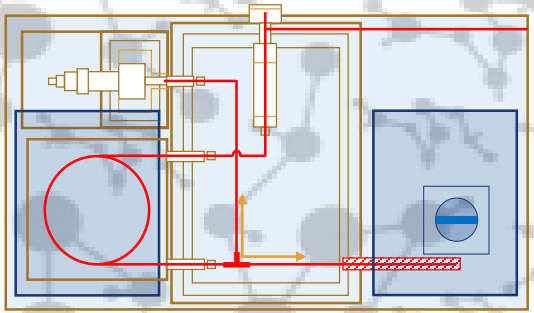
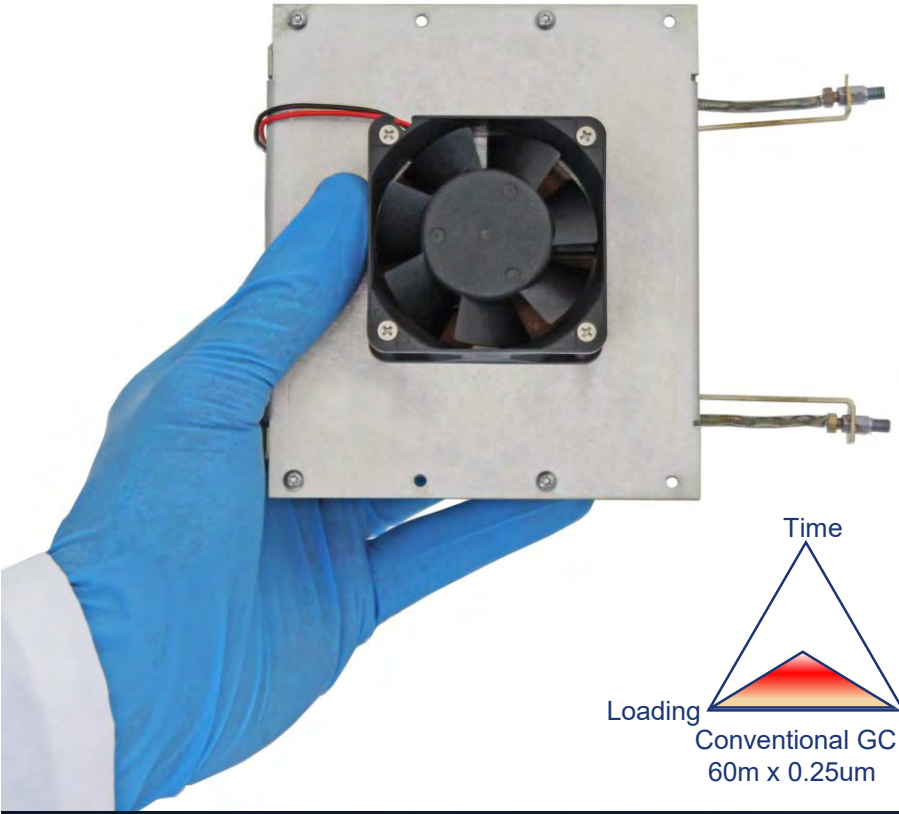
Fast Gas Chromatography High Pressure Mass Spectrometry (GC-HPMS) Technique, Software and Applications

Graham Shelver & James Roush - 908 Devices Inc.

Ultrafast GC-HPMS Technology

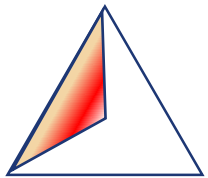


908devices// Fast Gas Chromatography

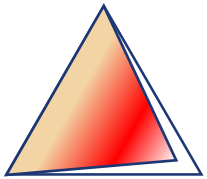


- Resistively heated SilcoSteel capillary columns
- Ultrafast heating (5°C/sec) & rapid cooling
- Retention times in seconds (0.06% RSD)
- Low power (<400W)
- Easy to exchange modules

Conventional GC
60m x 0.25um



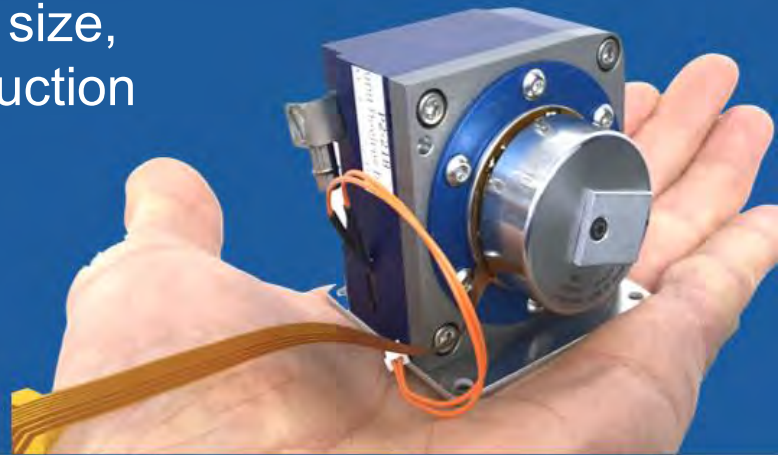
Conventional GC
4m x 0.25um



Ballistic GC
4m x 0.25um

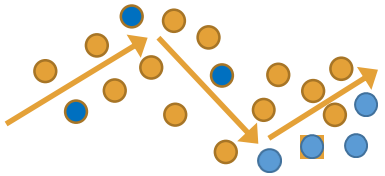
G908 eliminates need for outer space vacuum

Patented ion trap technology
makes for dramatic size,
weight, & power reduction

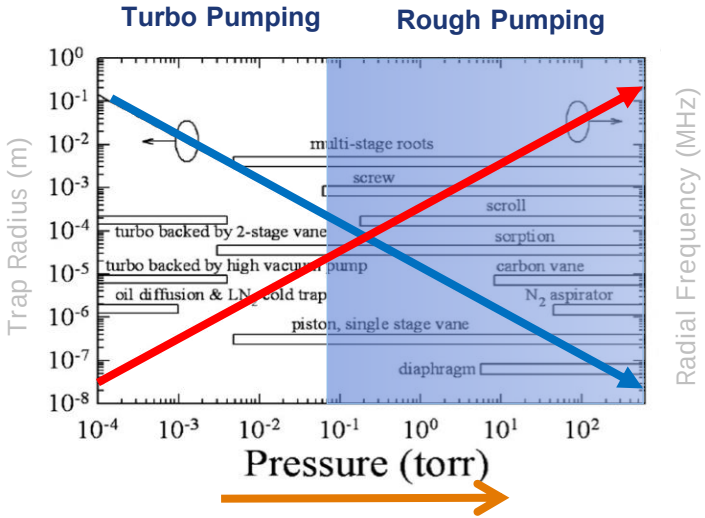


908devices// Measurement of Hydrocarbons in Process Streams

Conventional GC-MS has an absolute requirement for continuous high vacuum (0.0001 Torr) to ensure suitable mean-free path - average distance a particle travels between collisions with other particles



Atmospheric pressure (760 torr):	~ 100 nm
Low vacuum 1 torr:	~1 mm
Medium vacuum (1e^{-3} torr)	~ 10 cm
High vacuum 1e^{-6} torr:	100 m
Ultra high vacuum 1 e^{-12} torr:	100 km



908devices// Breaking Free with High Pressure MS

Conventional MS has an absolute requirement for continuous high vacuum

Outer Space → < 0.0001 torr → 1- 8 torr → Sea Level

1 Torr = 1mmHg
1 Atm = 760mmHg

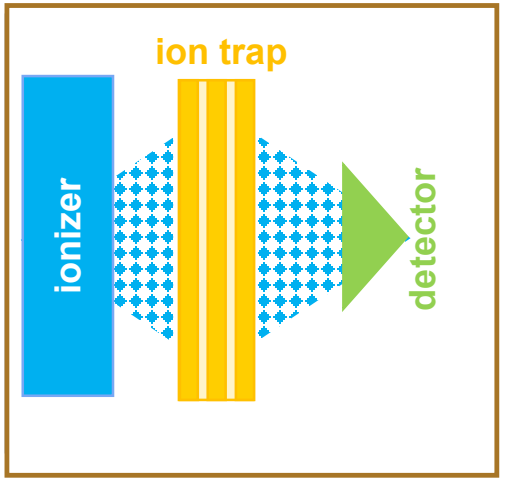
Power and Maintenance Requirements ← Low

The G908 HPMS requires only a miniature, on-board scroll pump to operate.

908devices// Going Micro with High Pressure Mass Spectrometry

‘All-in-one’ HPMS Concept integrates all three MS elements…..

- Ion Source -Glow Discharge
- Ion Trap – 3D Microscale
- Detector – Faraday plate



….into a single Compact Core (1”x1”x1”) designed to be easily exchangeable and/or cleaned by operators

'All-in-one' HPMS Concept integrates all three MS elements…..

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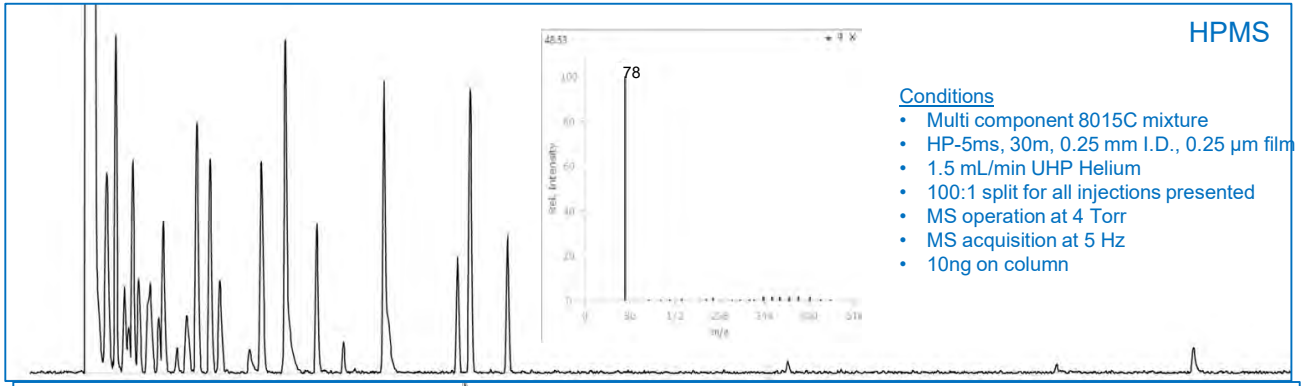
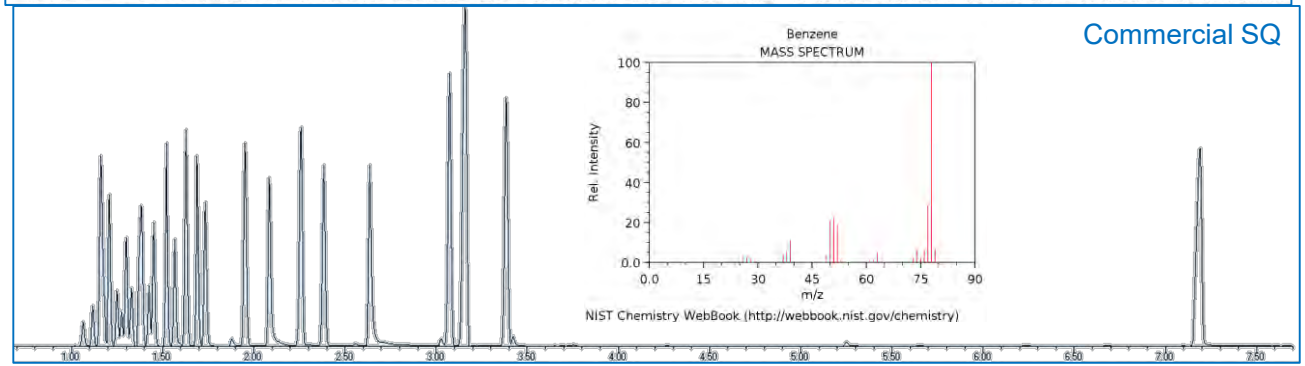
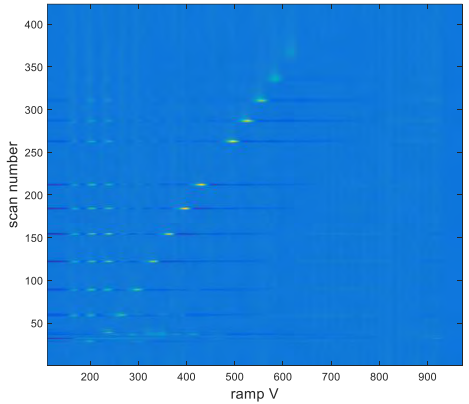
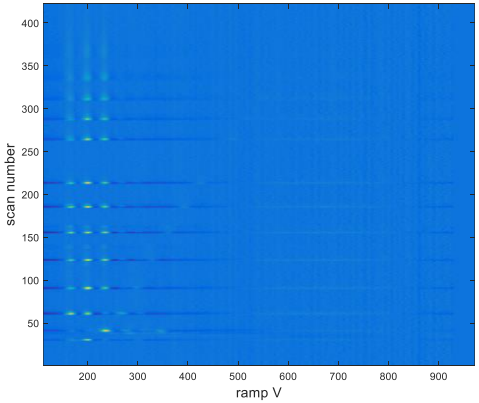
GC-MS vs GC-HPMS

- GDI equivalent to CI or soft ionization
- Spectra differ from EI NIST
- High trap pressure (1-4 Torr) can produce Reactive Ion Products (RIP)



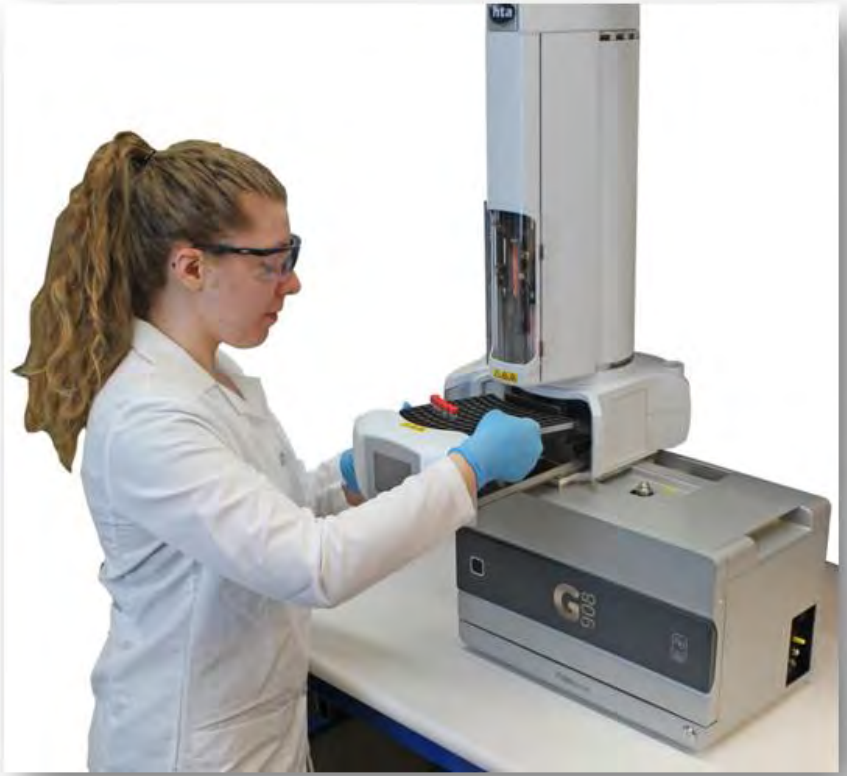






908devices// User serviceable modules

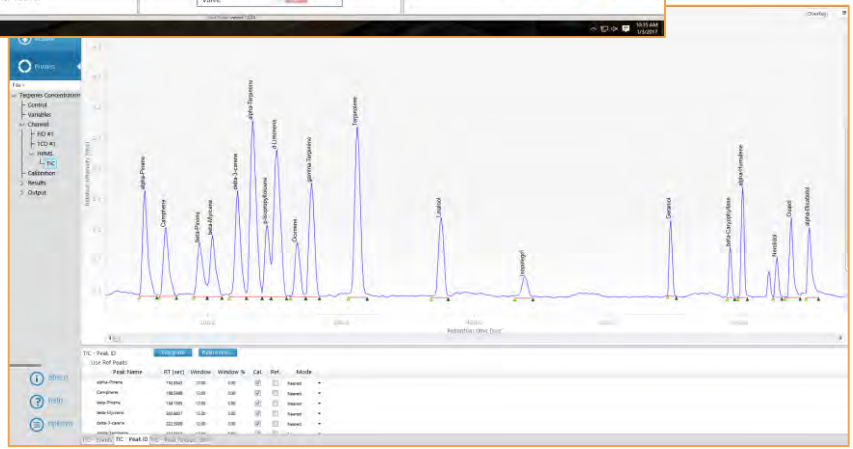
908devices// Start with Manual Injection, Upgrade to Automation



908devices// JetStream Software – Designed around Workflow

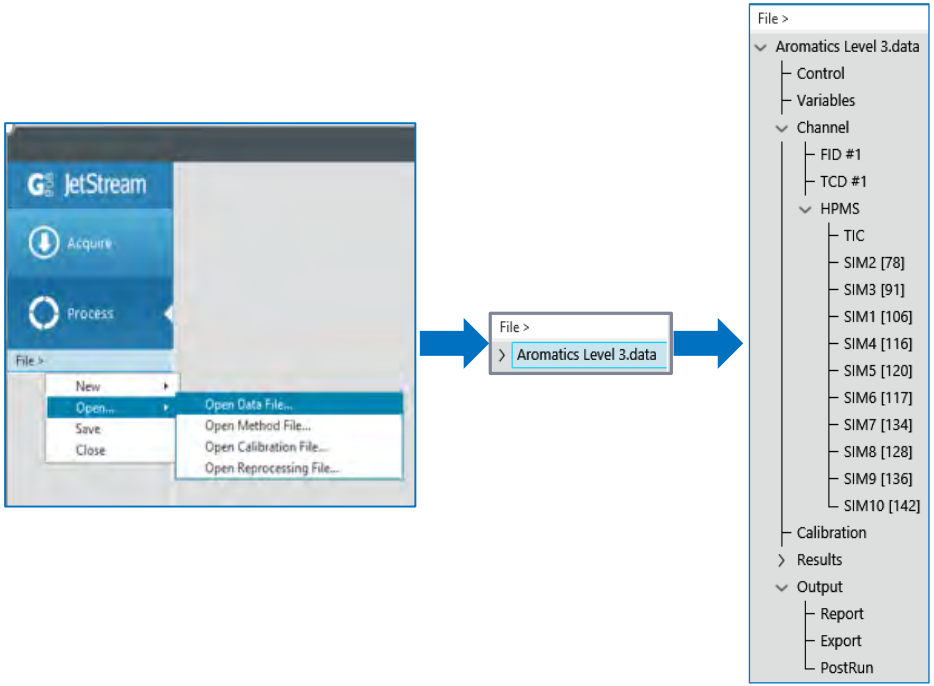
“Less is More”

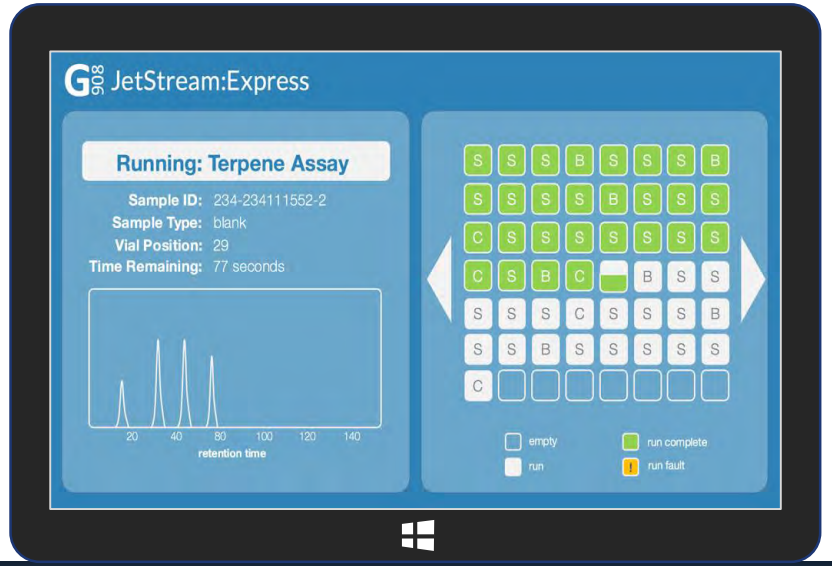
- Uncluttered User Interfaces
- All-in-one data file format (SQL)
- Unified data channel processing
- For Operators & Analytical Chemists



JetStream Software – Designed around Workflow

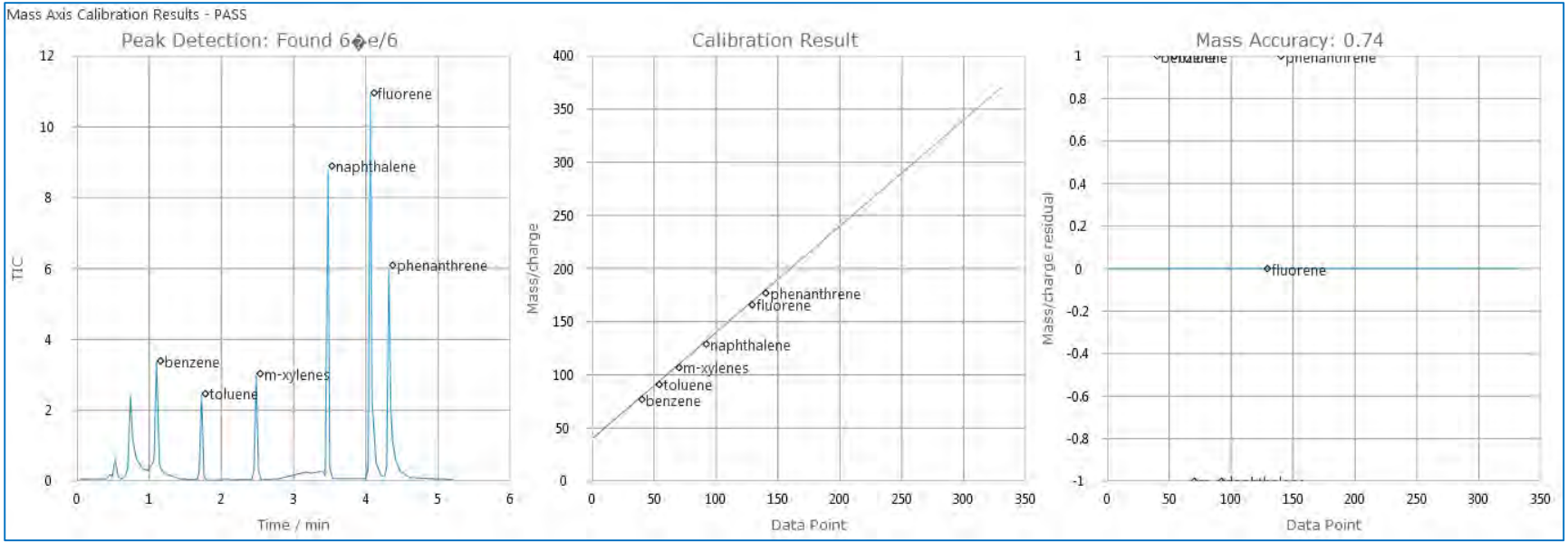
- All-in-one data file structure
- SQL – raw data, results, method, calibration, metadata
- Single button operation



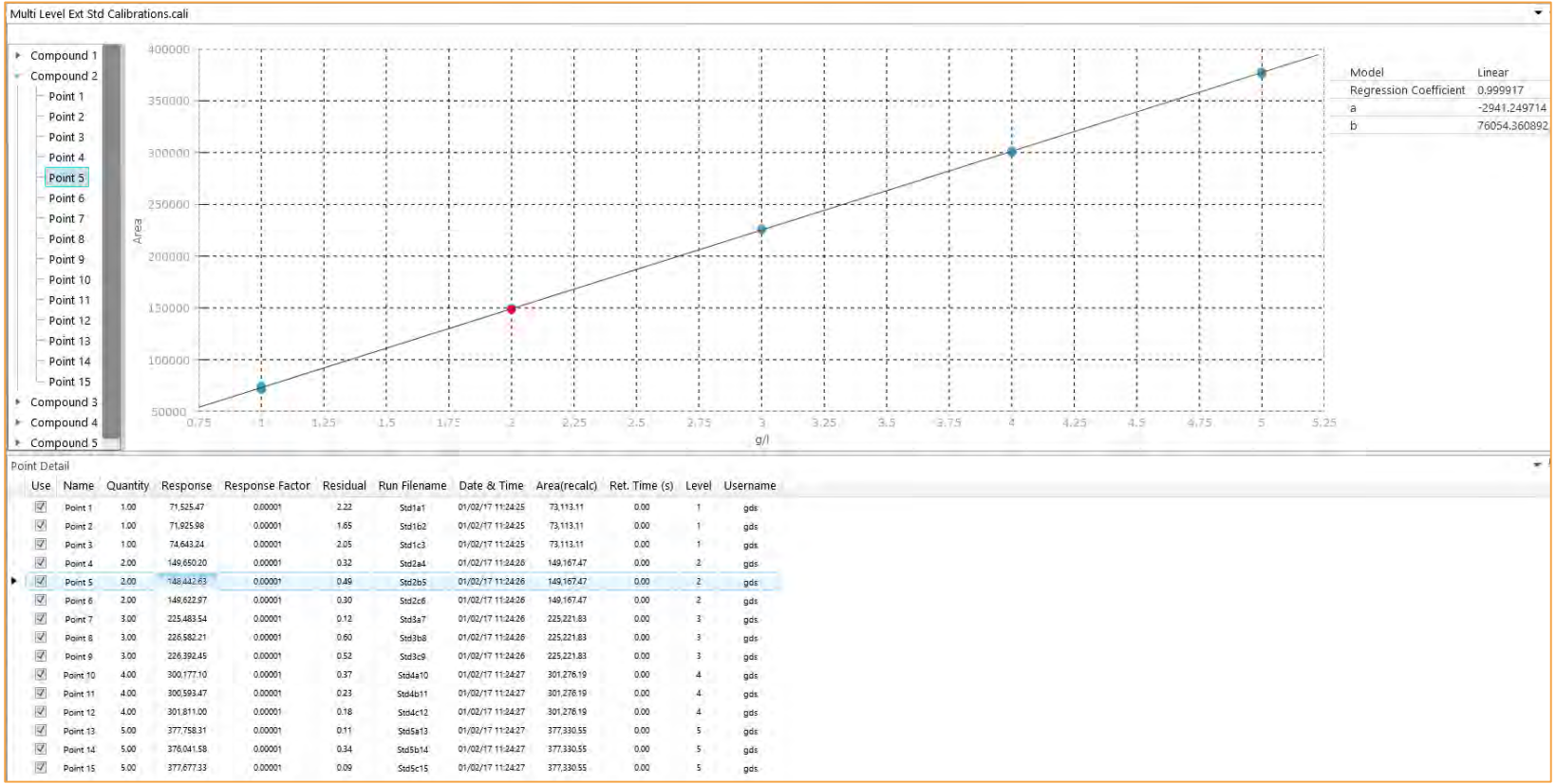


908devices // JetStream – Mass Axis Calibration Report

- Standardized MassCal Test Mixtures supplied with G908 System
- Single Injection with automated results calculation and Pass/Fail Report

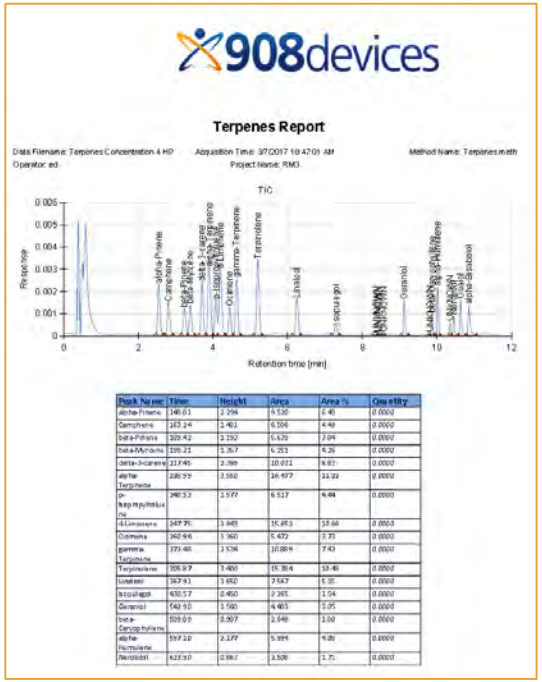


908devices // JetStream – Component Calibration



908devices // JetStream Output – Reporting, Export and PostRun

Template driven multi-channel JS report



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Terpenes Report

Data Filename: Terpenes Concentration 4 HP Acquisition Time: 3/7/2017 10:47:01 AM Method Name: Terpenes.meth
Operator: ed Project Name: RMG

TIC

Response

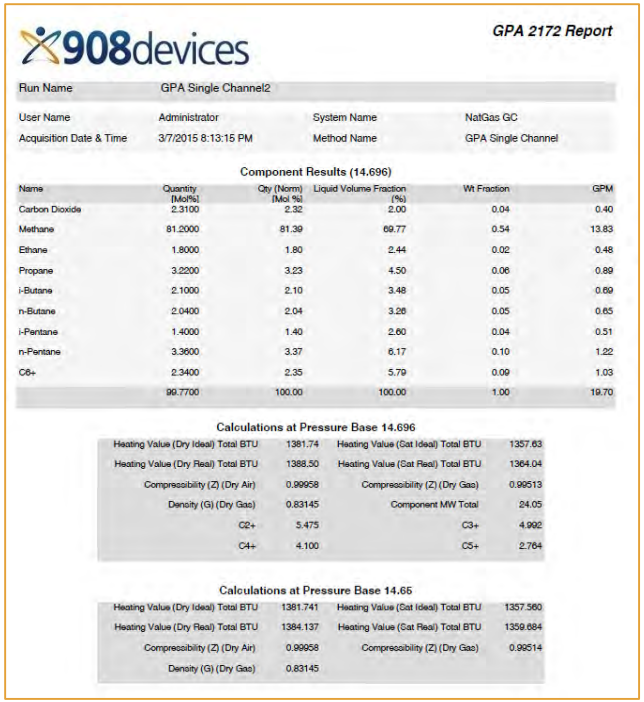
Retention time [min]

Peak Name	Time	Height	Area	Area %	Quantity
alpha-Pinene	140.01	2.256	9.526	6.46	0.0000
Camphene	153.24	1.401	6.596	4.48	0.0000
beta-Pinene	169.42	3.152	5.429	7.04	0.0000
beta-Myrcene	199.31	3.267	6.253	9.26	0.0000
delta-3-carene	217.45	2.389	10.021	9.83	0.0000
alpha-Terpinene	228.59	2.550	14.477	11.22	0.0000
p-isopropyltoluene	240.53	2.577	6.527	9.44	0.0000
d-Limonene	247.75	3.948	15.813	18.68	0.0000
Cumene	262.96	1.360	5.472	7.73	0.0000
gamma-Terpinene	273.48	2.536	10.884	7.43	0.0000
Terpinolene	306.87	3.480	15.364	18.46	0.0000
linalool	367.91	3.662	7.647	6.35	0.0000
isopulegol	430.57	2.460	2.365	1.54	0.0000
Geraniol	542.50	3.500	4.483	3.05	0.0000
beta-Caryophyllene	559.05	0.507	2.049	1.00	0.0000
alpha-Humulene	597.10	2.177	5.994	4.88	0.0000
Nerolidol	623.90	0.867	2.526	1.75	0.0000

Data export

- CSV
- ASCII
- XML

Postrun .exe for 3rd party plug-in applications



908devices

GPA 2172 Report

Run Name	GPA Single Channel2		
User Name	Administrator	System Name	NatGas GC
Acquisition Date & Time	3/7/2015 8:13:15 PM	Method Name	GPA Single Channel

Component Results (14.696)

Name	Quantity (Mol%)	Qty (Norm) (Mol %)	Liquid Volume Fraction (%)	Wt Fraction	GPM
Carbon Dioxide	2.3100	2.32	2.00	0.04	0.40
Methane	81.2000	81.39	69.77	0.54	13.83
Ethane	1.8000	1.80	2.44	0.02	0.48
Propane	3.2200	3.23	4.50	0.06	0.89
i-Butane	2.1000	2.10	3.48	0.05	0.69
n-Butane	2.0400	2.04	3.26	0.05	0.65
i-Pentane	1.4000	1.40	2.60	0.04	0.51
n-Pentane	3.3600	3.37	6.17	0.10	1.22
C6+	2.3400	2.35	5.79	0.09	1.03
	99.7700	100.00	100.00	1.00	19.70

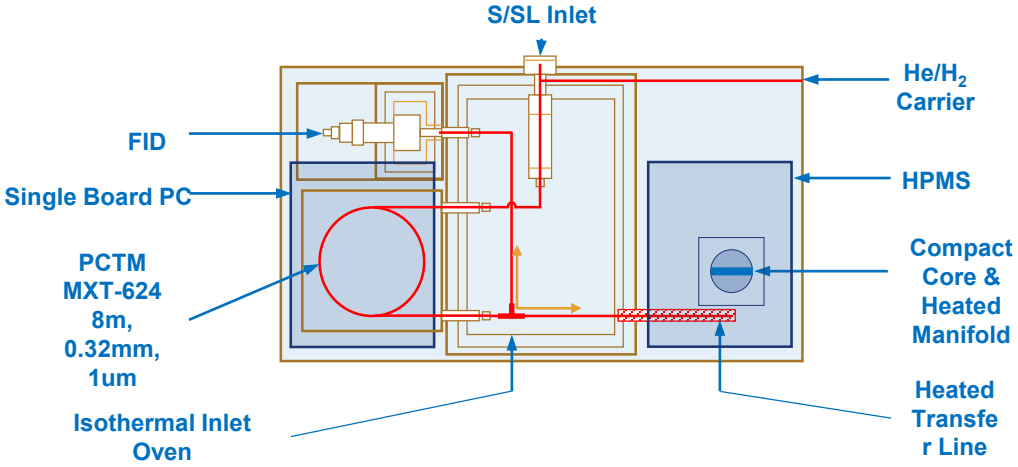
Calculations at Pressure Base 14.696

Heating Value (Dry Ideal) Total BTU	1381.74	Heating Value (Sat Ideal) Total BTU	1357.63
Heating Value (Dry Real) Total BTU	1388.50	Heating Value (Sat Real) Total BTU	1364.04
Compressibility (Z) (Dry Air)	0.99958	Compressibility (Z) (Dry Gas)	0.99513
Density (G) (Dry Gas)	0.83145	Component MW Total	24.05
C2+	5.475	C3+	4.992
C4+	4.100	C5+	2.764

Calculations at Pressure Base 14.65

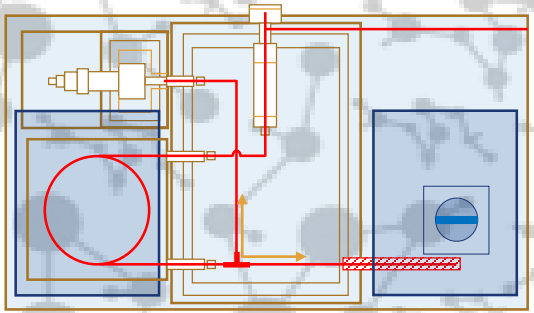
Heating Value (Dry Ideal) Total BTU	1381.741	Heating Value (Sat Ideal) Total BTU	1357.560
Heating Value (Dry Real) Total BTU	1384.137	Heating Value (Sat Real) Total BTU	1359.684
Compressibility (Z) (Dry Air)	0.99958	Compressibility (Z) (Dry Gas)	0.99514
Density (G) (Dry Gas)	0.83145		

908devices// G908 Ultrafast GC-HPMS



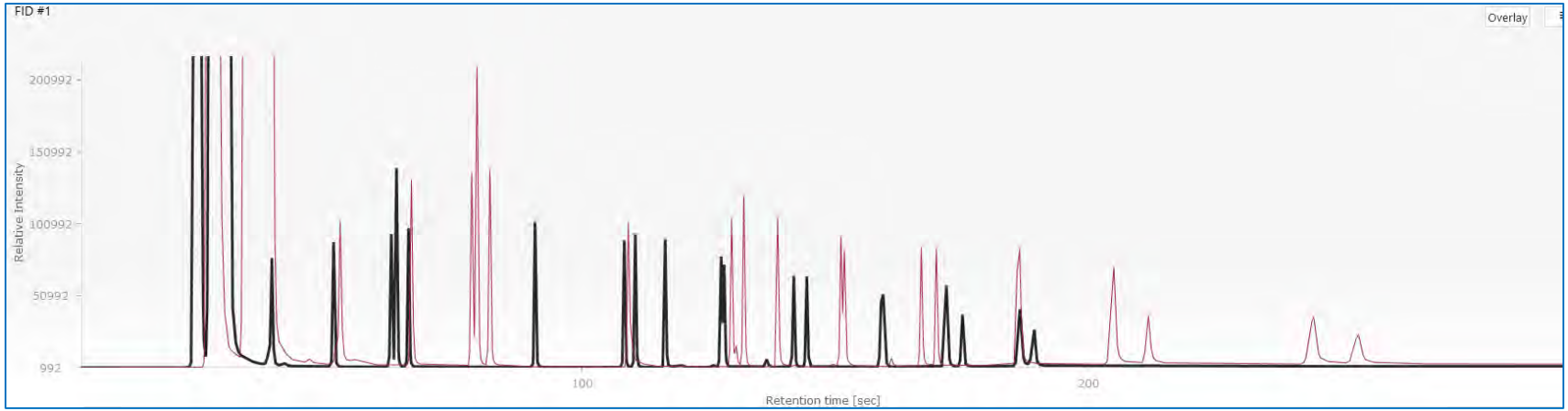
Technology	High Pressure Mass (HPMS)
Size	43 x 28 x 30cm (17.25 x 10.5 x in)
Weight	12.3kg (28lbs)
Power Requirements	24VDC from external power 100-240VAC 50/60Hz
Power Consumption	Startup 220W Maximum 350-480W Config Dependent
Operating Temperature	0-40°C (32-104°F)
Mass Spectrometer	Microscale Ion Trap
Ionization Source	Non-radioactive, internal glow discharge ionization (70eV), polarity
Low Mass Range	15-150 m/z
Full Mass Range	50-450 m/z
Mass Resolution	1 m/z (nominal)
Scan Rate	10-40Hz
Trap Operating	Ambient - 120°C
Operating Vacuum	1-4 Torr
Injector	Split/Splitless 1:1-1:200
Injector Manifold Temp & Pressure	350°C Max 50 psi Max
Sample Injection Modes	Manual/Valve/Autosampler
Carrier Gas	$He/H_2/N_2/Air$
Column Heating	Resistive, Ambient - 400°C Max
Column Temp Ramp Rate	0.1-5°C/second
GC Detectors	FID/TCD 350°C Max
Software	JetStream system control, data acquisition & processing

Technical Challenges

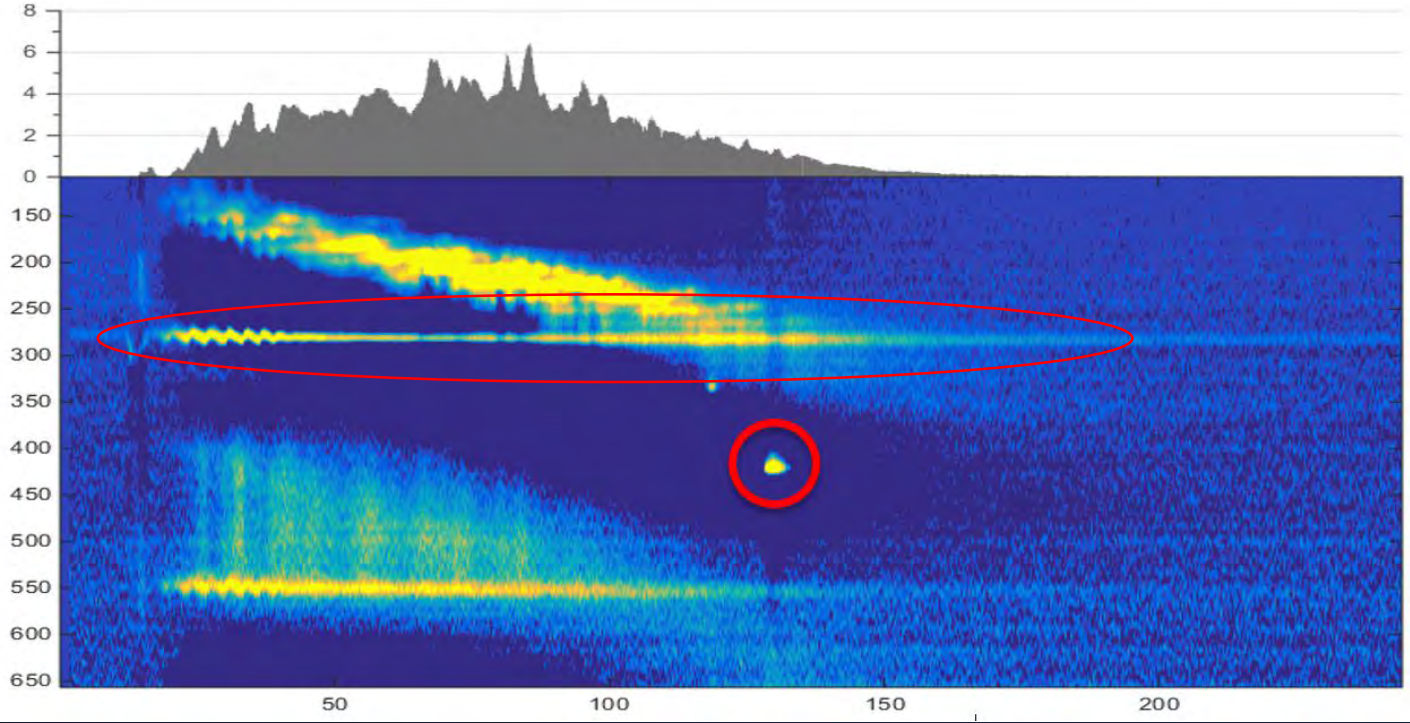


908devices// G908 – Balancing Sensitivity, Speed & Resolution

Column Length 4m……8m…….16m……?



Heated Compact Core – PEEK vs Polyimide



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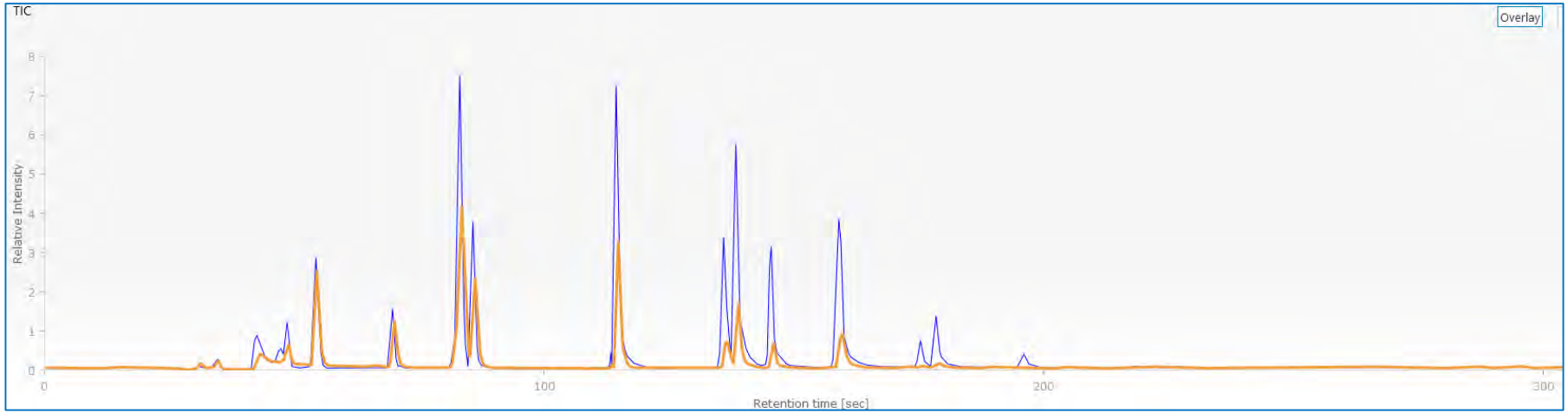
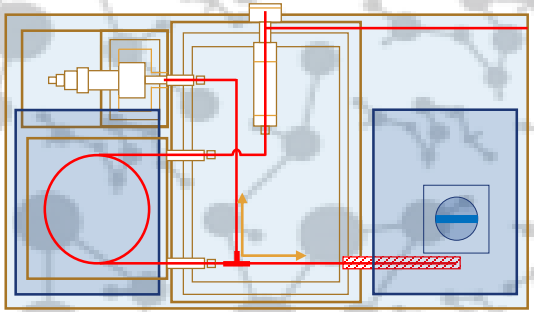
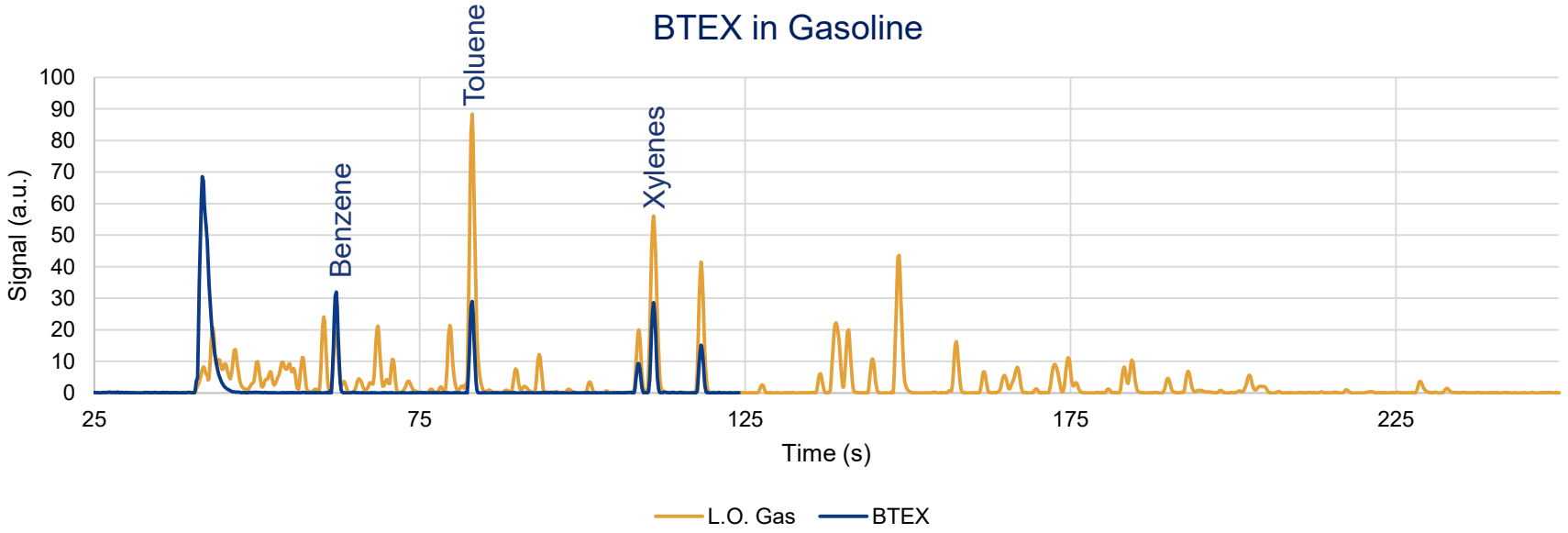


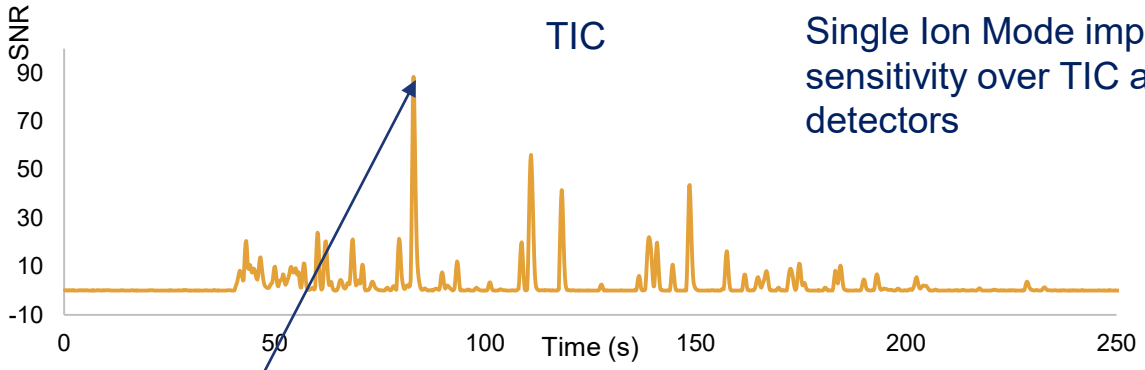
Applications



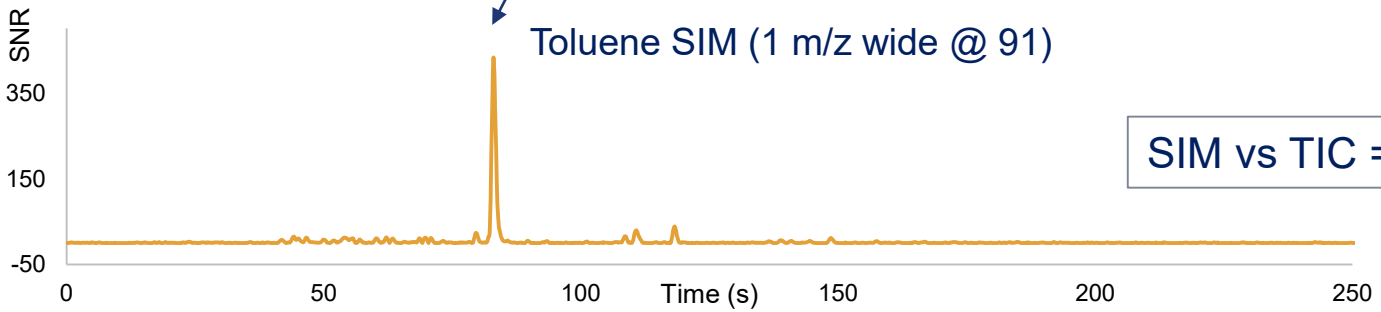
908devices// BTEX in Gasoline Total Ion Current



BTEX in Gasoline TIC vs SIM - Toluene

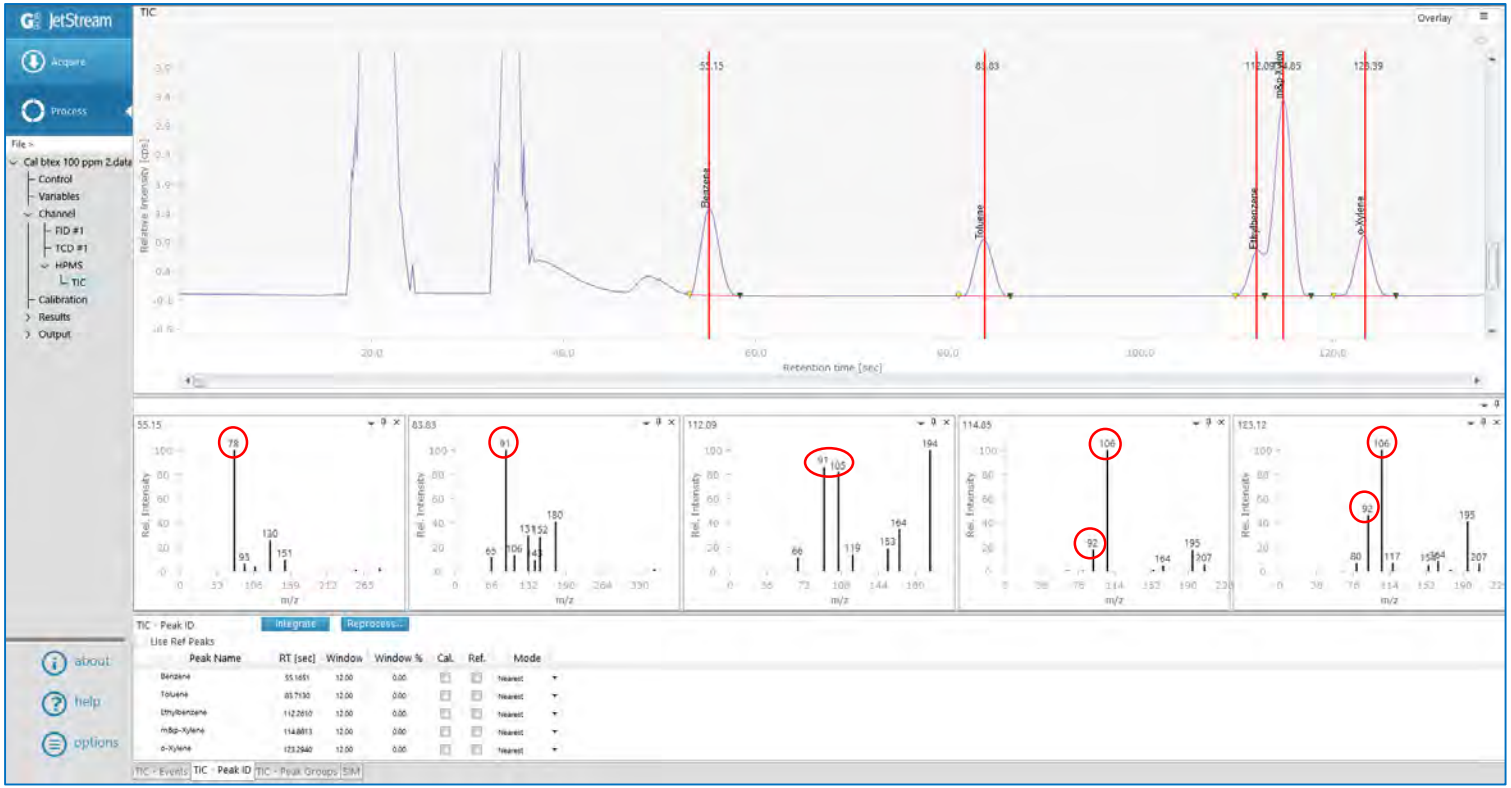


Single Ion Mode improves selectivity and sensitivity over TIC and conventional GC detectors

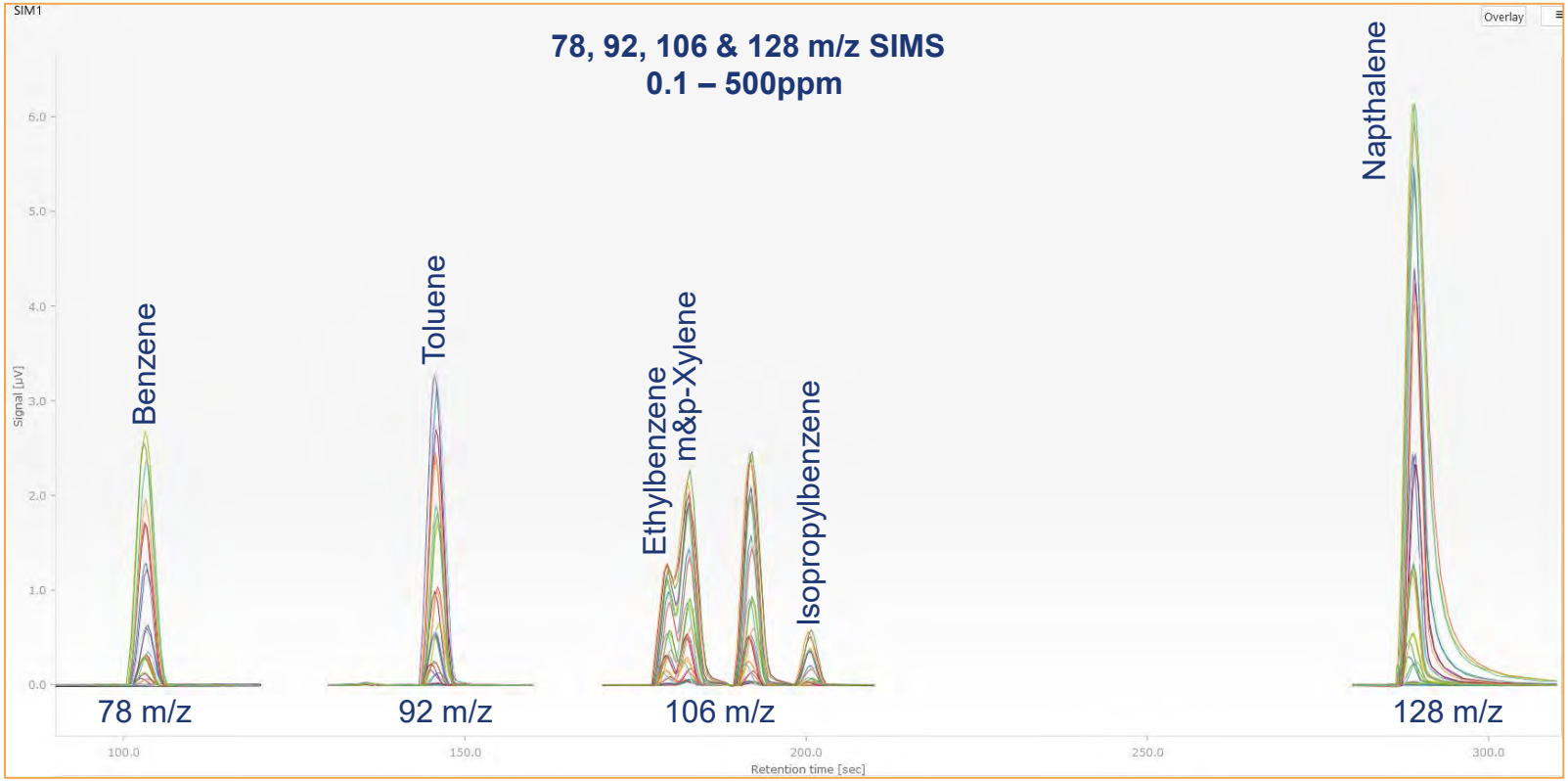


SIM vs TIC = 431:80 = 5.4:1

908devices// BTEX – GDI Spectra

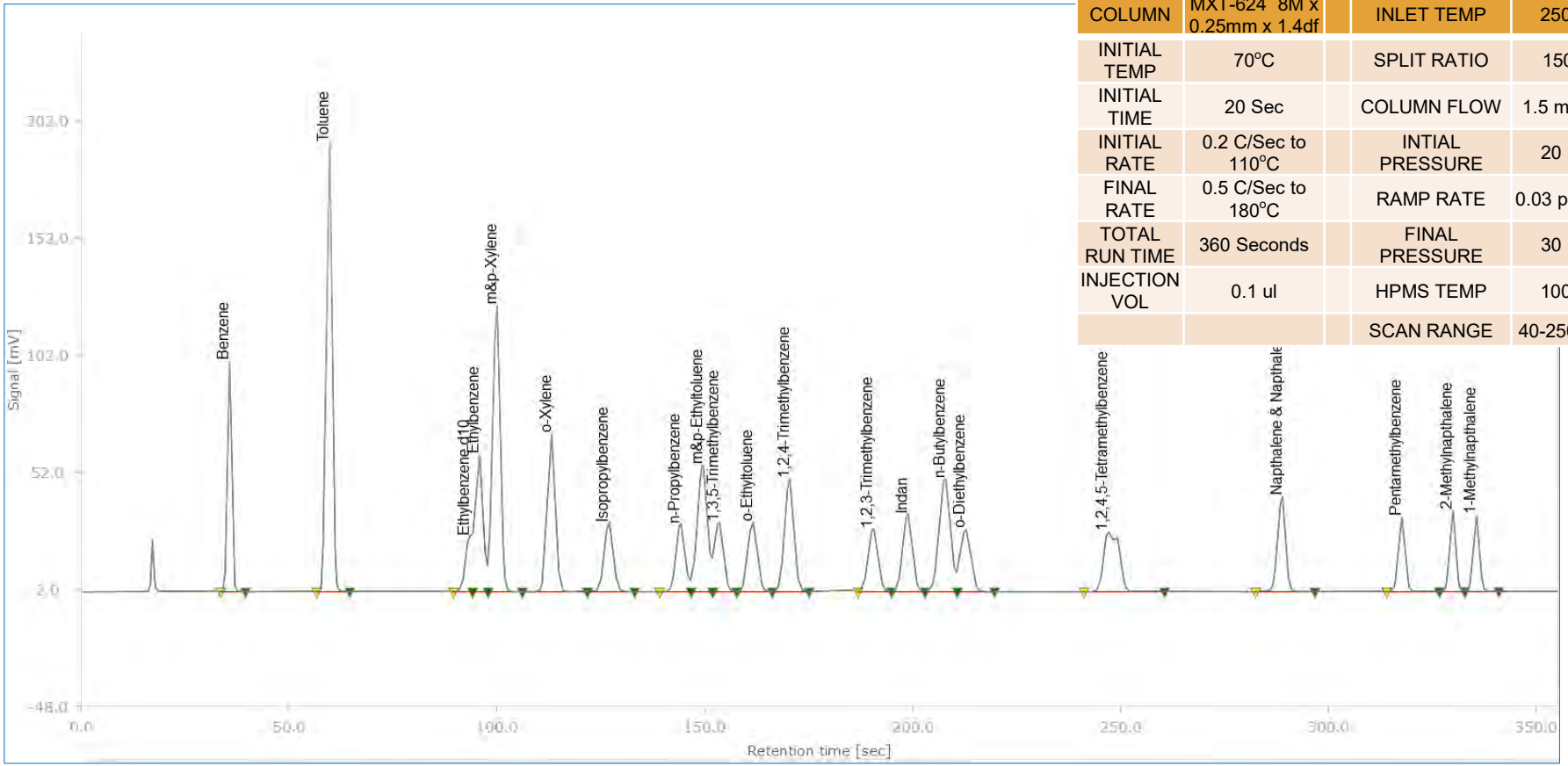


908devices// BTEX Selected Ion Mode (SIM)



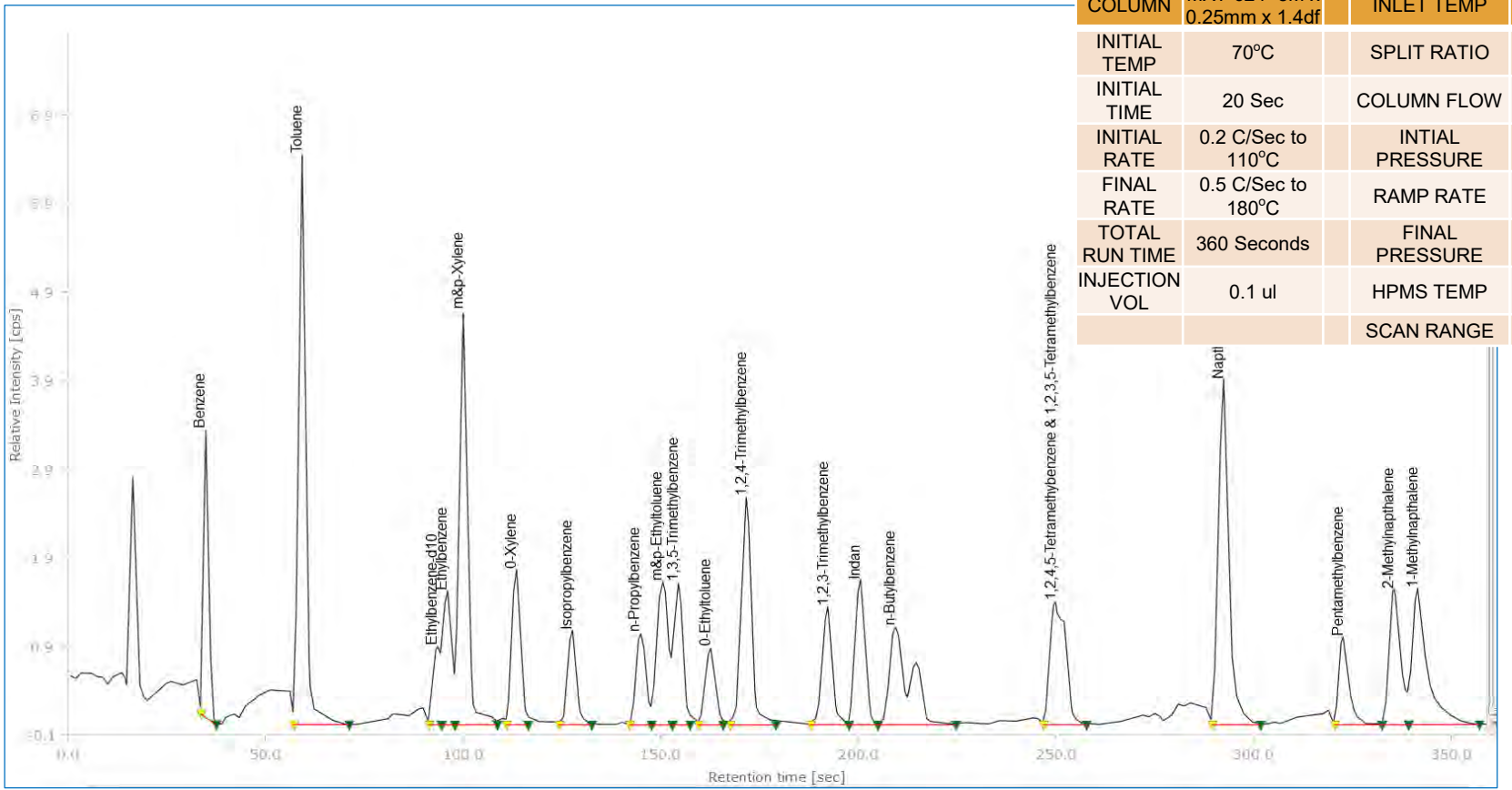
908devices// Aromatics in Finished Gasoline - FID

COLUMN	MXT-624 8M x 0.25mm x 1.4df		INLET TEMP	250°C
INITIAL TEMP	70°C		SPLIT RATIO	150:1
INITIAL TIME	20 Sec		COLUMN FLOW	1.5 ml/min
INITIAL RATE	0.2 C/Sec to 110°C		INTIAL PRESSURE	20 psi
FINAL RATE	0.5 C/Sec to 180°C		RAMP RATE	0.03 psi/sec
TOTAL RUN TIME	360 Seconds		FINAL PRESSURE	30 psi
INJECTION VOL	0.1 ul		HPMS TEMP	100°C
			SCAN RANGE	40-250 m/z

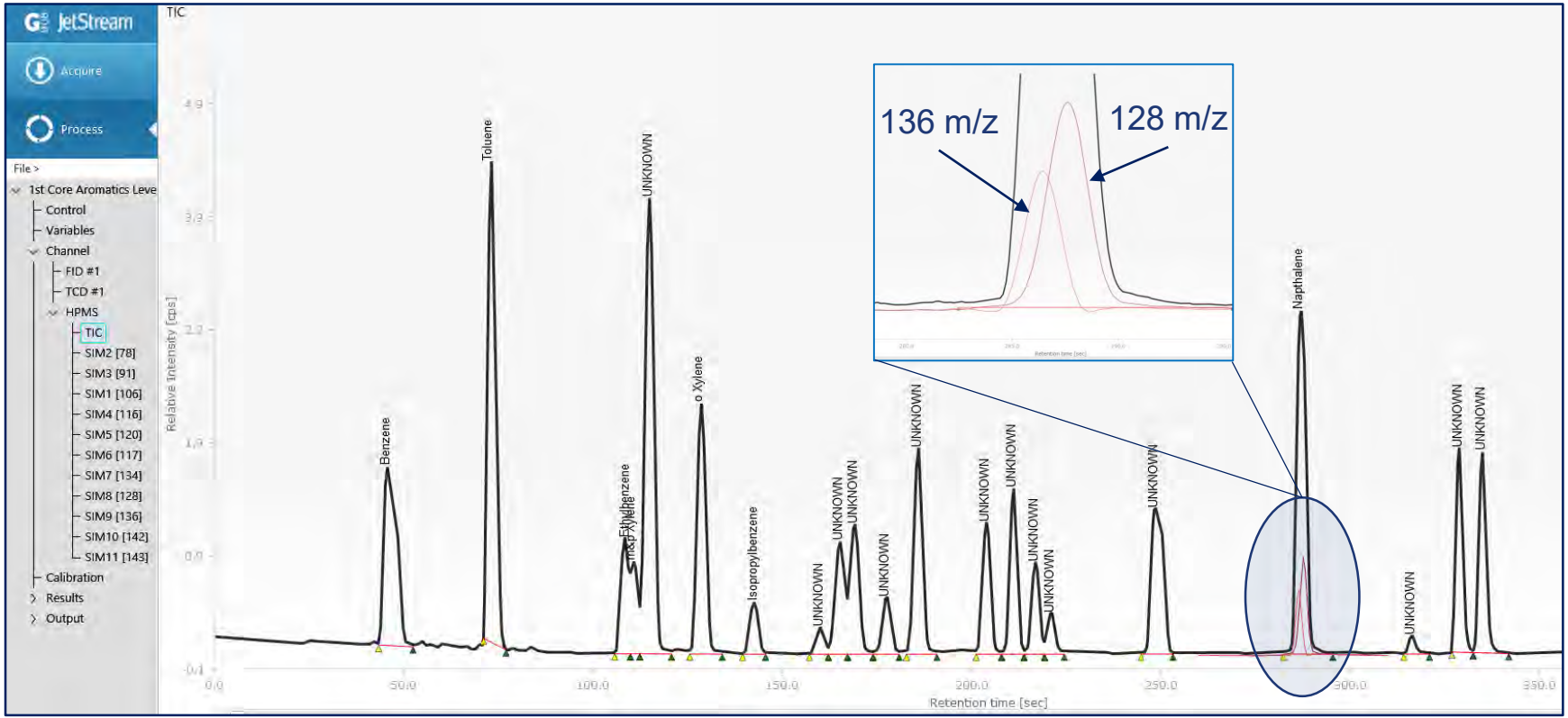


908devices// Aromatics in Finished Gasoline - TIC

COLUMN	MXT-624 8M x 0.25mm x 1.4df		INLET TEMP	250°C
INITIAL TEMP	70°C		SPLIT RATIO	150:1
INITIAL TIME	20 Sec		COLUMN FLOW	1.5 ml/min
INITIAL RATE	0.2 C/Sec to 110°C		INTIAL PRESSURE	20 psi
FINAL RATE	0.5 C/Sec to 180°C		RAMP RATE	0.03 psi/sec
TOTAL RUN TIME	360 Seconds		FINAL PRESSURE	30 psi
INJECTION VOL	0.1 ul		HPMS TEMP	100°C
			SCAN RANGE	40-250 m/z



908devices// Aromatics in Finished Gasoline - SIM



908devices// G908 GC-HPMS

- Fast, Accurate Compound ID & Measurement
- Small Footprint & Low Maintenance
- In-line, At-line, Lab & Portable
- Operator centric

IDEAL FOR RAPID, QUANTITATIVE POINT-OF-NEED HYDROCARBON ANALYSIS