

Agilent GC/MS Hardware, Software, and Consumables optimized for the Analysis of US EPA Method 8270

Fred Feyerherm
GCMS Applications
Houston, Tx

Agenda

Hardware – New GC and MSD: 7890B / 5977A

Higher sensitivity – More Inert – Still very robust

Performance Data

Chromatography – Initial Calibration

Software – Both Chemstation and Mass Hunter

Added capabilities – Universal cross training

Ultra Inert Sample Pathway Components

Inlets – Columns – Liners – Source

Helium Shortage

Choices – Hydrogen carrier or Helium Conservation

7890B / 5977A GCMS

New Pumps
Extractor Source
Low Energy Sleep Mode
Low Femtogram Detection Limits



Ultimetal Inert Inlets
Helium Conservation Mode
Easy Switch to H2 Carrier

New Extractor Ion Source for 5977



Increase in ion count

- ✓ True increase in sensitivity

Better trace level precision

- ✓ Lower IDL and MDL

Performance Data: Many Different 8270 Methods

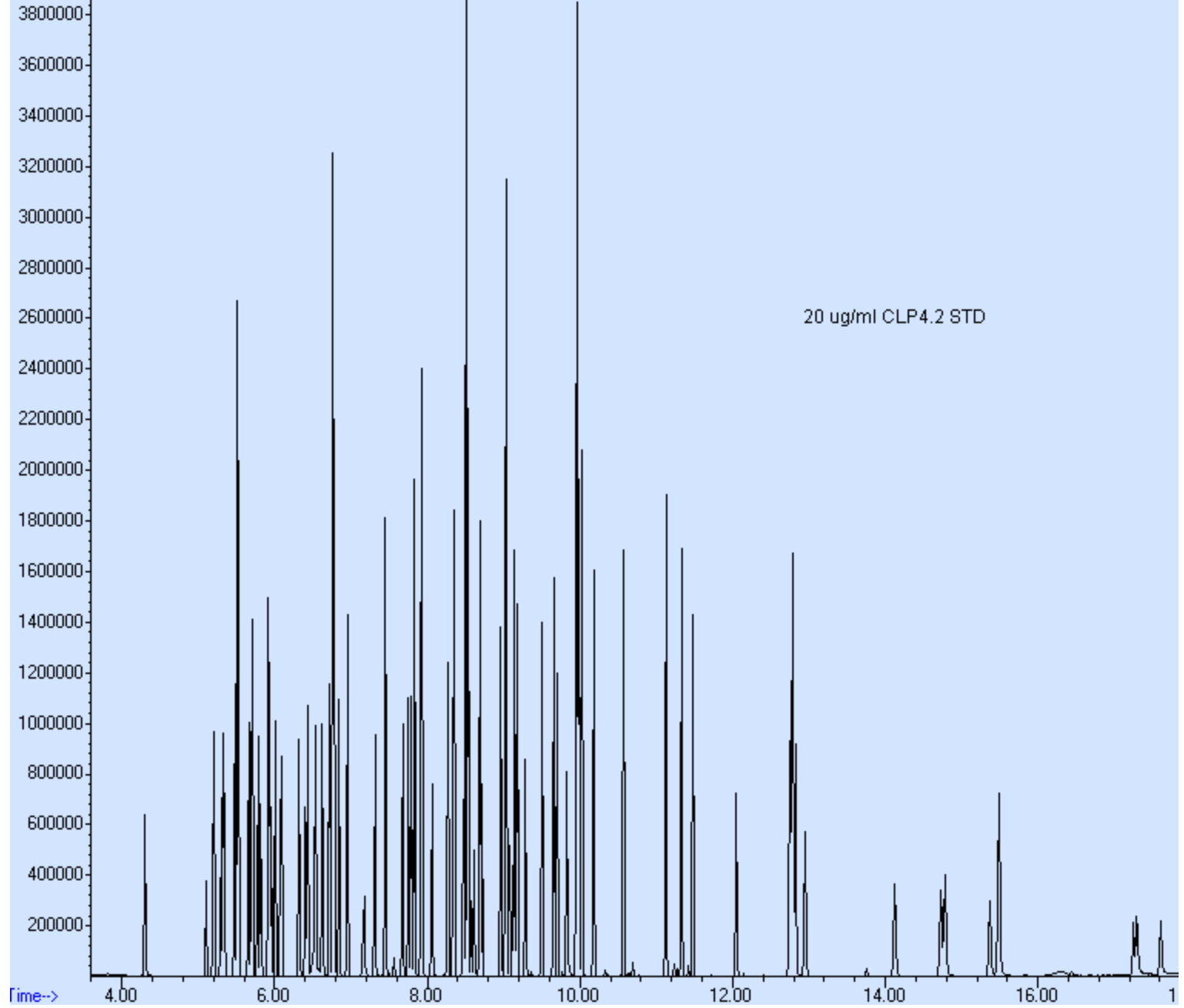
Different compound lists

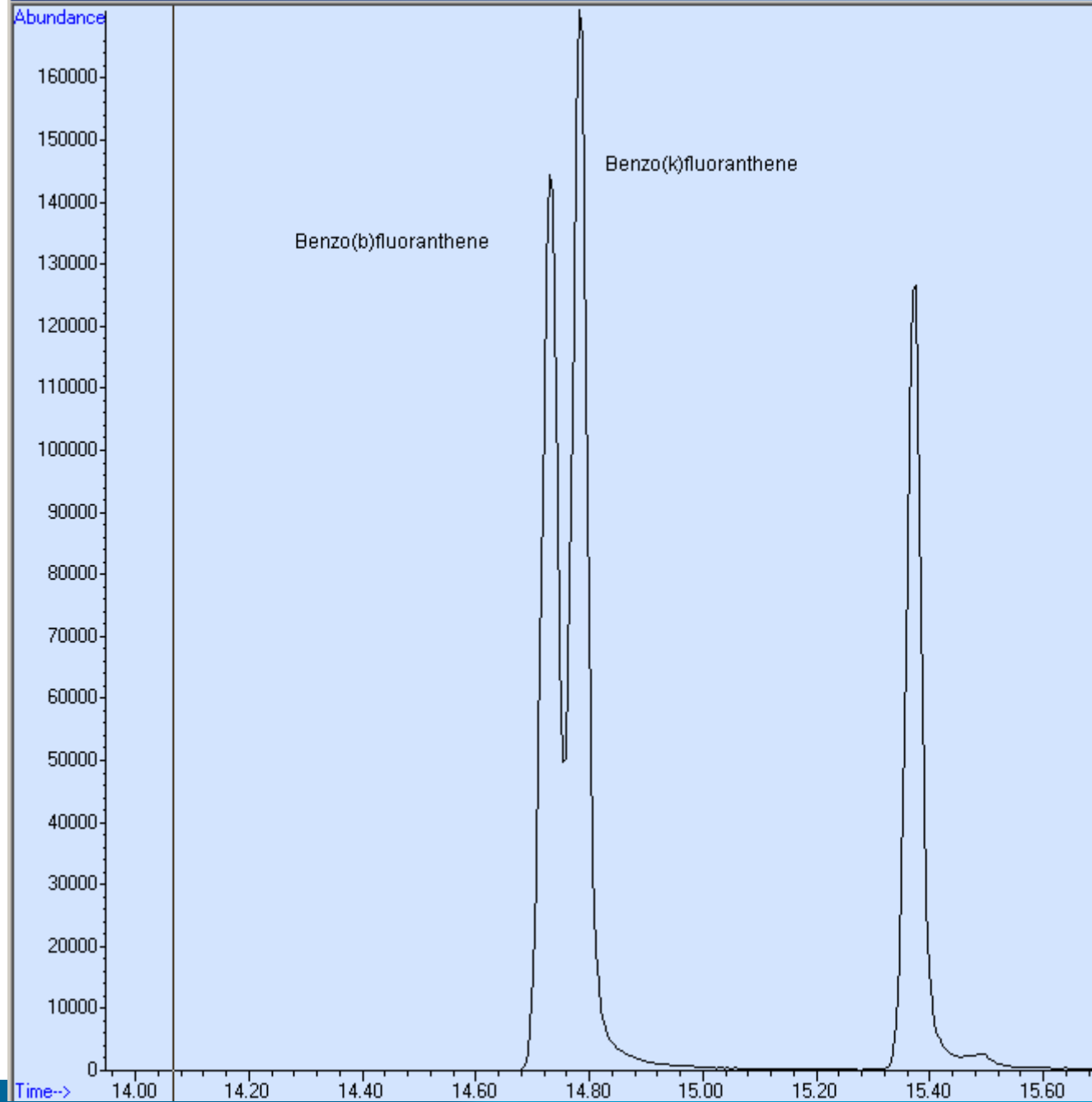
Different calibration ranges

For example: High	2 – 100 ug/ml
Low	0.1 – 10 ug/ml

Different reporting limits

Data shown is from EPA Region 6 Lab in Houston





Performance Data – most critical: ical & Perf Eval

Compound	100	80	50	20	10	5	2	Avg	%RSD
1) I 1,4-Dichlorobenzen...	-----ISTD-----								
2) SCP 2-Fluorophenol...	1.013	1.001	0.994	0.999	1.000	1.013	0.983	1.000	1.04
3) SCP Phenol-d5 (surr2)	1.237	1.221	1.231	1.247	1.225	1.235	1.233	1.233	0.68
4) MCP Phenol	1.275	1.288	1.289	1.301	1.304	1.310	1.315	1.297	1.09
5) SCP 2-Chlorophenol...	1.179	1.161	1.168	1.177	1.177	1.172	1.169	1.172	0.53
6) TCP bis(2-Chloroet...	1.071	1.081	1.077	1.088	1.089	1.084	1.111	1.086	1.16
7) MCP 2-Chlorophenol	1.200	1.219	1.213	1.216	1.209	1.222	1.223	1.215	0.65
8) TCP 1,3-Dichlorobe...	1.399	1.417	1.412	1.418	1.407	1.439	1.447	1.420	1.22
9) MCP 1,4-Dichlorobe...	1.406	1.427	1.439	1.440	1.453	1.442	1.472	1.440	1.42
10) TCP Benzyl Alcohol	0.904	0.905	0.900	0.873	0.852	0.838	0.834	0.872	3.60
11) SCP 1,2-Dichlorobe...	0.832	0.844	0.842	0.861	0.861	0.875	0.893	0.858	2.45
12) TCP 1,2-Dichlorobe...	1.326	1.353	1.366	1.369	1.376	1.385	1.398	1.368	1.70
13) TCP 2-Methylphenol	0.959	0.972	0.975	1.000	0.988	0.972	1.000	0.981	1.60
14) TCP bis(2-Chlorois...	1.110	1.153	1.174	1.209	1.203	1.219	1.266	1.191	4.23
15) TCP Acetophenone	1.539	1.535	1.541	1.577	1.554	1.569	1.618	1.562	1.89
16) TCP 3-&/or 4-Methy...	1.284	1.293	1.287	1.310	1.287	1.301	1.299	1.294	0.73
17) MCP N-Nitroso-di-p...	0.748	0.759	0.758	0.769	0.754	0.754	0.781	0.761	1.46
18) TCP Hexachloroethane	0.487	0.505	0.505	0.502	0.501	0.512	0.518	0.504	1.91
19) I Naphthalene-d8 (IS...	-----ISTD-----								
20) SCP Nitrobenzene--...	0.294	0.297	0.297	0.298	0.305	0.303	0.307	0.300	1.60
21) TCP Nitrobenzene	0.299	0.304	0.308	0.307	0.317	0.317	0.319	0.310	2.48
22) TCP Isophorone	0.548	0.547	0.543	0.541	0.549	0.547	0.556	0.547	0.93
23) TCP 2-Nitrophenol	0.177	0.182	0.180	0.174	0.171	0.165	0.154	0.172	5.78
24) TCP 2,4-Dimethylph...	0.265	0.268	0.266	0.255	0.260	0.264	0.264	0.263	1.58
25) TCP bis(2-Chloroet...	0.354	0.357	0.358	0.359	0.361	0.365	0.368	0.360	1.34
26) TCP Benzoic Acid	0.165	0.193	0.178	0.144	0.097	0.060	0.032	0.124	50.01#
27) TCP 2,4-Dichloroph...	0.292	0.293	0.290	0.284	0.282	0.276	0.268	0.283	3.20
28) MCP 1,2,4-Trichlor...	0.333	0.336	0.337	0.333	0.341	0.340	0.342	0.337	1.13
29) TCP Naphthalene	0.900	0.919	0.928	0.938	0.954	0.972	0.987	0.943	3.23
30) TCP 4-Chloroaniline	0.374	0.376	0.374	0.369	0.359	0.347	0.304	0.357	7.23
31) TCP Hexachlorbutad...	0.210	0.211	0.210	0.207	0.210	0.212	0.213	0.211	0.89
32) TCP Caprolactam	0.068	0.068	0.079	0.076	0.073	0.069	0.065	0.071	7.15
33) MCP 4-Chloro-3-met...	0.260	0.258	0.254	0.248	0.241	0.235	0.235	0.247	4.26
34) TCP 2-Methylnaphth...	0.556	0.562	0.564	0.560	0.565	0.565	0.585	0.565	1.68

Software – Both Chemstation and Mass Hunter

Chemstation - Enviroquant

Classical tools for analysis and reporting

Mass Hunter

New platform with new capabilities

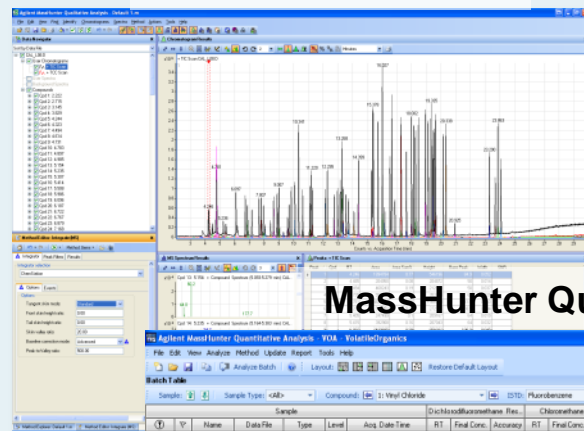
Batch mode calibration tools

All Agilent MS platforms (GCMS, GC-QQQ, LCMS, ICP-MS)

GC/MSD Software



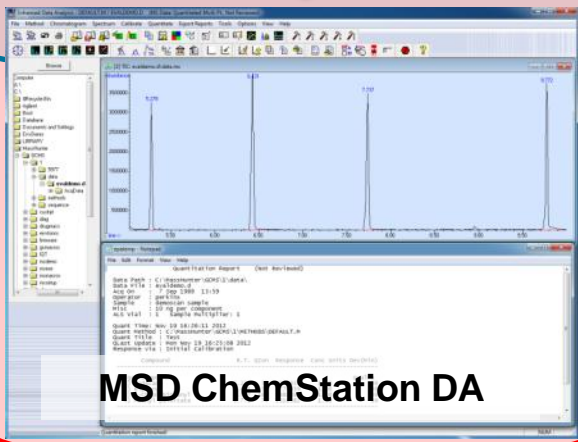
MassHunter Qual



MassHunter Quant

The MassHunter Quant software interface displays a data table with columns for Sample, Name, Data File, Type, Level, Acq. Date/Time, Dichloromethane Results, Chloroform Results, Vinyl Chloride Results, and Benzene Results. The table contains multiple rows of data for various samples and compounds.

Sample	Name	Data File	Type	Level	Acq. Date/Time	Dichloromethane Results	Chloroform Results	Vinyl Chloride Results	Benzene Results								
1	CAL_L03	CAL_L03.D	Cal	3	6/20/2008 4:53 AM	4.237	0.1755	14.4	4.490	0.2574	570	5.231	1.0162	203.9			
2	CAL_L04	CAL_L04.D	Cal	4	6/20/2008 9:20 AM	4.261	0.7450	14.4	4.432	1.0026	100.4	4.728	0.7992	740	5.237	1.2902	130.8
3	CAL_L05	CAL_L05.D	Cal	5	6/20/2008 8:06 AM	4.248	1.7252	46.8	4.470	0.7826	103.5	4.721	1.7260	251.3	3.259	2.4502	124.8
4	CAL_L06	CAL_L06.D	Cal	6	6/20/2008 4:44 AM	4.267	4.5071	90.58	4.496	0.9113	115.2	4.720	4.8911	670.9	6.240	5.2638	159.3
5	CAL_L07	CAL_L07.D	Cal	7	6/20/2008 7:21 AM	4.269	10.2071	103.1	4.493	4.730	0.8101	96.2	5.231	6.3125	93.1		
6	CAL_L08	CAL_L08.D	Cal	8	6/20/2008 3:04 AM	4.244	15.1922	126.51	4.494	15.1203	101.3	4.725	15.4384	103.9	5.225	13.3244	95.2
7	CAL_L09	CAL_L09.D	Cal	9	6/20/2008 8:41 AM	4.240	20.2929	101.5	4.484	15.5605	97.0	4.719	20.6427	103.2	5.240	20.9922	103.8
8	CAL_L10	CAL_L10.D	Cal	10	6/20/2008 9:19 AM	4.265	29.791	99	4.489	20.2294	97.6	4.726	20.2257	103.9	5.229	21.4263	101.4
9	CAL_L11	CAL_L11.D	Cal	11	6/20/2008 8:59 AM	4.260	46.8998	102.61	4.493	25.1868	98.11	4.725	46.9464	102.4	5.227	25.6464	95.1
10	CAL_L12	CAL_L12.D	Cal	12	6/20/2008 10:35 AM	4.246	48.9354	97.9	4.489	55.1927	102.4	4.722	48.7623	97.6	5.226	50.5471	101.1
11	CAL_L13	CAL_L13.D	Cal	13	6/20/2008 11:13 AM	4.247	10.1253	4.493	10.1248	4.765	10.6784	4.764	10.6784	4.764	10.6784	4.764	10.6784
12	QC_L06	QC_L06.D	QC	6	6/20/2008 11:50 AM	4.240	2.6322	61.4	4.493	4.2648	95.3	4.729	4.8199	88.4	5.225	3.9632	70.1
13	Blank01	BLANK01.D	Blank	6/20/2008 12:28 PM	4.499	0.0416	4.738	0.1991	5.256	1.2038							
14	Blank02	BLANK02.D	Blank	6/20/2008 1:07 PM	4.482	0.2476	4.722	0.0000	5.120	0.8479							
15	SAMPLE01	SAMPLE01.D	Sample	6/20/2008 1:44 PM	4.500	0.29237	4.740	0.1038	5.295	0.9868							
16	SAMPLE02	SAMPLE02.D	Sample	6/20/2008 2:22 PM	4.496	0.1038	4.740	0.1038	5.145	0.9011							
17	SAMPLE03	SAMPLE03.D	Sample	6/20/2008 3:08 PM	4.491	0.2923	4.740	0.2923	5.262	1.1762							
18	SAMPLE04	SAMPLE04.D	Sample	6/20/2008 3:38 PM	4.471	0.1729	4.740	0.1729	5.262	1.0291							
19	SAMPLE05	SAMPLE05.D	Sample	6/20/2008 4:18 PM	4.496	0.2624	4.734	0.2624	5.265	0.9061							



MSD ChemStation DA

MassHunter GC/MS Acquisition

And Use Either
MassHunter Data Analysis

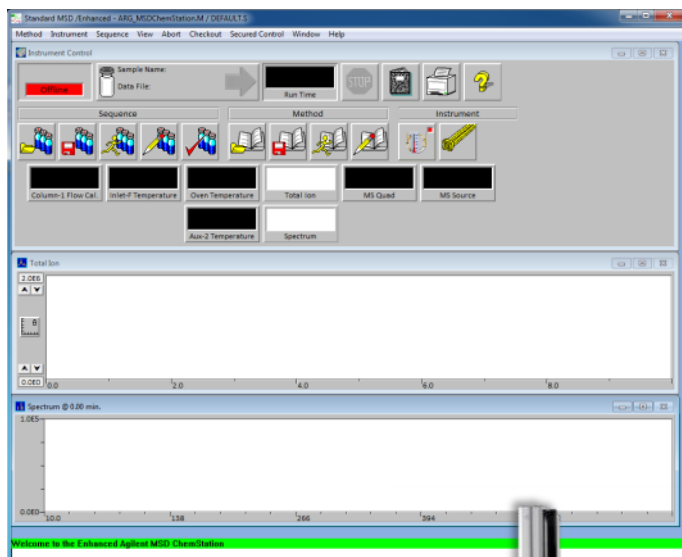
OR

MSD ChemStation Data Analysis

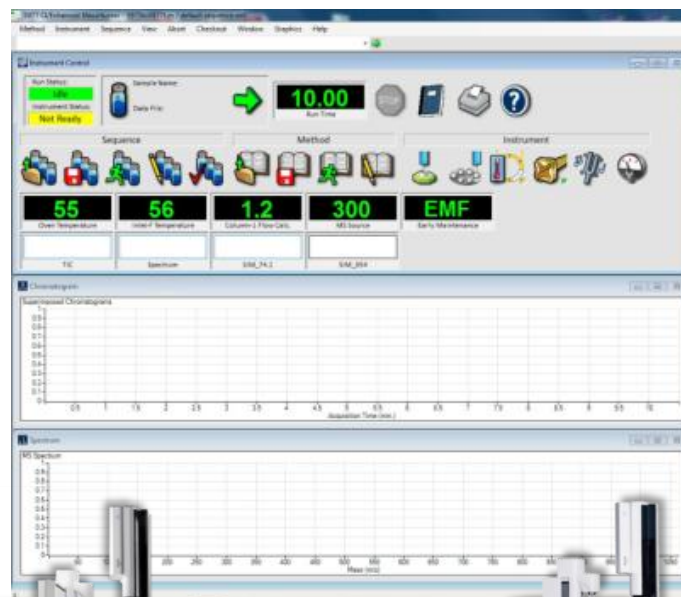
G1701FA

GC/MSD Acquisition Methods

MSD Productivity ChemStation



MassHunter GC/MS Acquisition



GC/MS Acquisition Methods are Transparent
from MSD ChemStation to MassHunter GC/MS (Except PAL Autosampler)

Agilent Inert Flow Path Solution

Ultimetal Plus Inlet Weldment, Shell and Transfer Lines



Ultra Inert Inlet Liner



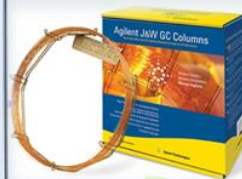
Ultimetal Plus Ferrules



Ultimetal Capillary Flow Technology Devices, Ultimate Union



Ultra Inert Gold Seal



Ultra Inert GC Column



Inert Flow Path Split/Splitless Inlet

UltiMetal Plus treatment creates inert surface
7890 inlet weldment & shell

- Limit adsorption / degradation active analytes in contact with hot metal
- Target trace GC/MS active compound analysis
- Combine with Agilent's UI Liners, UI gold seals, UI GC columns



UltiMetal Plus surface treatment

Helium Shortage Issue

What can we do?

- There are only two realistic choices:
 - Switch to a different carrier gas such as Hydrogen
 - Implement Helium conservation measures

Hydrogen Carrier – brief summary

Agilent has advised H₂ carrier for 8270 for over 15 years

Mainly for faster runs and better GC resolution

Easy to convert with a little guidance

Use a 20m x 0.18 column with 0.5 ml/min flow

Set inlet temp to 230C (avoids HCl formation with MeCl₂)

EPA Region 8 in Golden, Co has been using H₂ for over a year

Both for VOA's and 8270

But methods have to be re-validated – new RT's

New Approach: Helium Conservation

While the GC is just sitting there, it is blowing gas out the vents 24/7

- Minimum flow is about 25 ml/min per S/SL inlet
- $1440 \text{ min/day} \times 25 \text{ ml} = 36,000 \text{ ml/day} = 36 \text{ liters/day}$ per inlet

If the GC is idle, you can switch to a cheaper standby gas such as nitrogen

- Helium cost is 17 cents per cubic foot, N₂ is 0.03 cents per cubic foot (prices vary by area)
- Cheapest source of N₂ is liquid LN₂ dewars

Nitrogen Switching

- Manual valve (any GC)
- Electronic valve (5890, 6890, 7890)
- Fully Automatic EPC (7890B option) (7890A in July)

Helium Conservation Tools

Helium Conservation

- Smarter helium use with new hardware/software tools
- No need to revalidate existing GCMS methods
 - RT's are the same
 - Performance is the same

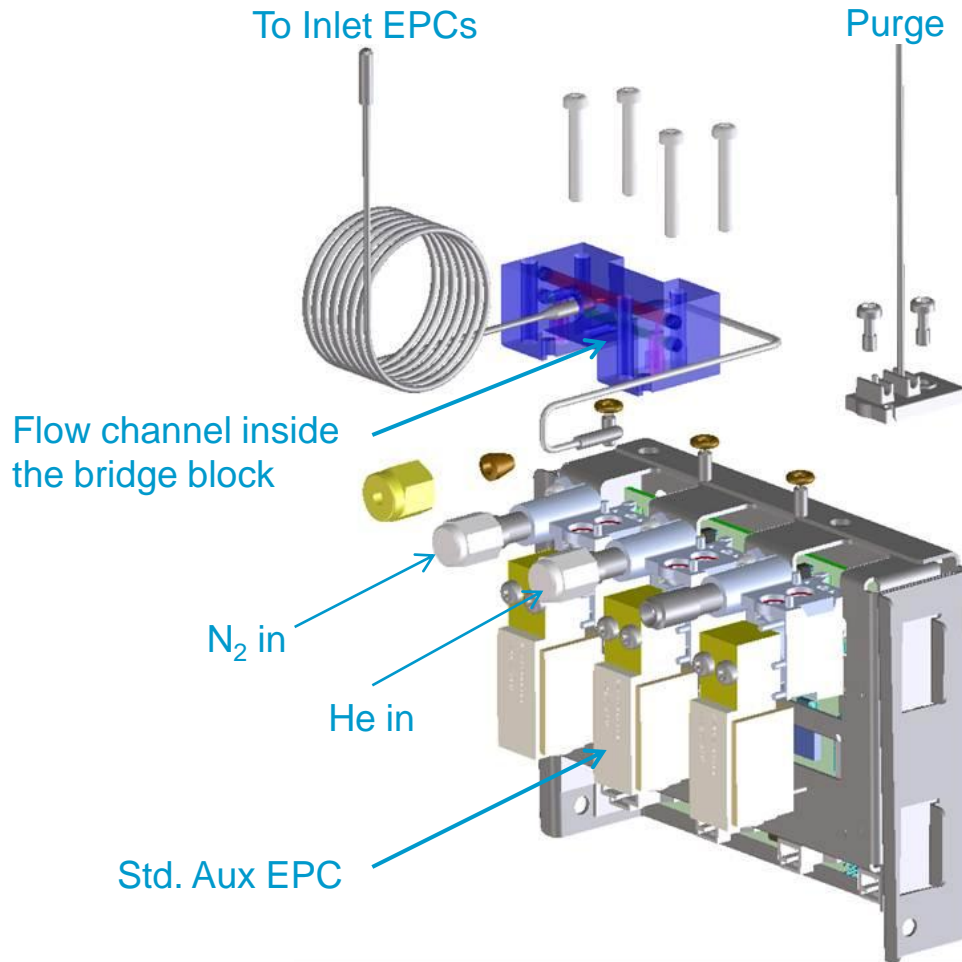
Reducing Helium Use With Conservation

New 7890B Helium Conservation Module

- Automatically switches carrier gas supply to N₂ Standby during idle time
- Integrates into the new 7890B Sleep and Wake function
- Combined with Helium Gas Saver to ***GREATLY*** reduce helium consumption

Helium Conservation Module

Seamlessly integrated onto 7890 GC hardware and software



- Based on EPC module
- Fully controlled by Agilent data systems
- Precise pressure control between tank and GC
- Switch between gases within 2-5 min depending on flow setting

How It Works: Configuring Sleep/Wake Operation

Simple, Straight Forward Setup

Agilent 7890B Configuration: Instrument 1

Connection Configuration **Resource Conservation**

Reduce gas and power consumption by setting gas saver and instrument schedule options

Instrument Schedule

Select a schedule that best matches how you use this instrument:

Custom

Schedule

Day	Set Wake Method	Wake Time	Set Sleep Method	Sleep Time
Sunday	<input type="checkbox"/>		<input type="checkbox"/>	
Monday	<input type="checkbox"/>		<input type="checkbox"/>	
Tuesday	<input type="checkbox"/>		<input type="checkbox"/>	
Wednesday	<input type="checkbox"/>		<input type="checkbox"/>	
Thursday	<input type="checkbox"/>		<input type="checkbox"/>	
Friday	<input type="checkbox"/>		<input type="checkbox"/>	
Saturday	<input type="checkbox"/>		<input type="checkbox"/>	

Wake Method: Sleep Method:

Wake to last active method before sleep

Perform a conditioning run on Wake

Future Developments

Self-cleaning ion source

Improved PAH peak shape at 1.0 picogram levels

Micro-extraction with LVI

Acknowledgements

David Spencer, Diane Gregg

EPA Region 6 Houston, Tx

Vince Marti

EPA Region 8 Golden, Co

Call or email me for specific guidelines:

Fred Feyerherm

- fred_feyerherm@agilent.com
- 713-392-8493 cell