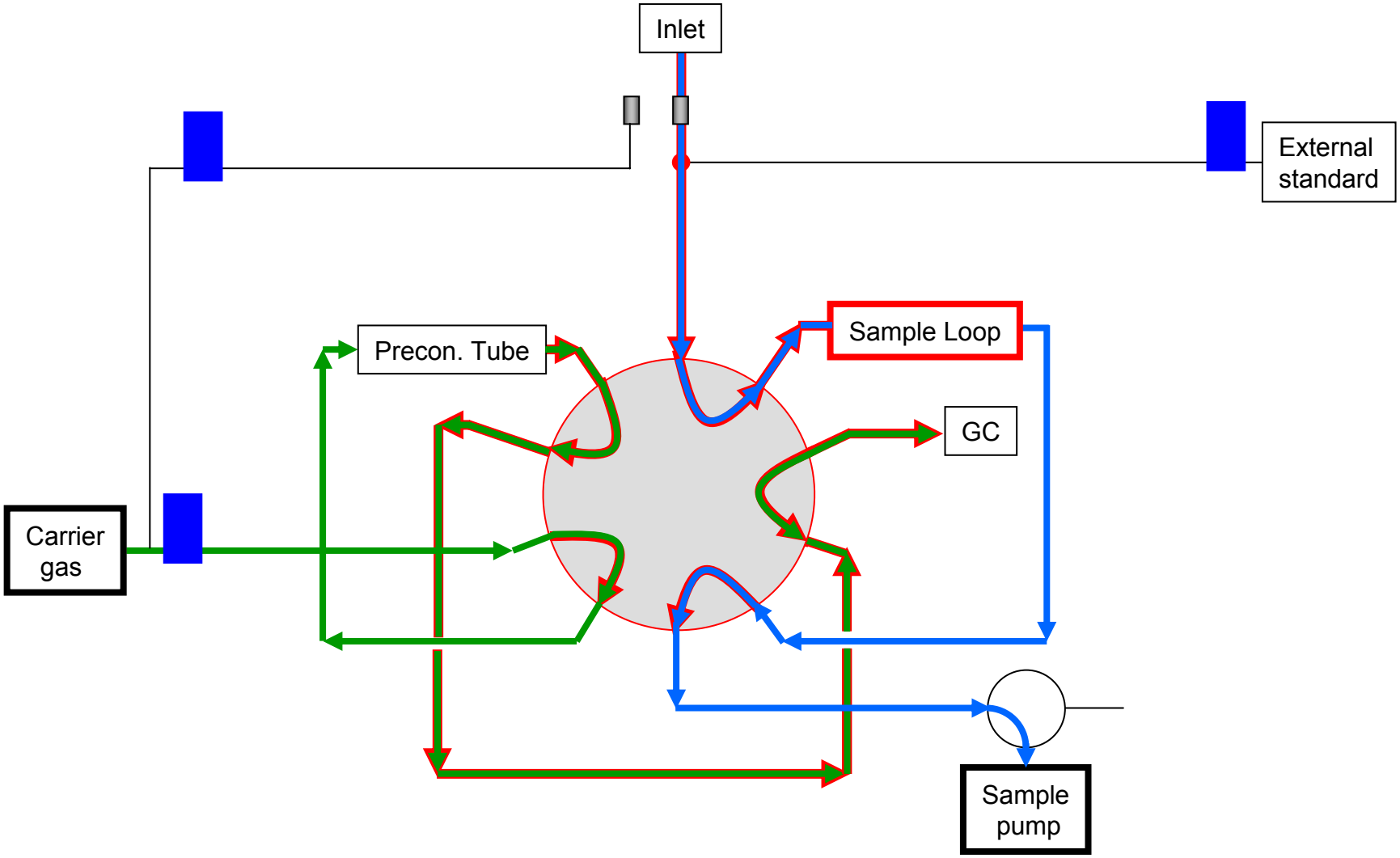
Operator Level – Method Wizard



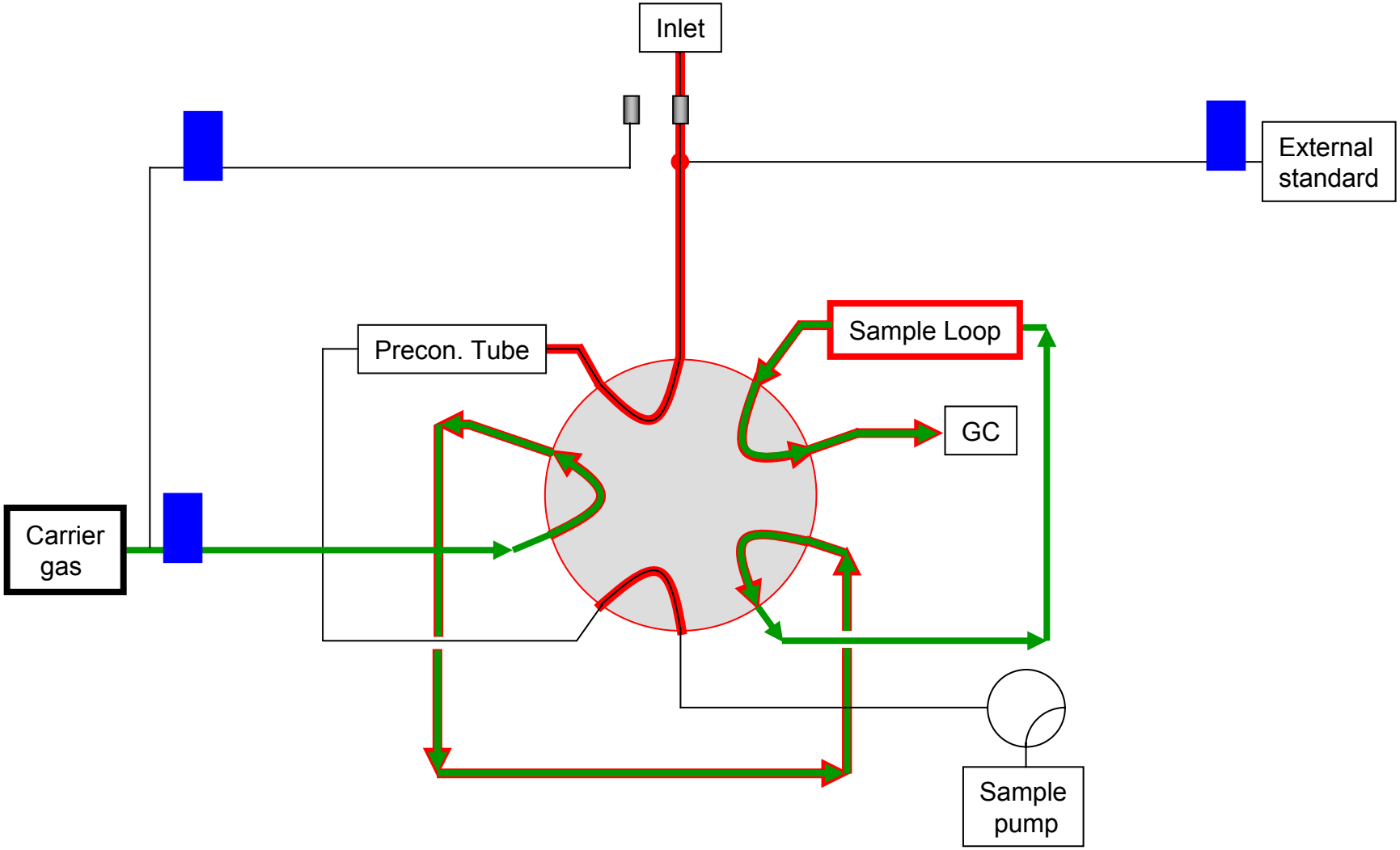
Method WIZARD!

Intuitive step-by-step process.

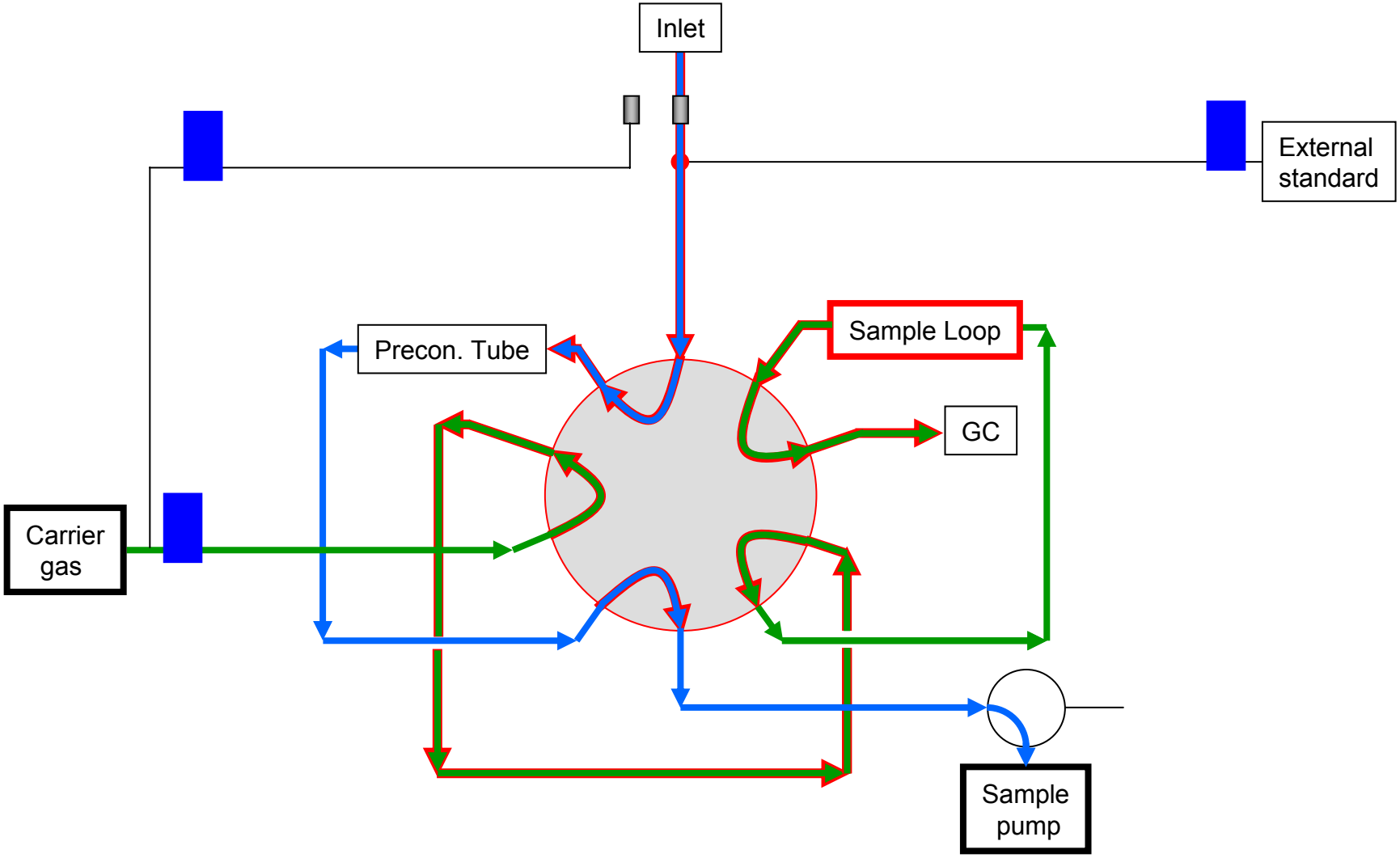
Flow schematic for loading the sample loop



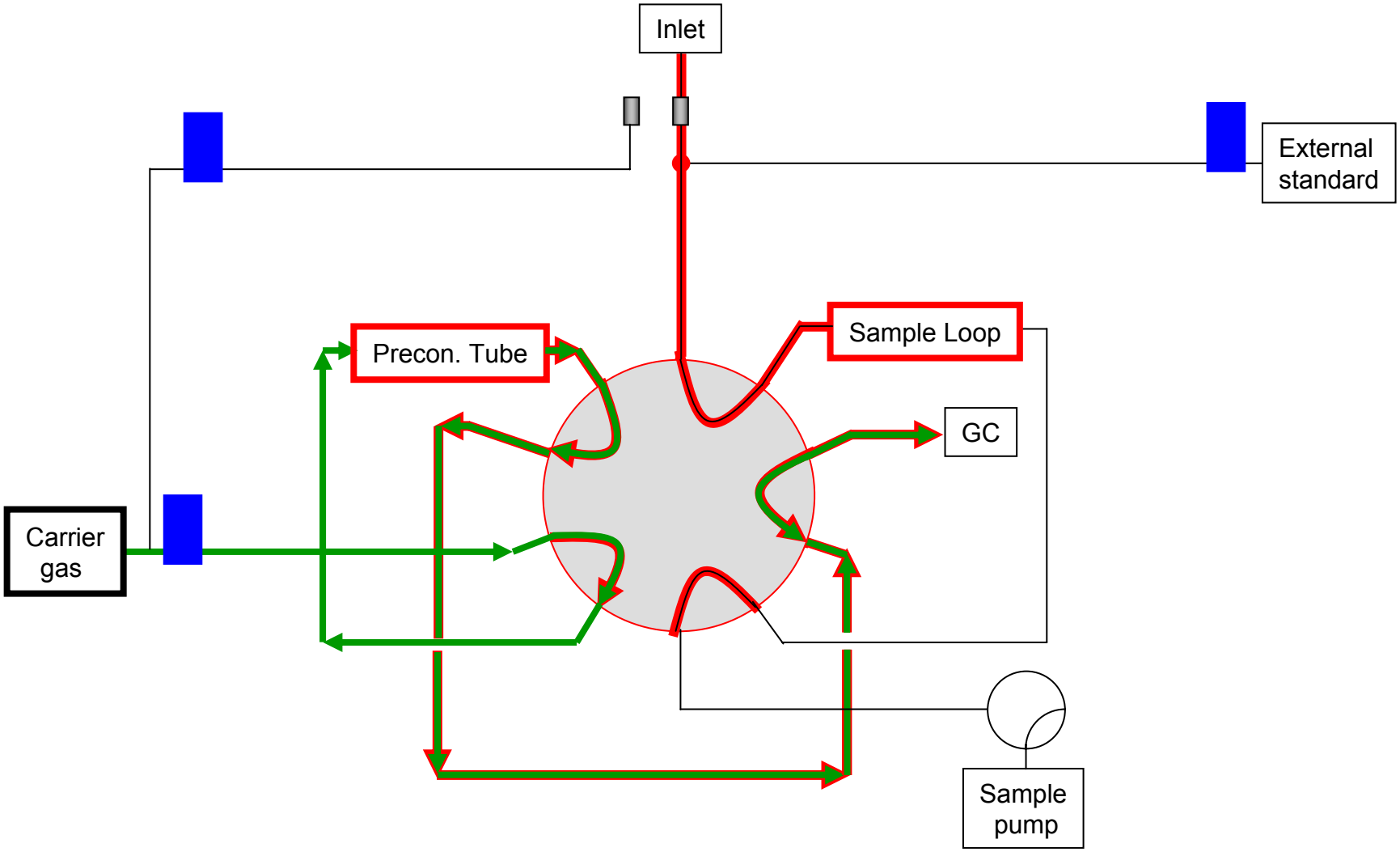
Flow schematic for flushing and analyzing the sample loop



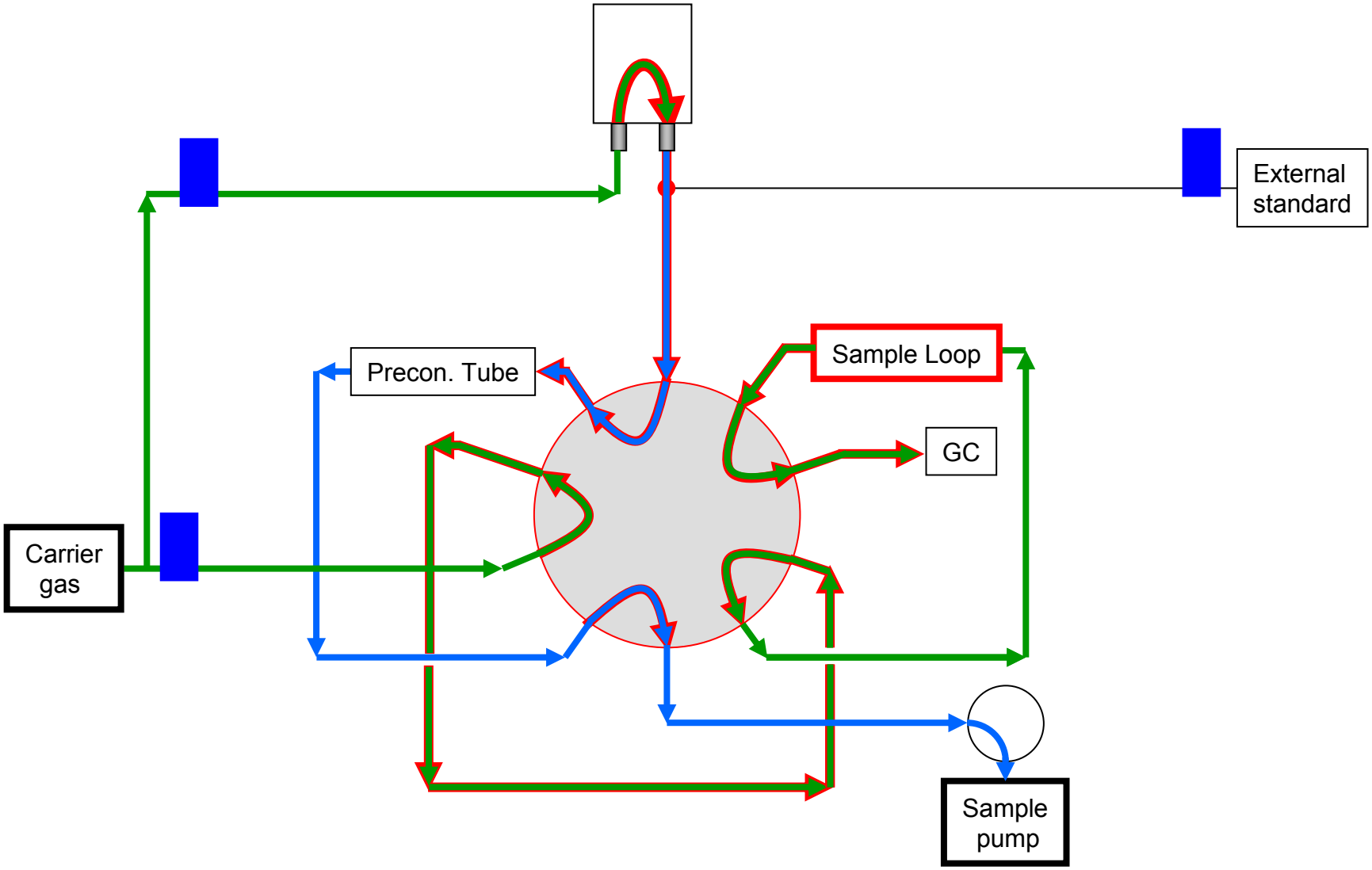
Flow schematic for sample preconcentration



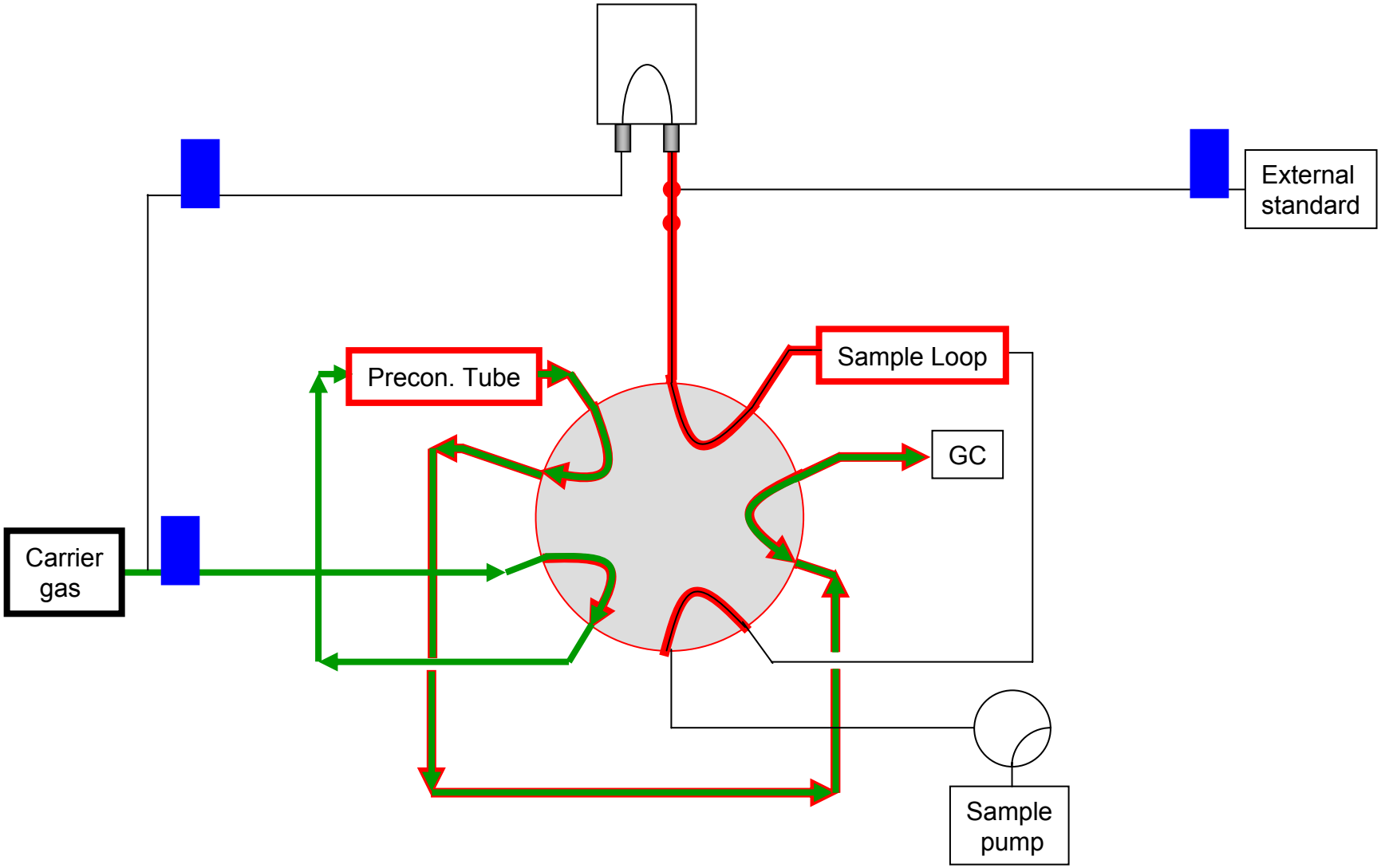
Flow schematic for sample desorption



Flow schematic for focusing of X-Sorber with Griffin 450



Flow schematic for injection after focusing from the X-Sorber with Griffin 450



GROB Mixture Analysis

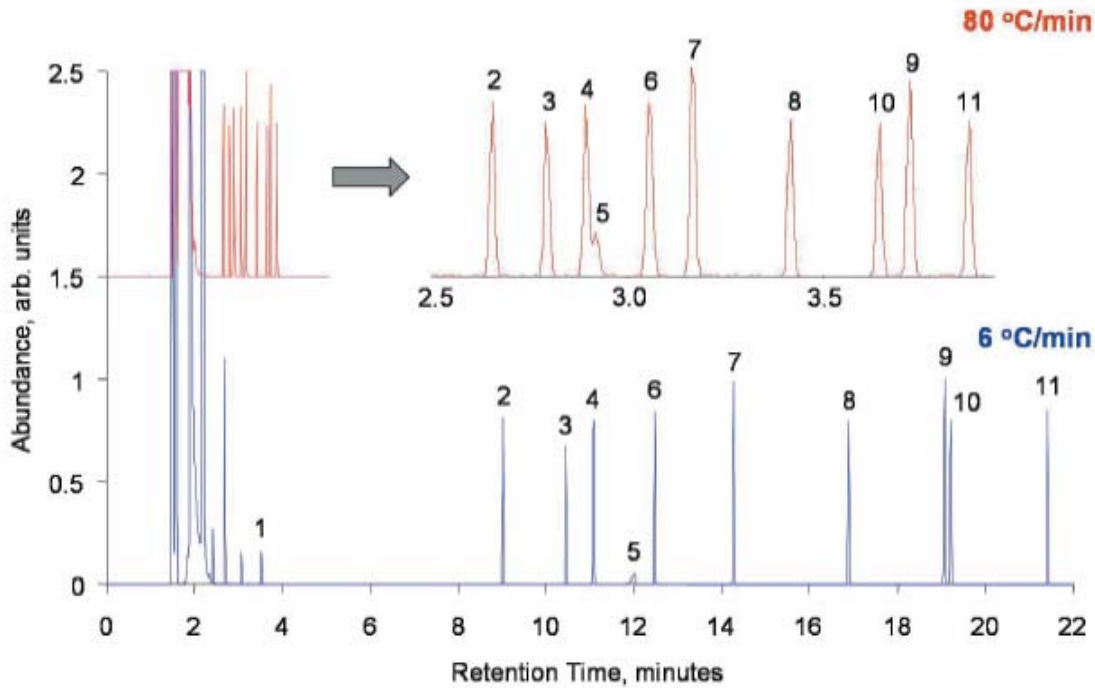


Figure 3. Total ion current traces for injections of Grob test mixture on the Griffin LTM-GC/MS with GC temperature ramps of 6° C/min (blue) and 80° C/min (red).

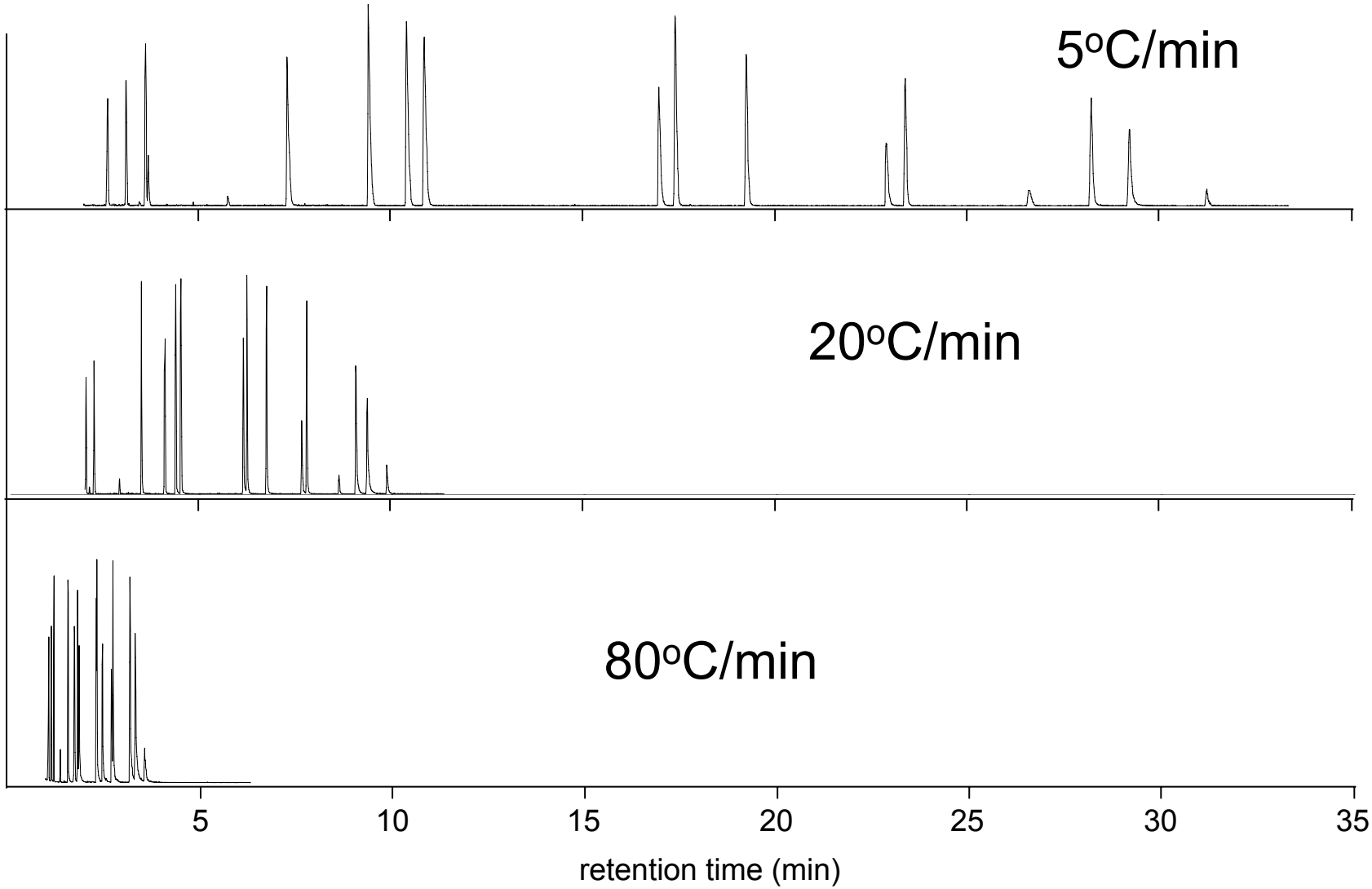
GC column: Rtx-1MS, 30 m
0.25 mm i.d.
0.25 µm df

Carrier Gas: He, 1 mL/min
15:1 split ratio

Grob Mixture Components:
1) 2,3-butanediol
2) n-decane
3) 1-octanol
4) 2,6-diphenylphenol
5) 2-ethylhexanoic acid
6) 2,6-dimethylbenzenamine
7) n-dodecane
8) methyl decanoate
9) N-cyclohexanamine
10) methyl undecanoate
11) methyl decanoate

Explosives Analysis

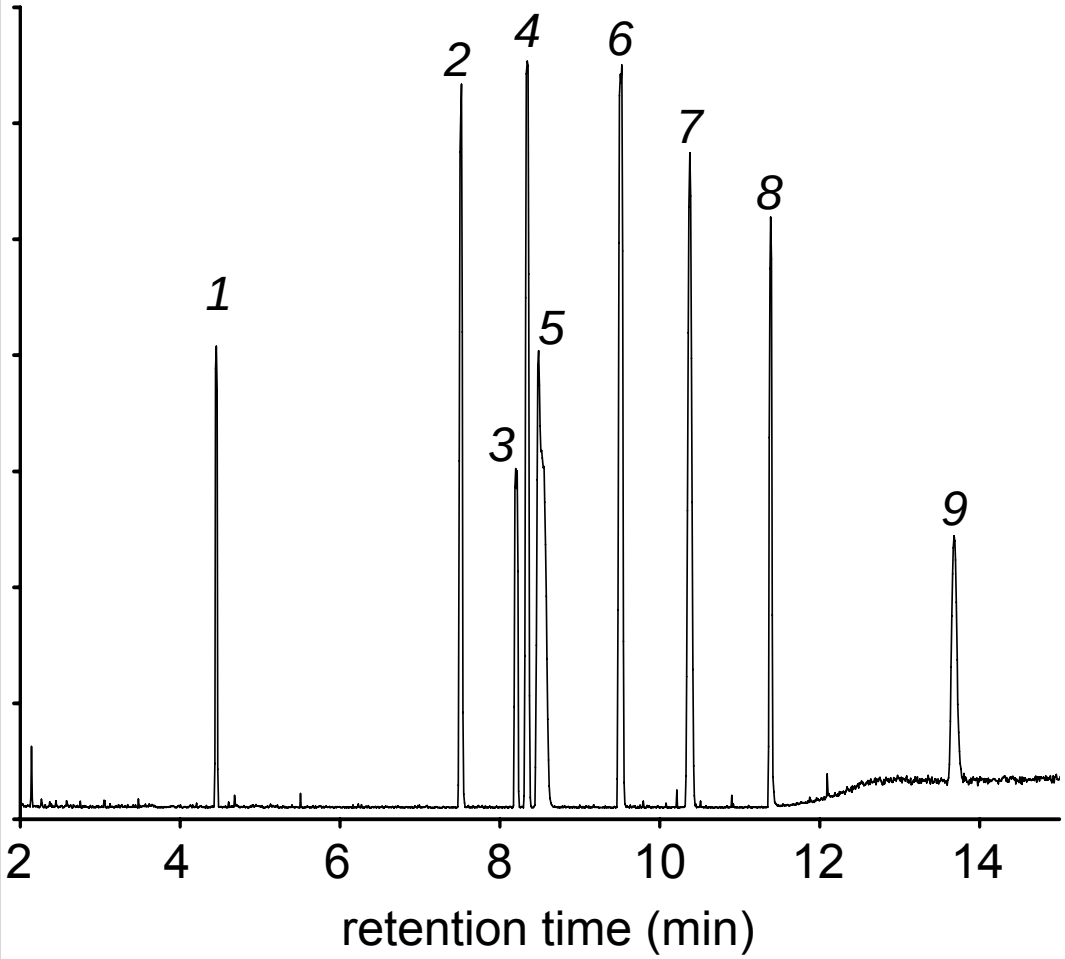
Explosives separation at faster ramp rates



Pesticides Analysis

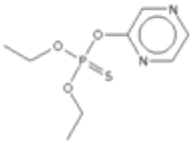
Separation of 9 organophosphorus pesticides

30 m x 0.25 mm Rtx-5MS columns

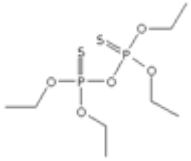


1) O,O,O-triethyl thiophosphate

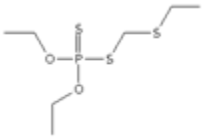
2) Thionazin



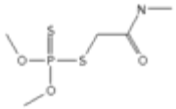
3) Sulfotep



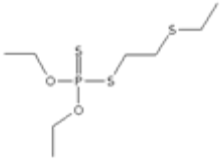
4) Phorate



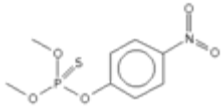
5) Dimethoate



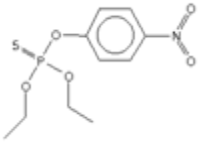
6) Disulfoton



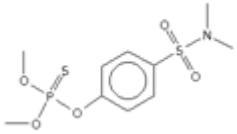
7) Methyl Parathion



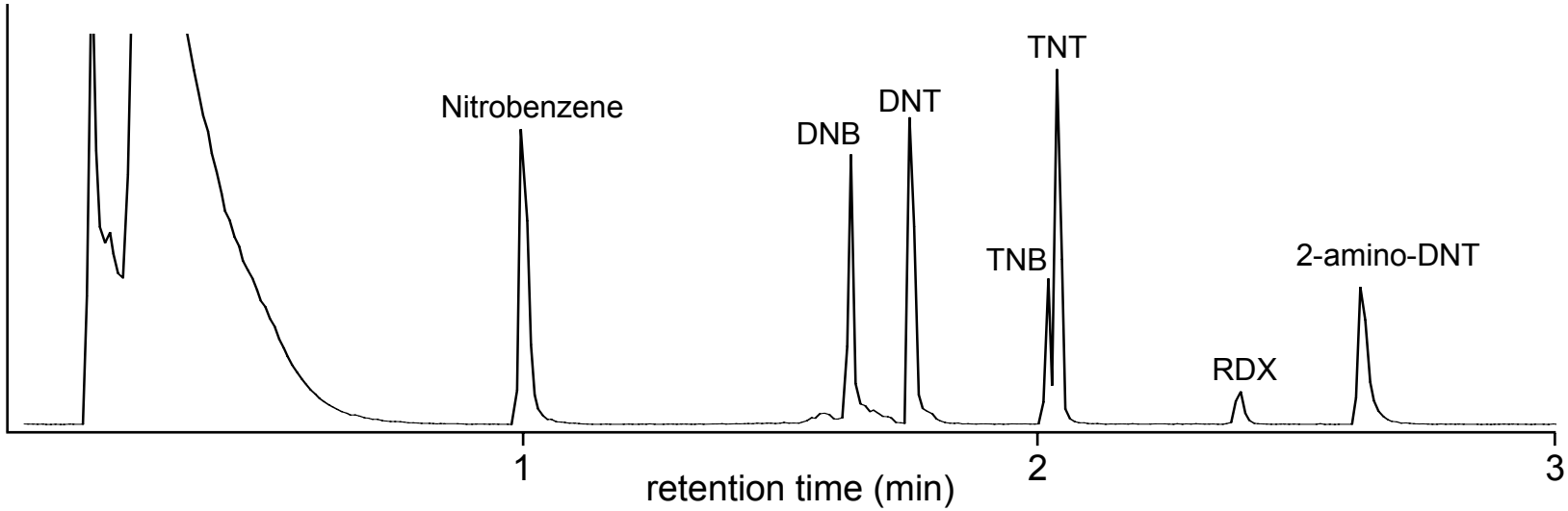
8) Parathion

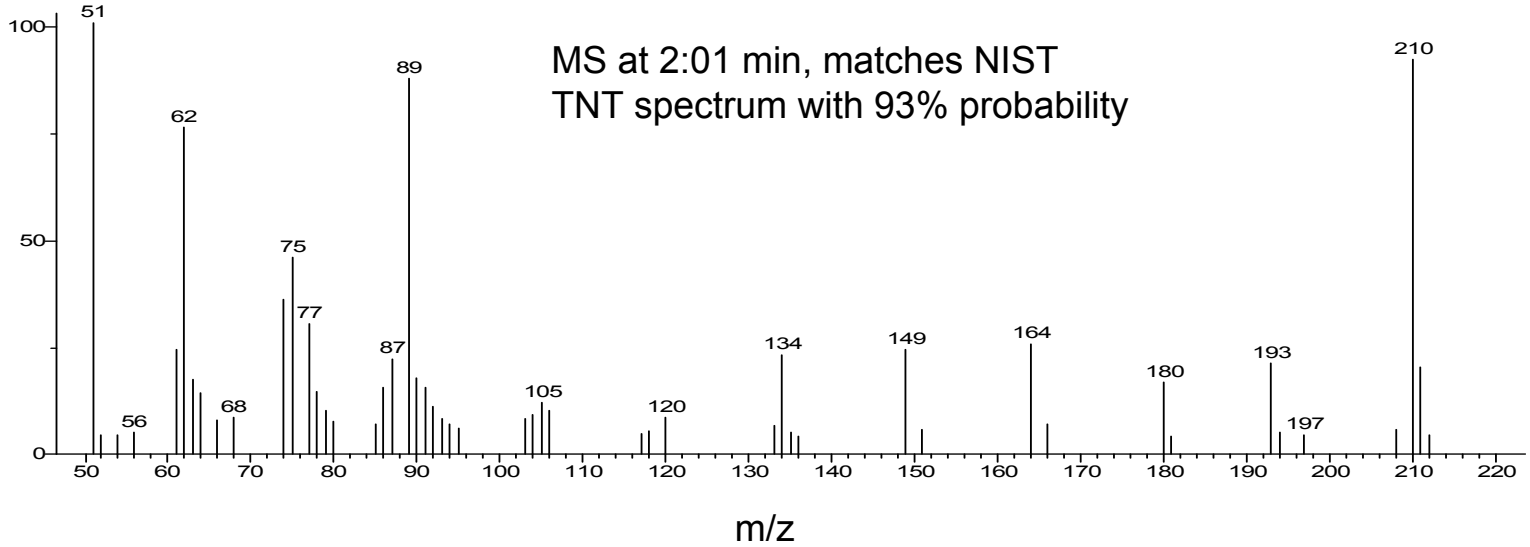


9) Famphur

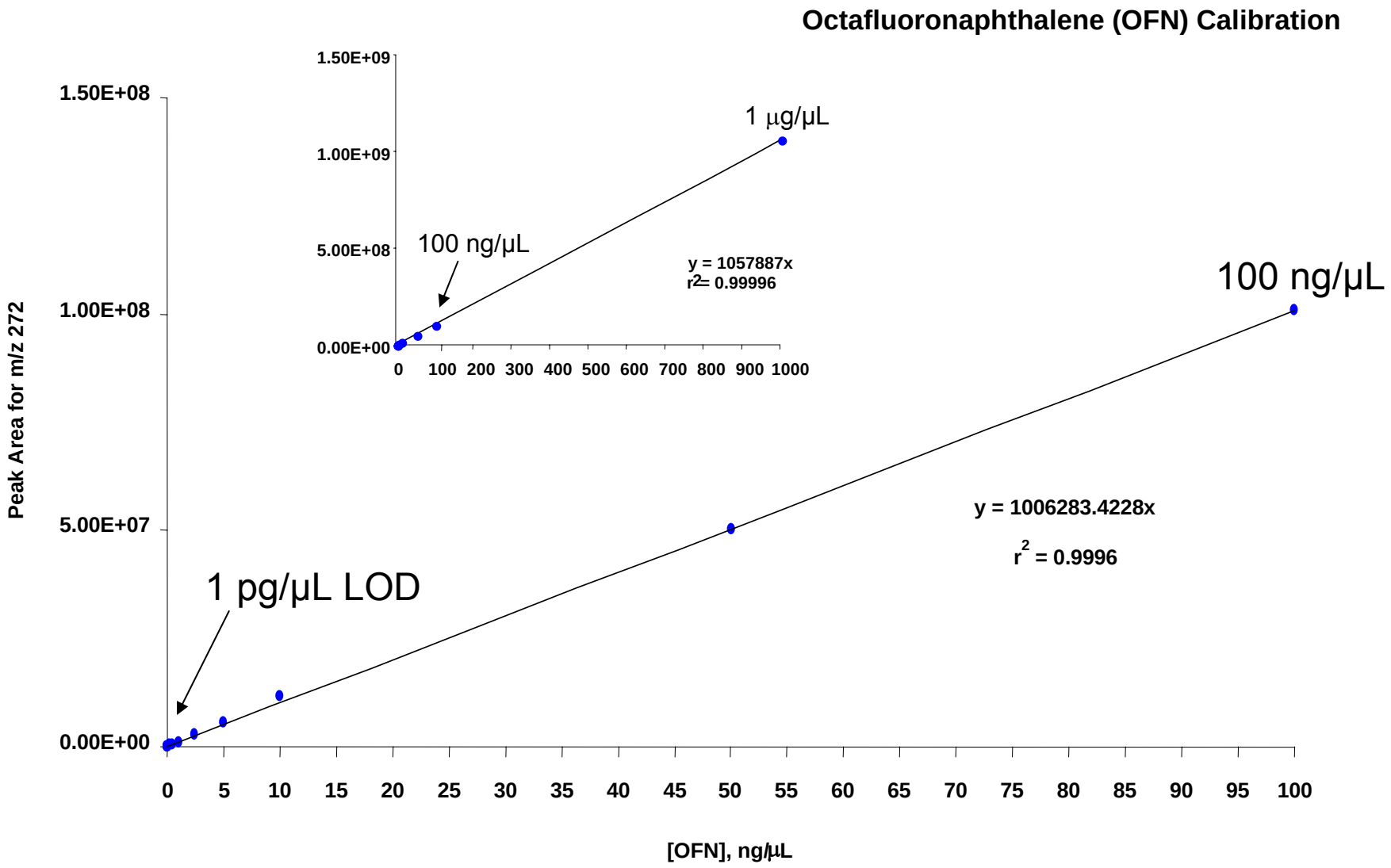


Explosive separation on a 5 m Rtx-5MS column



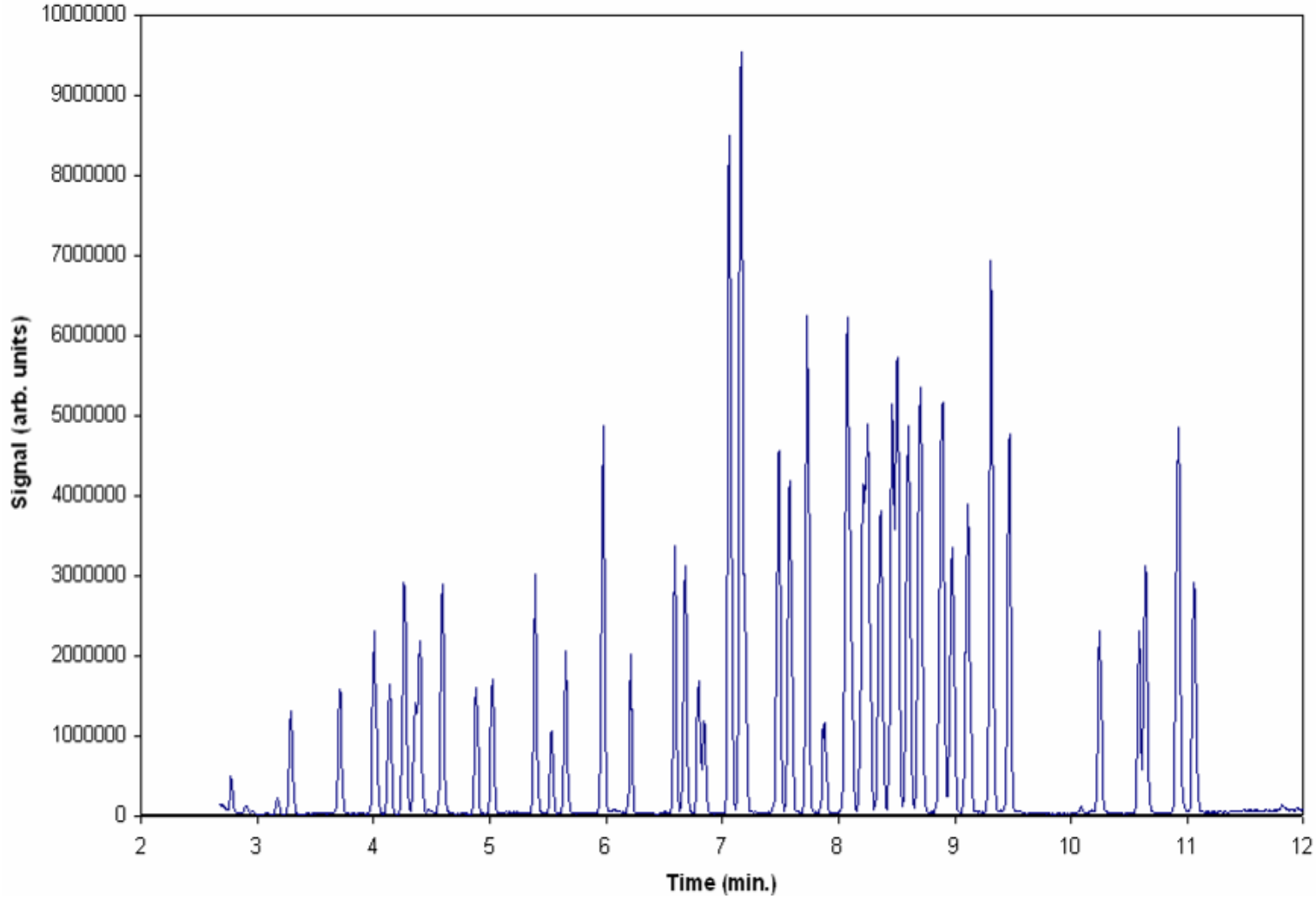


Dynamic Range with Automatic Level Control (ALC)™

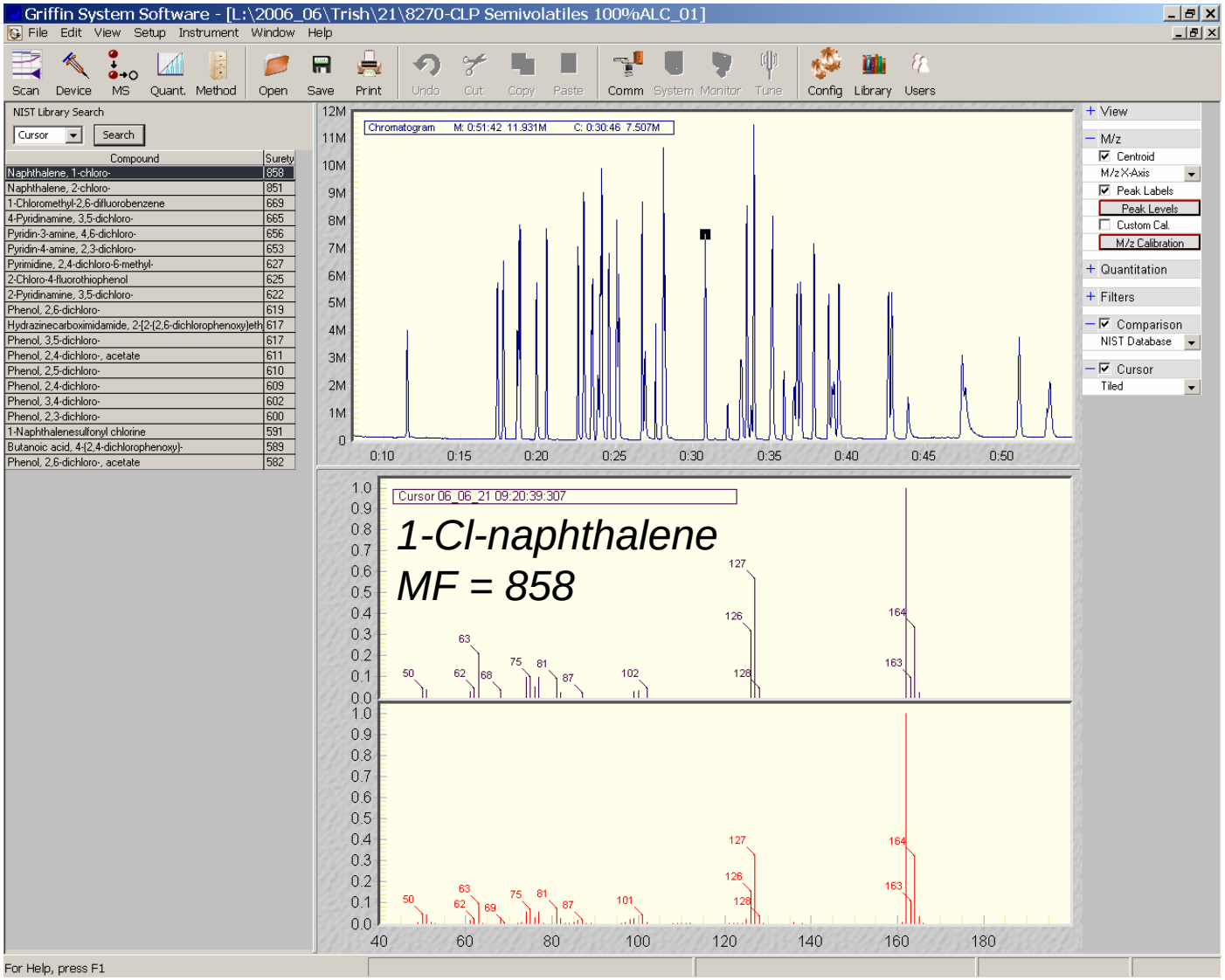


EPA Method 8260

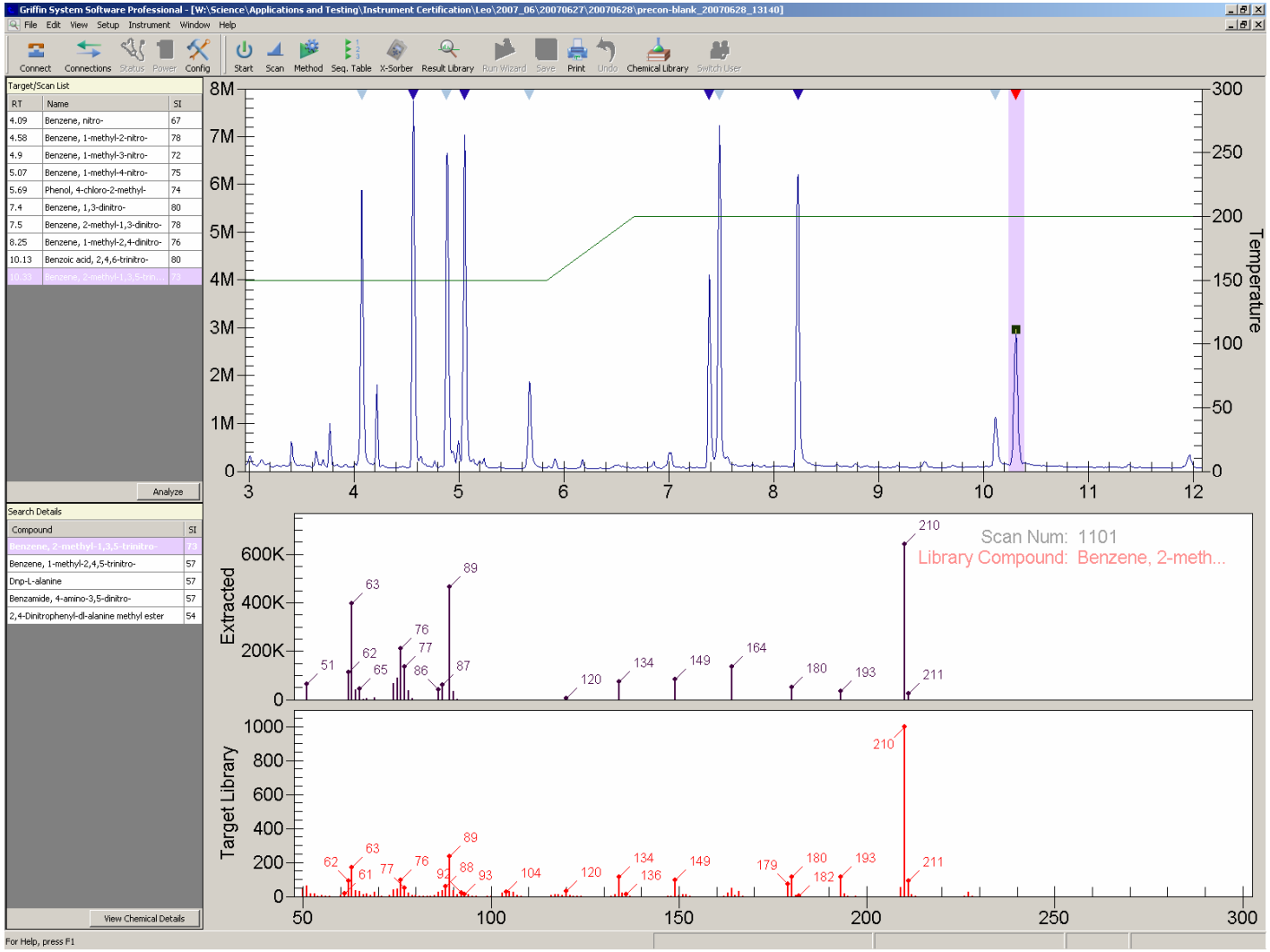
Chromatogram (TIC) for 52 component standard (liquid injection via autosampler)



Complex mixture analysis: EPA 8270 semivolatiles



X-Sorber + explosives mixture



Screen capture from the Griffin System Software (GSS) showing EPA 529 chromatogram and overlaid temperature trace (green stair step line).

Initial temperature 40° C, hold 0.5 min,
Ramp 40° to 150° C at 60° C/min, hold 3.5 min,
Ramp 150° to 200° C at 60° C/min, hold 13.5 min,
Ramp 200° to 250° C at 60° C/min, hold 4 min

X-Sorber + TNT

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Griffin System Software Professional - [W:\Science\Applications and Testing\Instrument Certification\Jethro\ASM\TNT 1000 ng _1 Jethro]

File Edit View Setup Instrument Window Help

Connect Connections Status Power Config Start Scan Method Seq. Table X-Sorber Result Library Run Wizard Save Print Undo Chemical Library Switch User

Target/Scan List

Target List | Scan List | Scans

RT	Name
14.58	2,4,6-Trinitroto...

Details
2,4,6-Trinitrotoluene
RT..... 14.58
PRT..... n/a
RTSI..... n/a
Match SI..... n/a
Quant Area... 2.22M
Quant Conc... n/a

Edit Target | Delete Target | Delete All

Graph Options

RICs | Options

TIC | Quant (90, 210, 211) ...

M/z 90 | Enable

Baseline

Add RIC | Delete RIC

Search Details

Target Results | Spectral Results | Comparison

Compound	SI
2,4,6-Trinitrotoluene	

View Chemical Details

Target: 2,4,6-Trinitrotoluene
Area: 2.22M

RIC Data | TIC Data | Temperature

Spectrum | Scan Num: 2661 | Background Subtracted

View Options
- Target/Scan List
- Graph Options
- Search Details

Graphs
- Chromatogram
- Detailed Chromatogram
- Both

Original Data

Display Method | Display X-Sorber Data | View Quant. Report | View Qual. Report

Analysis
Search Options | Reprocess

Calibration
Import Custom Quant. | View Custom Quant. | Use Custom Quant.

Spectrum Options
Spectrum: Background Extracted
Comparison Spectrum: Library
Show Comparison
View Options: Tiled
Peak Floor: 100000

For Help, press F1

X-Sorber + MES

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Griffin System Software Professional - [W:\Science\Applications and Testing\Instrument Certification\Jethro\ASM\Jethro Precon 16.6 ppb MES_1]

File Edit View Setup Instrument Window Help

Disconnect Connections Status Power Config Start Scan Method Seq. Table X-Sorber Result Library Run Wizard Save Print Undo Chemical Library Switch User

Target/Scan List

Target List | Scan List | Scans

RT	Name
6.63	16.6 ppb MES

Details
16.6 ppb MES
RT..... 6.63
PRT..... n/a
RTSI..... n/a
Match SI..... n/a
Quant Area... 27.16M
Quant Conc... n/a

Edit Target | Delete Target | Delete All

Graph Options

RICs | Options

TIC | Quant (92, 120, 152)

M/z 92 | Enable

M/z 120 | Enable

Baseline

Add RIC | Delete RIC

Search Details

Target Results | Spectral Results | Comparison

Compound	Surety
Benzoic acid, 2-hydroxy-, me...	76
Benzoic acid, 2-(acetyloxy)-, ...	71
o-Aminobenzohydroxamic acid	64
2-Propenoic acid, 3-(1H-imida...	58
Methylparaben	55
3-Pyridinecarboxylic acid, 4-a...	54
2-Amino-nicotinic acid methyl ...	54
Urocanic acid, methyl ester	54
Benzoic acid, 2-hydroxy-, 2-...	53
Benzoic acid, 3-hydroxy-, me...	53
2-Hydroxyethyl salicylate	52

Perform Search | Max Results: 25

Temperature

16.6 ppb MES

RIC Data

TIC Data

Target: 16.6 ppb MES
Area: 27.16M

Background Subtracted

Scan Num: 860
Library Compound: Benzoic acid, 2...

Spectral Library

View Options
Target/Scan List
Graph Options
Search Details
Graphs
Chromatogram
Detailed Chromatogram
Both
Original Data
Display Method
View Quant. Report
View Qual. Report

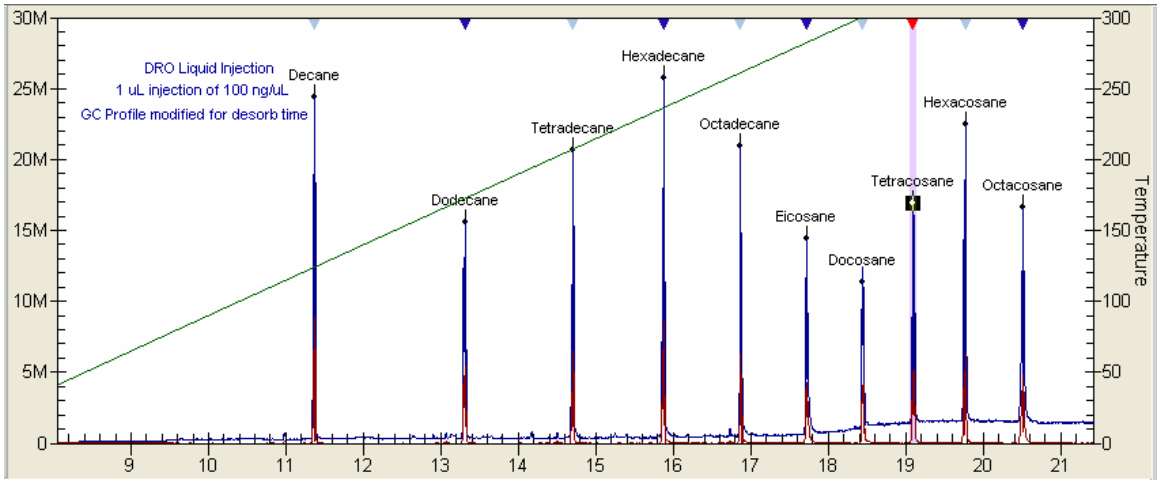
Analysis
Search Options
Reprocess

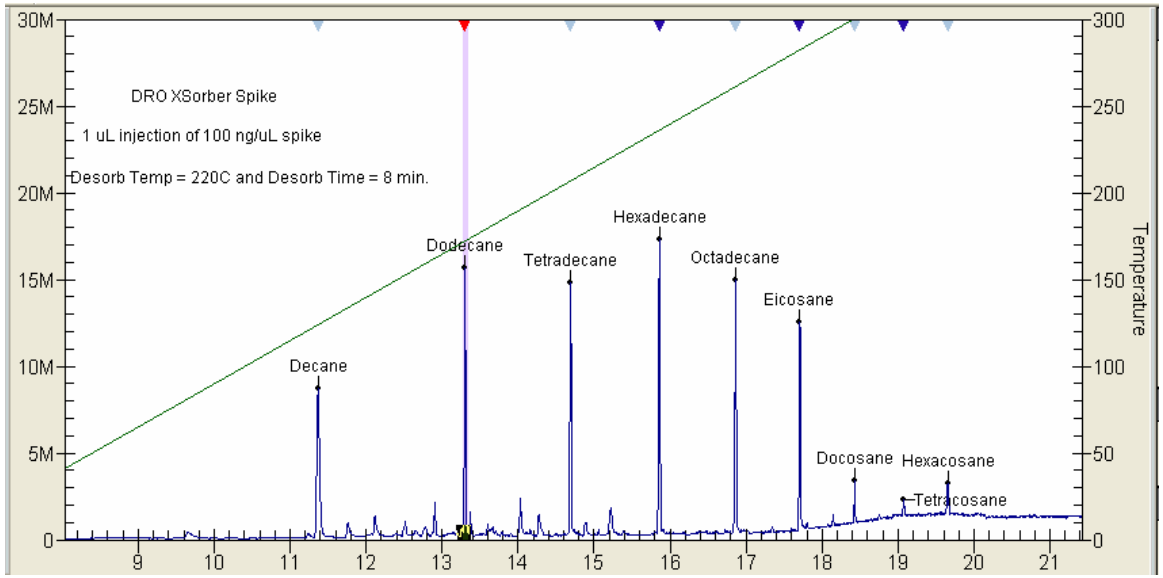
Calibration
Import Custom Quant.
View Custom Quant.
Use Custom Quant.

Spectrum Options
Spectrum: Background Extracted
Comparison Spectrum: Library
Show Comparison
View Options: Tiled
Peak Floor: 0

For Help, press F1 | LEO_407 G450 450-00005 v5.5 | Ready | Pressure: 8.21e-5 Torr

X-Sorber Injection Efficiency





Conclusions

- Fully integrated sampling design
  - Liquid injection
  - SPME
  - Air Sampling
  - Air Preconcentration
  - X-Sorber
- Rugged design
- Flexible and usable user software