



5975 inert MSD



Agilent Technologies

What Has Changed?

What's the same?

- *Reliability*
- *Quality*
- *Inertness*



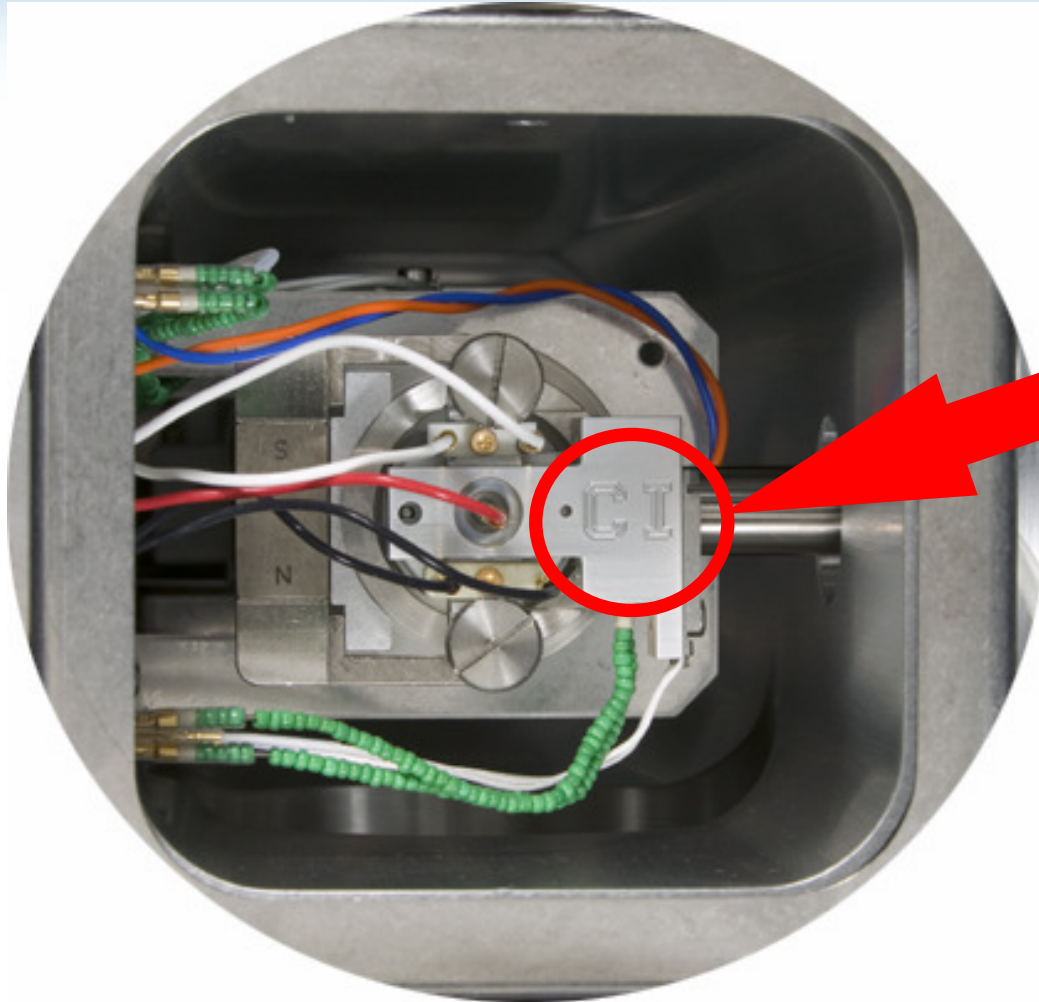
But NOT Performance – it's better!

What's Different?

- ***Functional industrial design***
- ***More efficient vacuum system***
- ***Extended mass range***
- ***AutoCI***
- ***New sensitivity specifications***
- ***Synchronous SIM/Scan***
- ***EI with CI ion source***
- ***6850 GC control***
- ***QuickSwap MSD interface***
- ***Review of differentiators***

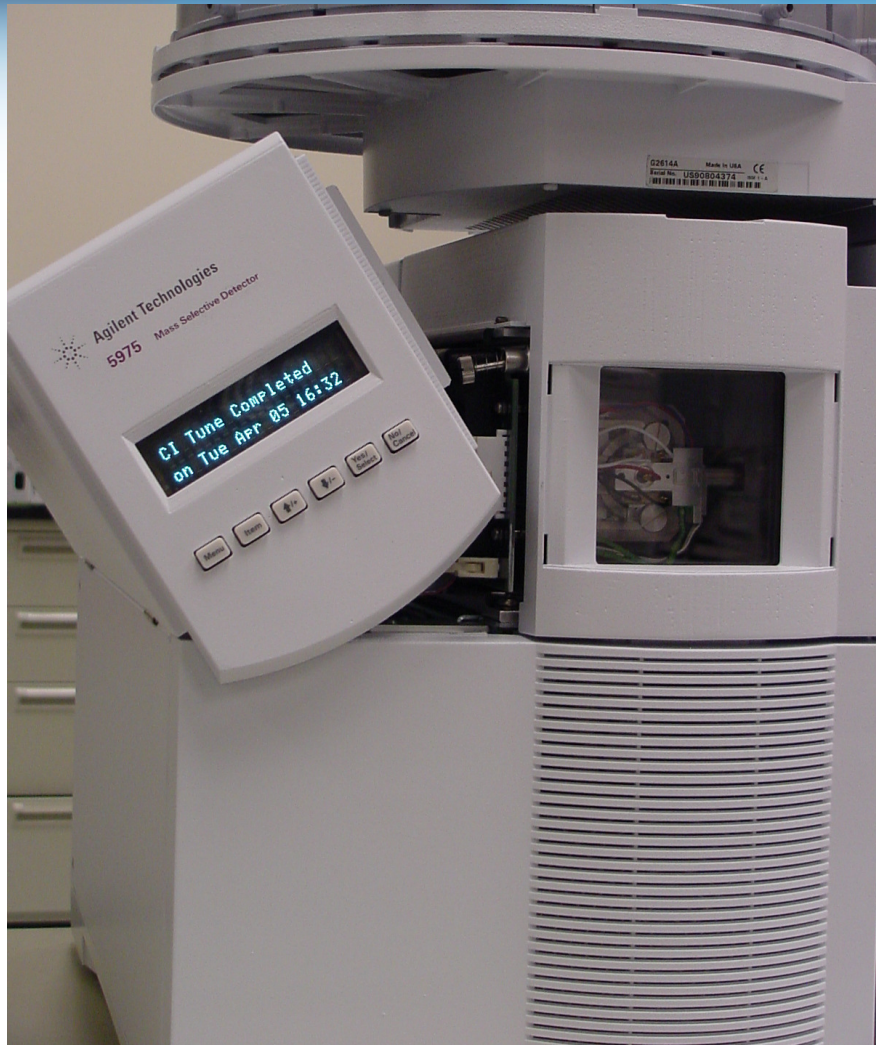


Functional Front Window



- **Wire connections**
- **Filament operation**
- **Column insertion**
- **CI Source identification**

Quick Remove Top Cover



Easy analyzer access

Modified Mainframe



Modified MSD mainframe
for quick/easy turbo pump
maintenance

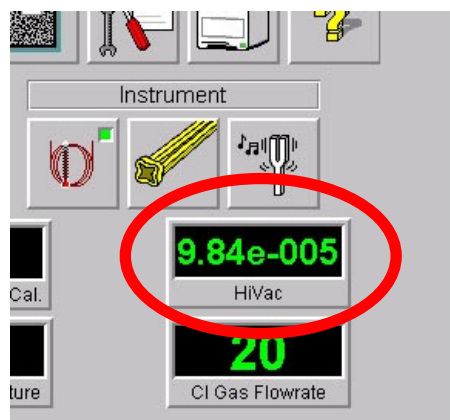
New turbo and mechanical vacuum
pumps are more efficient for Helium
and Hydrogen

- New 70 L/sec standard pump
- New 262 L/sec performance pump
- New 2.5 m³/hour mechanical pump
(67% more capacity)

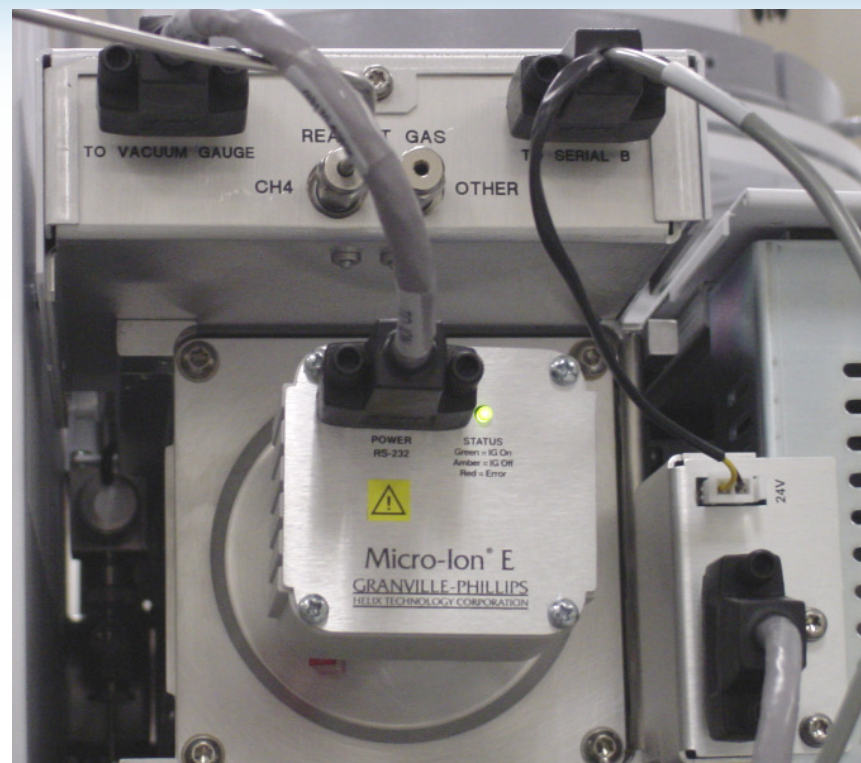


Integrated Ion Gauge/Controller

- **Greater vacuum precision**
- **Excellent for trouble shooting small leaks – every system should have one!**



Software display



G3397A – optional gauge/controller



Extended Mass Range

- **1050 m/z for 5975 inert MSD**

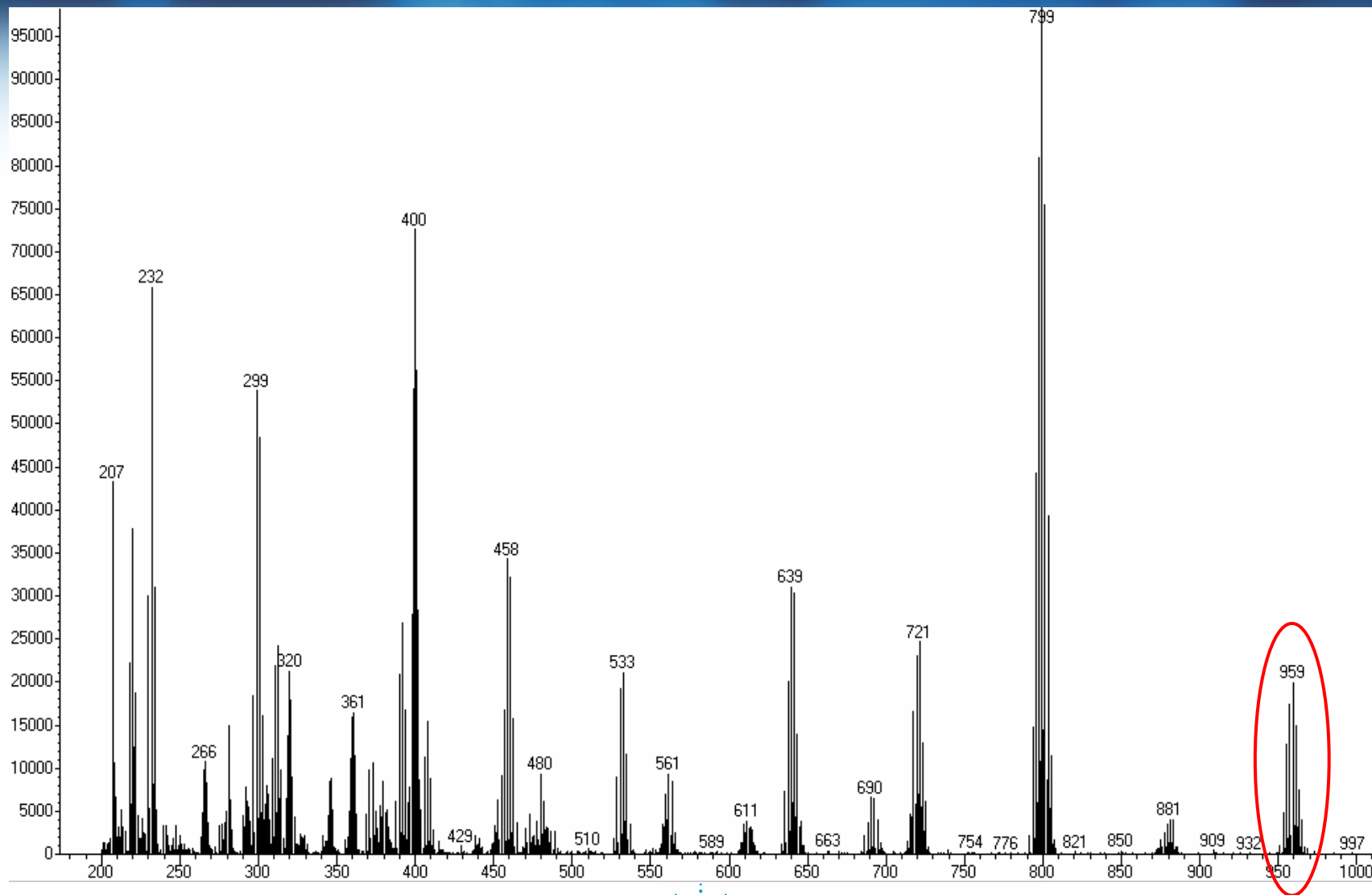
- Quadrupole modified
- New electronics

- **800 m/z for all 5973 MSDs**

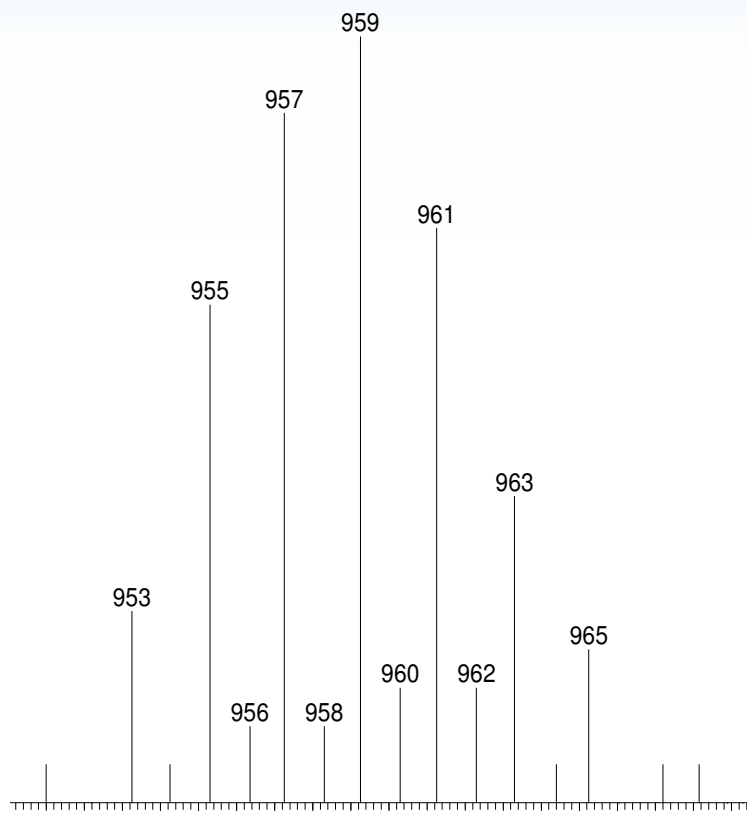
(Software upgrade does not enable 1050 m/z)



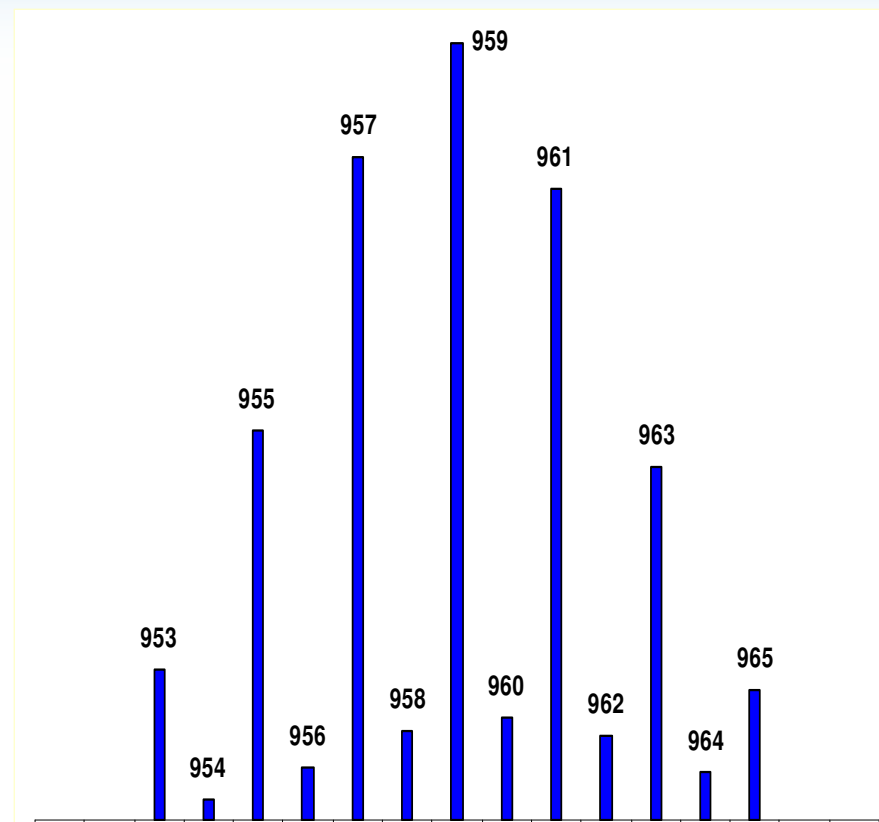
Extended Mass Range – PBDE 209



Extended Mass Range – PBDE 209



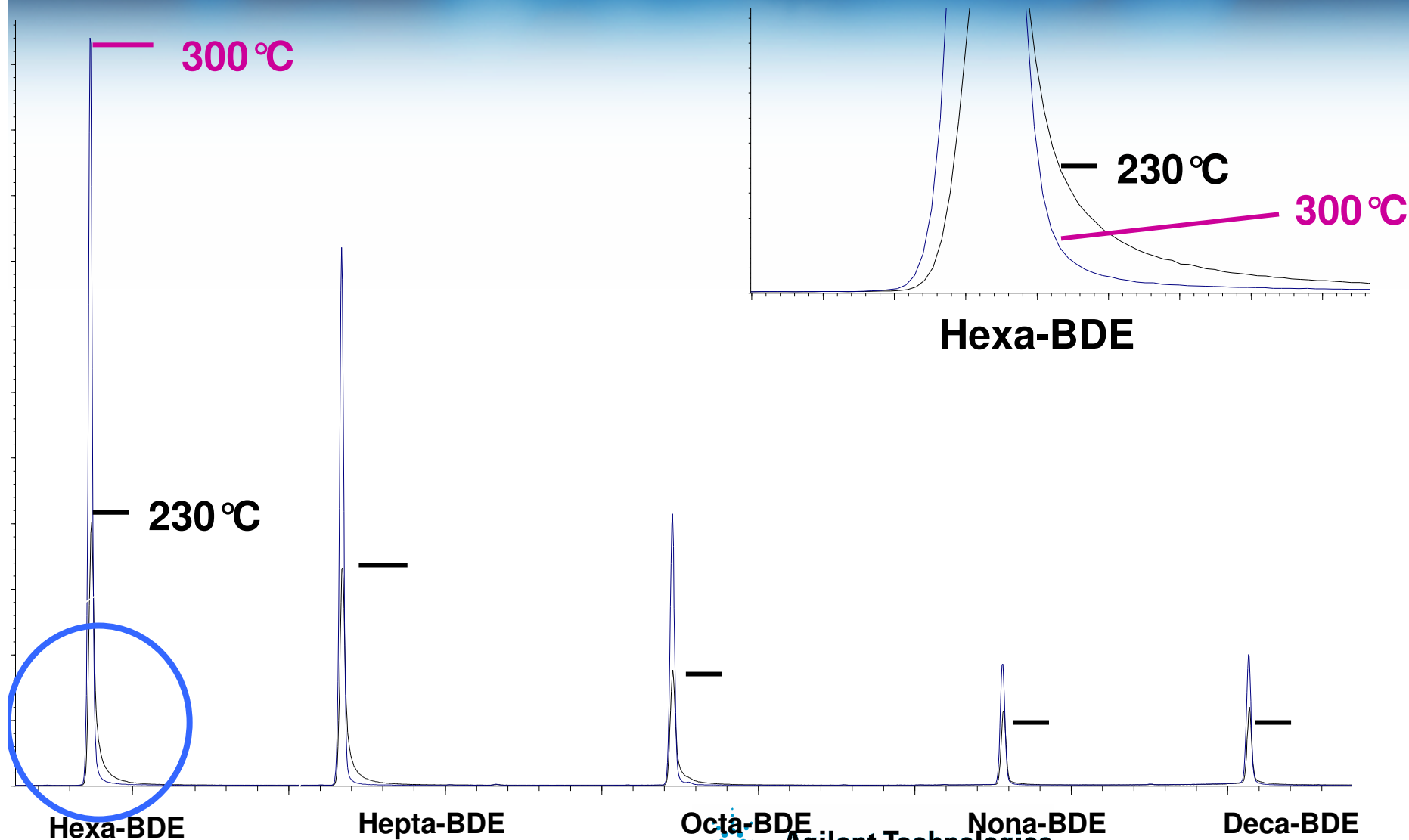
5975 inert MSD



Theoretical

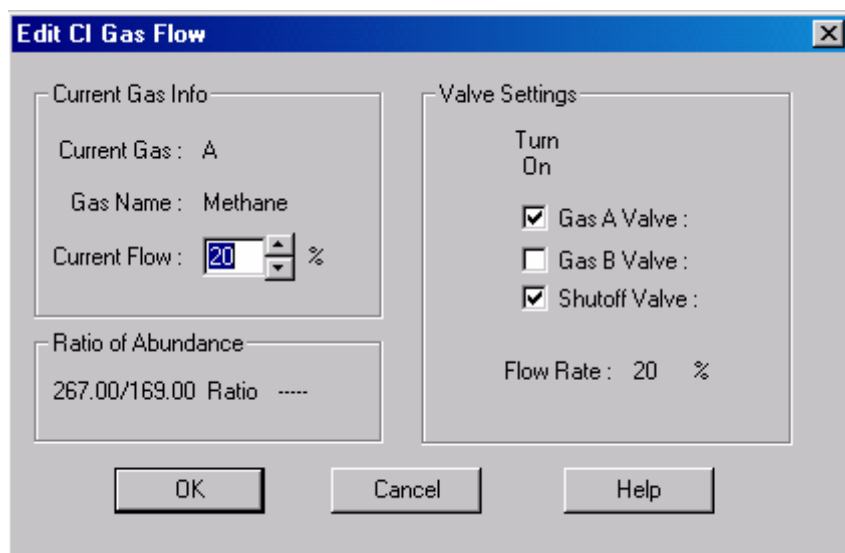


Comparing Source Temperatures – 230 °C vs 300 °C



AutoCI

- AutoCI – Fully automated setup/tuning
 - No external manual control
 - CI made as easy as EI!

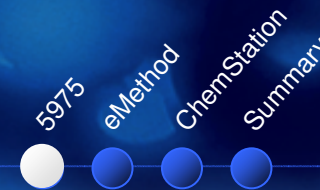


The new 5975
CI interface



The old 5973 manual
CI interface

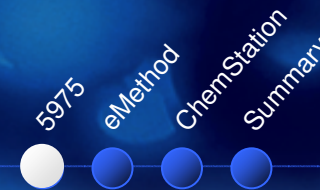
Automated EI with CI Source



- **March 2004:**
Application note on EI with CI ion source
- **Now:**
Automated switching between EI and CI in a sequence



Automated EI with CI Source

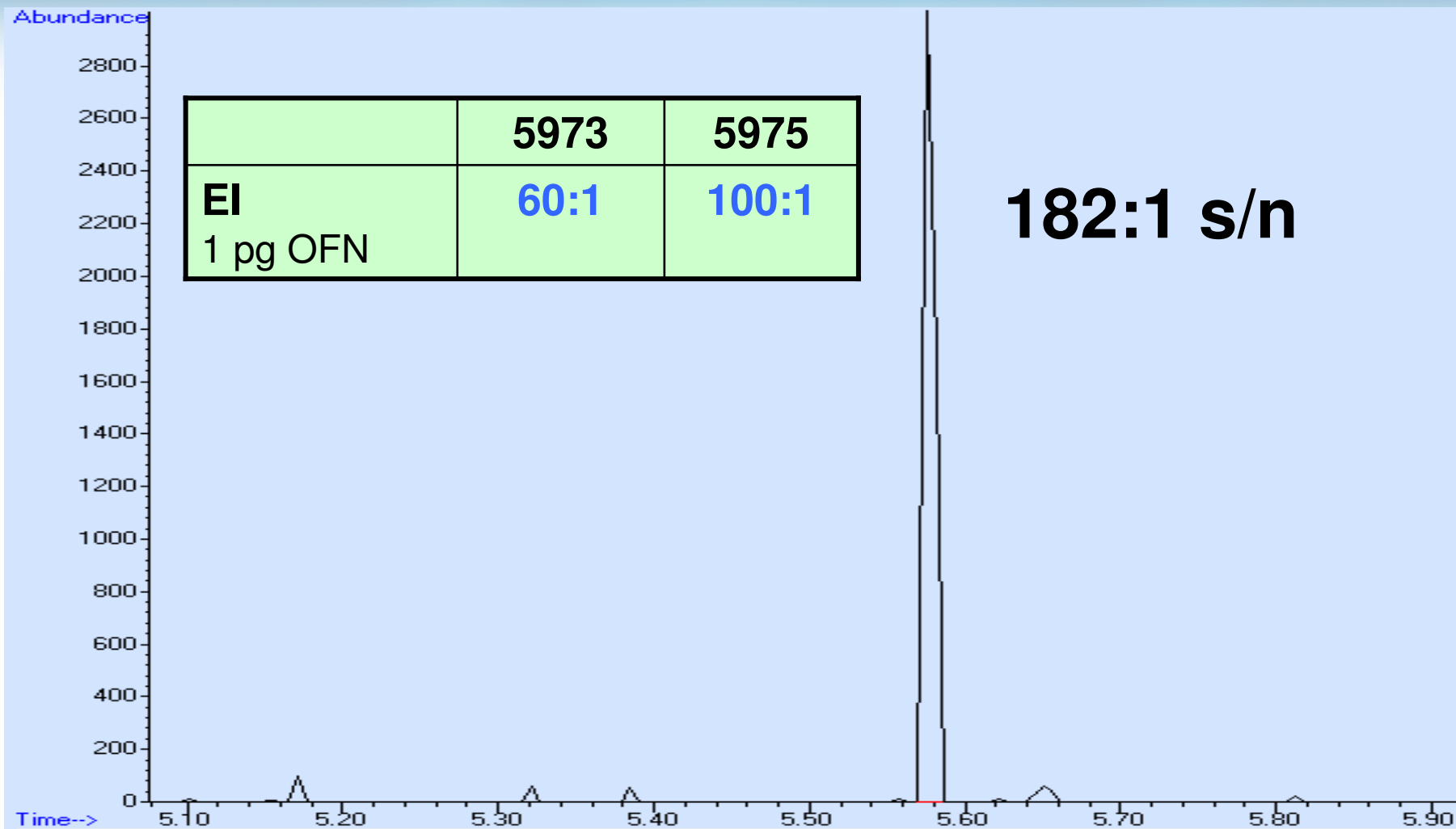


Setup steps:

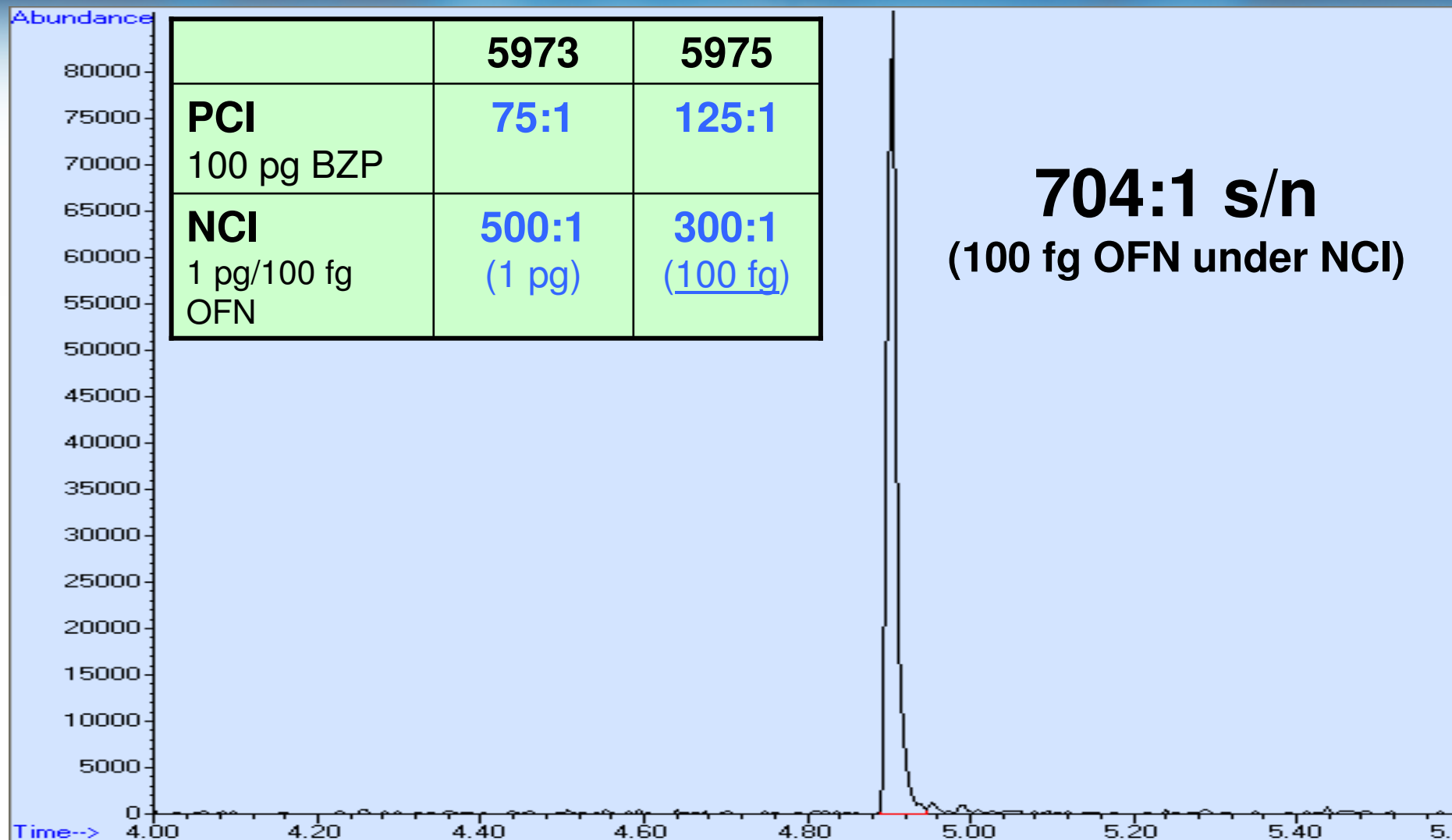
- 1. Tune instrument in PCI – create PCI_{CH4}.u***
- 2. Auto create EI tune file – create ei-cisource.u***
- 3. Tune instrument in NCI – NCI_{CH4}.u***
- 4. Assign tune file with method and run in sequence***



New Sensitivity Specifications – EI Scan



New Sensitivity Specifications – CI Scan



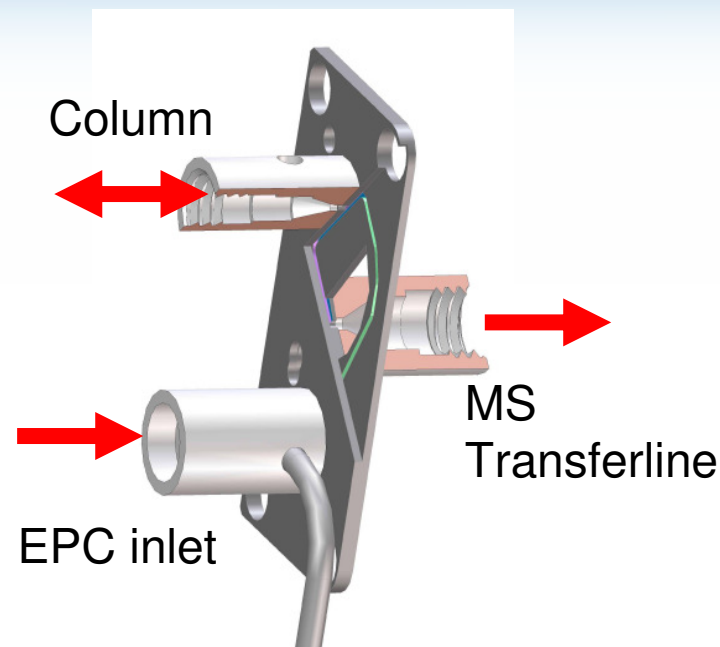
6850 GC Control via ChemStation

- **5973N MSD (G2570A)**
- **5973 inert MSDs**
- **5975 inert MSDs**



QuickSwap MSD interface

- ***Replacement for NoVent***
- ***Remove column w/o venting***
- ***Backflush mode***
- ***Inlet maintenance reverse flow***
- ***Removes heavies from column***
- ***Maintain constant flow to MSD***



Microfluidic technology

Requires performance turbo for flow rates > 2 cc/min

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Presentation

AUDIO INFORMATION

+44 20 7 182 0 125

e-Seminar

Slide 4 of 4

Question for Presenter:

There are no questions pending.

Question & Answer Session

Please type your question into the Question Box at any time during the presentation.

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Powered By Live Meeting

AutoSIM Setup for SIM/Scan

- ***Convert any scan method to SIM method***
- ***Automatic, no manual setup***

MS SIM/Scan Parameters

MS Instrument Parameters

Sample Inlet: GC

EM Voltage: 0 Rel = 1200

Solvent Delay: 3.00 min.

Acq. Mode: SIM

Acquire Scan and SIM data

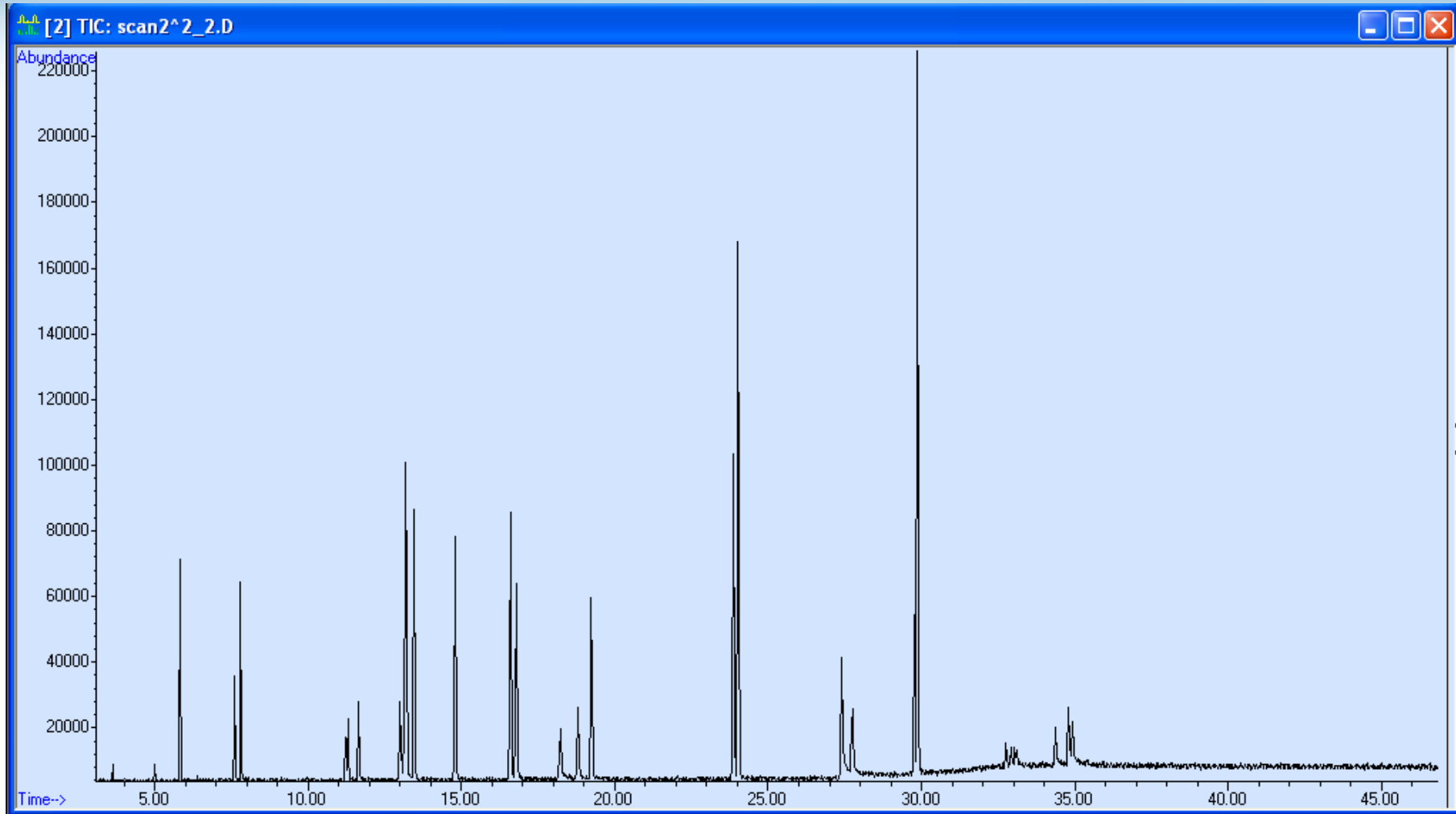
Tune File
ATUNE.U

Edit SIM Params Zone

OK Cancel



Inject Standard



Run AutoSIM

1. ***Load data file***
2. ***Run AutoSIM***

METHOD	CHROMATOGRAM
RUN METHOD...	
RUN CUSTOMANALYSIS	
<hr/>	
LOAD METHOD...	
SAVE METHOD...	
<hr/>	
EDIT METHOD...	
EDIT CUSTOMANALYSIS...	
<hr/>	
GENERATE AUTOSIM METHOD.	
EDIT SIM PARAMETERS...	
<hr/>	
1	
2	
3	
<hr/>	
BATCH MODE...	

Edit SIM Method

Enhanced Data Analysis - DEFAULT.M / SCAN2^2_2.D (MS Data: Not Quantitated)

File Method Chromatogram Spectrum Calibrate Quantitate Tools View Toolbars Help

Execute

Sim Group Table

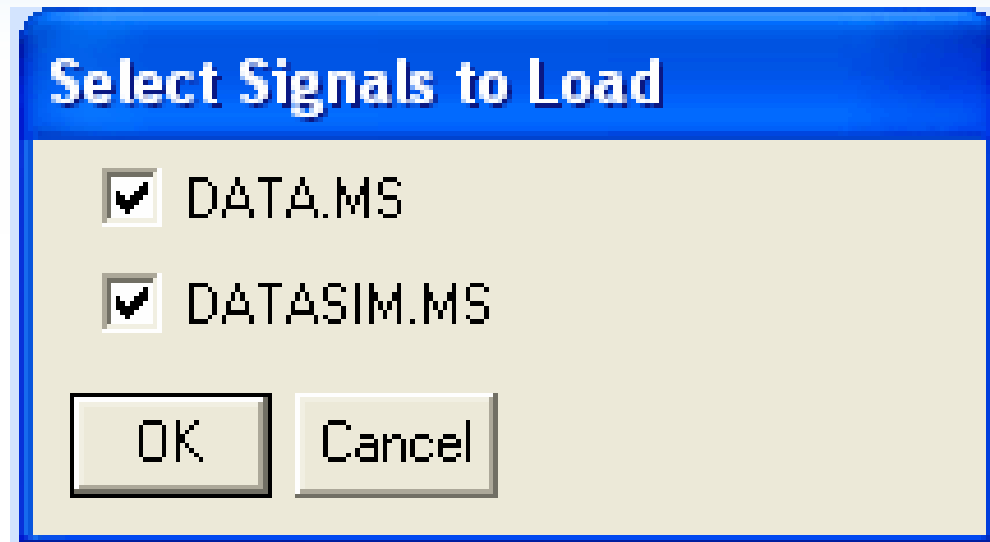
	Start Time (min)	Default Dwell (ms)	Group Label	Calc Cycles/Sec	Ion1	Ion2	Ion3	Ion4	Ion5	Ion6	Ion7	Ion8
1	3.043	85	Auto_1	2.5	180.85	182.85	216.85	218.85				
2	5.816	40	Auto_2	3.6	108.9	110.9	180.95	182.85	218.85			
3	6.298	95	Auto_3	2.2	180.95	182.85	216.85	218.85				
4	7.003	95	Auto_4	2.2	100	269.75	271.75	273.75				
5	7.826	125	Auto_5	1.8	66.05	260.75	262.8	264.8				
6	8.797	95	Auto_6	2.2	80.95	182.85	184.9	236.7				
7	9.773	95	Auto_7	2.2	194.85	236.8	238.8	240.8				
8	10.550	65	Auto_8	1.6	79.05	80.95	81.95	245.95	247.95	262.8	315.9	317.9
9	11.548	150	Auto_9	1.5	194.85	236.8	240.8	242.85				
10	12.146	180	Auto_10	1.3	165	234.95	236	237				
11	13.032	65	Auto_11	1.6	165	226.8	228.8	234.95	236	237	271.75	273.75
12												
13												
14												
15												
16												

Fill down using increment OK Cancel Help

AutoSIM automatically creates SIM groups and populates ions in each group

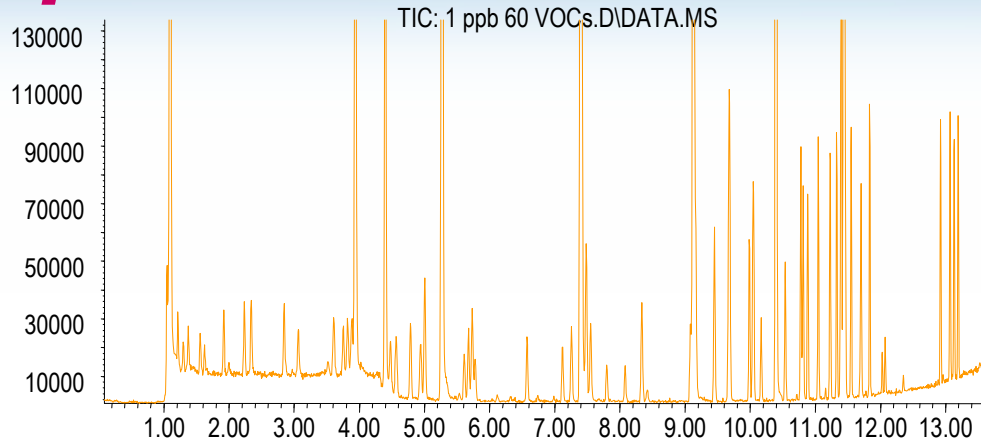
Set Up Synchronous SIM/Scan

- ***SIM/Scan data analysis requires mixed mode data view.***
- ***SIM/Scan data is saved in the same data file directory.***



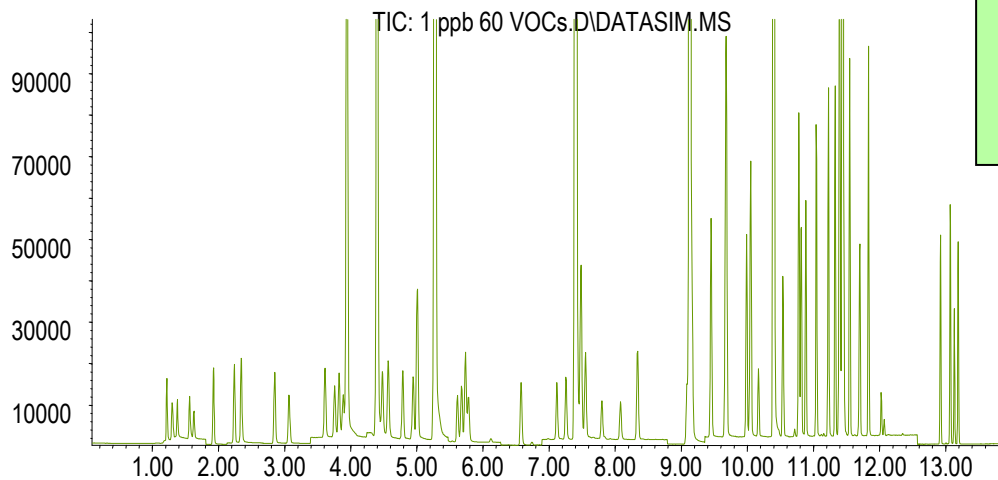
Scan and SIM Chromatograms from SIM/Scan Analysis of 60 VOCs at 1 ppb Each

Scan

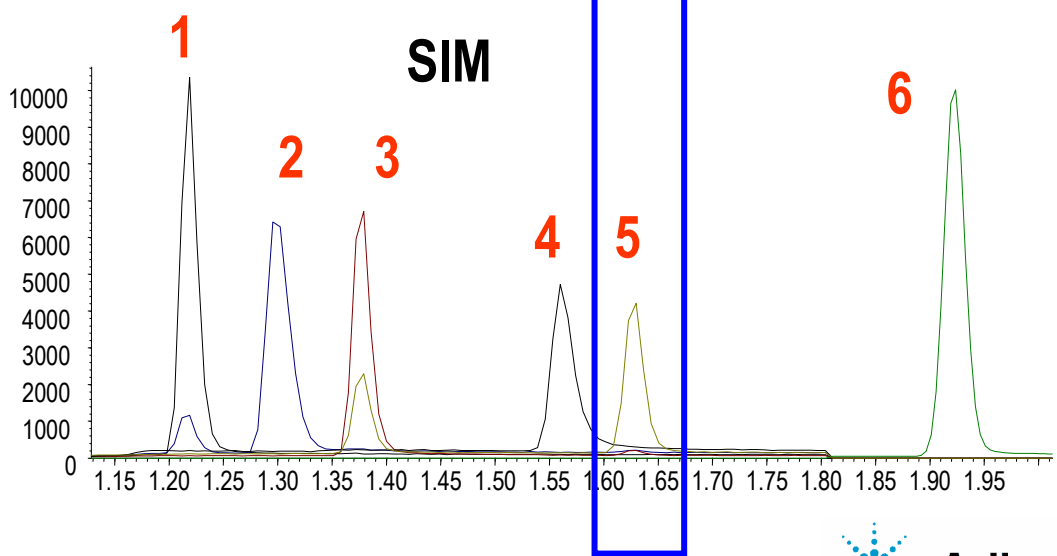
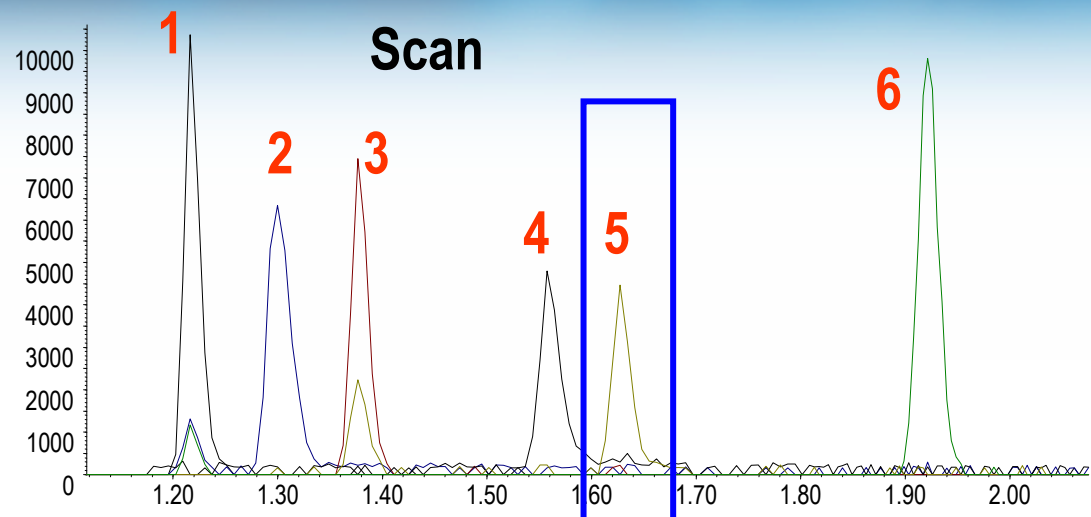


- Velocity XPT/6890N/5975 P&T/GC/MS system
- 20-m X 0.18 mm X 1.0 μ m DB-VRX column
- Scan sampling rate = 2; Dwell = 20 ms for SIM

SIM



Synchronous SIM/Scan Analysis of VOC Target Gases at 1 ppb each



- VOC Gases (1 ppb each)
- 1. Dichlorodifluoromethane
 - 2. Chloromethane
 - 3. Vinyl chloride
 - 4. Bromomethane
 - 5. Ethyl chloride**
 - 6. Trichlorofluoromethane

SIM/Scan and Scan-Only Sensitivity

Comparison: 5-mL Purge of 1 ppb

Ethyl Chloride (a Low Responding Gas)

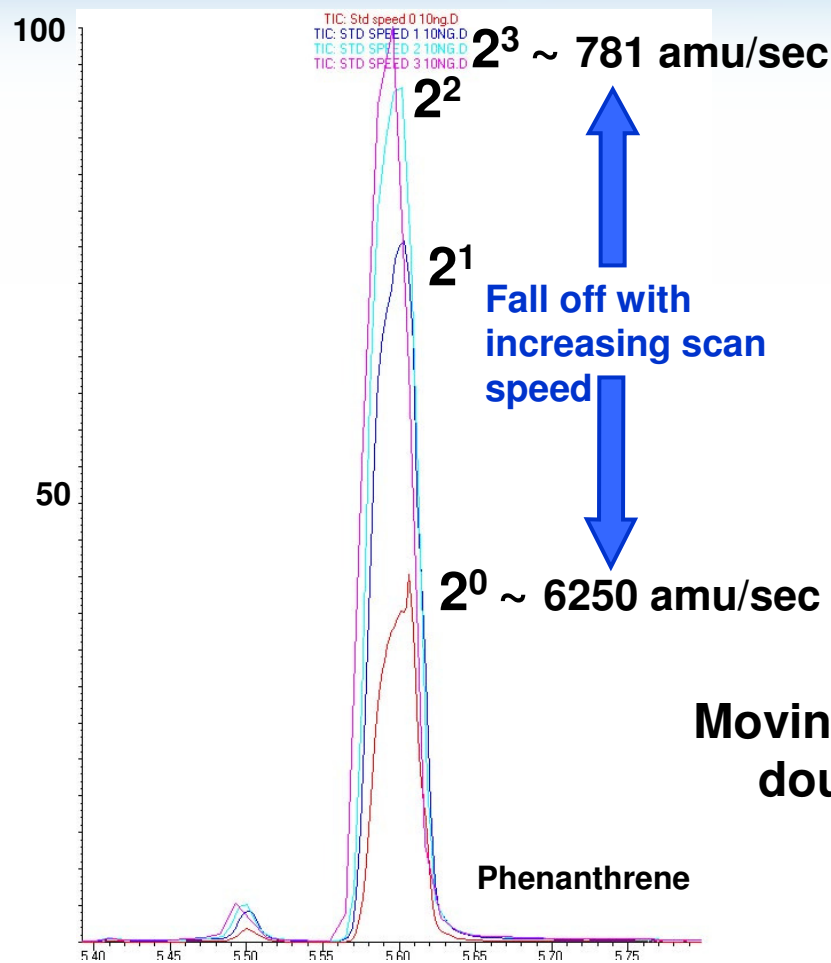
	<i>RMS S/N</i>	<i>Peak/Peak S/N</i>
<i>SIM</i> (SIM/Scan)	749	254
<i>Scan</i> (SIM/Scan)	75	20
<i>Scan</i> (Scan only)	73	17

- SIM as part of SIM/Scan run gives 10X greater sensitivity
- Still get ≥ 8 scans across peak using same scan rate ($n = 2$)

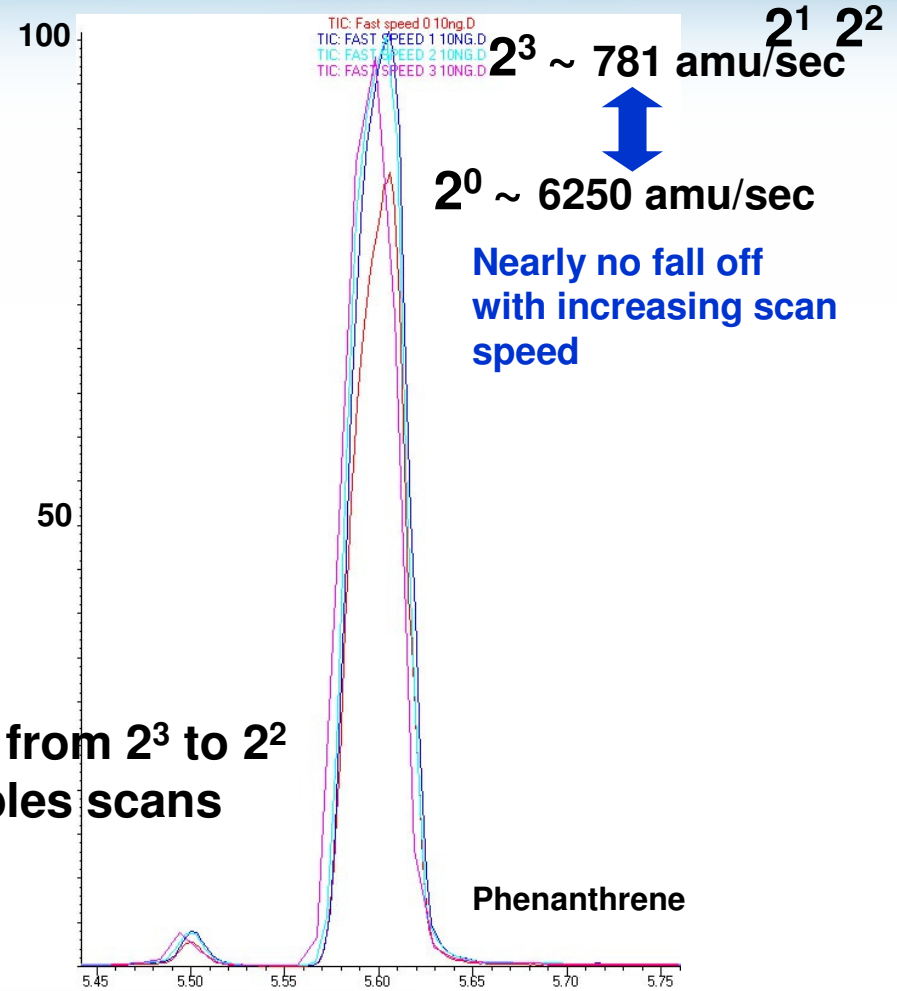


Why Our SIM/scan is So Good

Standard Electronics



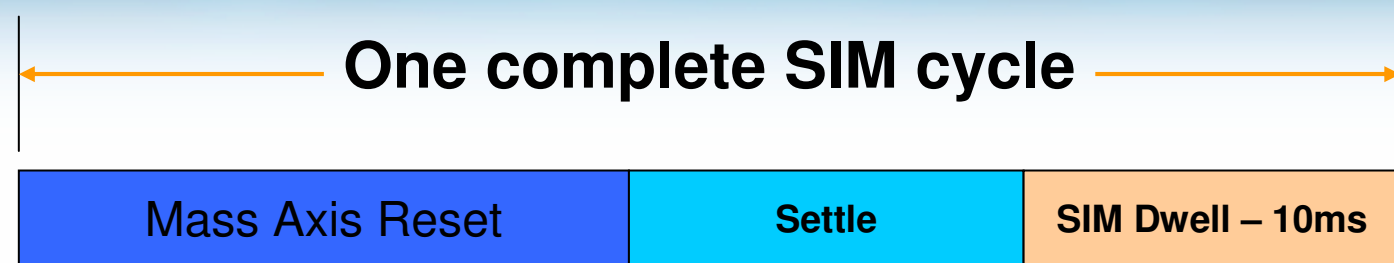
Performance Electronics



Moving from 2^3 to 2^2 doubles scans



Why Our SIM/scan is So Good



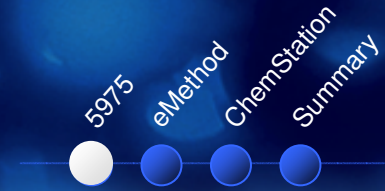
Standard Electronics

20% cycle efficiency improvement = more cycles

Performance Electronics = More Points



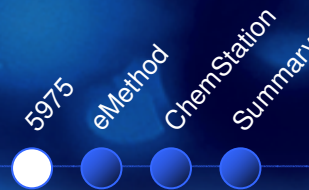
Synchronous SIM/Scan – Key Features



- ***Performance Electronics really make the difference***
- ***SIM Improvements – 100 groups and 60 ions per group***
- ***Minimum dwell time is reduced by half to 5 ms***
 - Even more data points per SIM peak
- ***Synchronous SIM/Scan available on 5973 MSDs with performance electronics (req. Smart Card 3+)***
 - Upgrades: G1088A and G1088B AND SW upgrade



Application examples



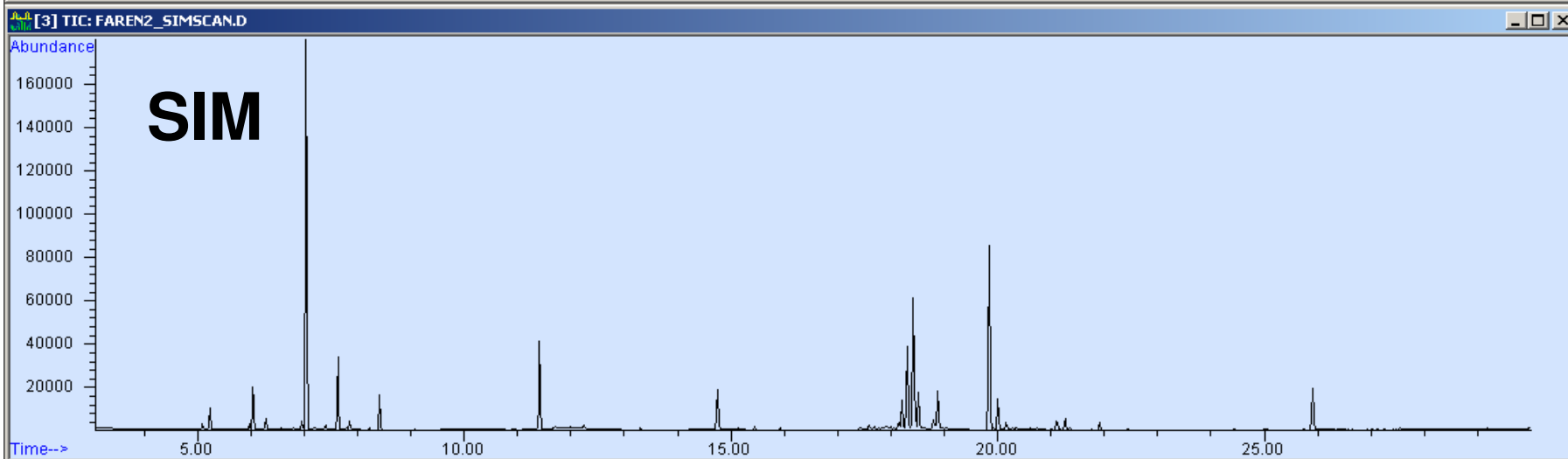
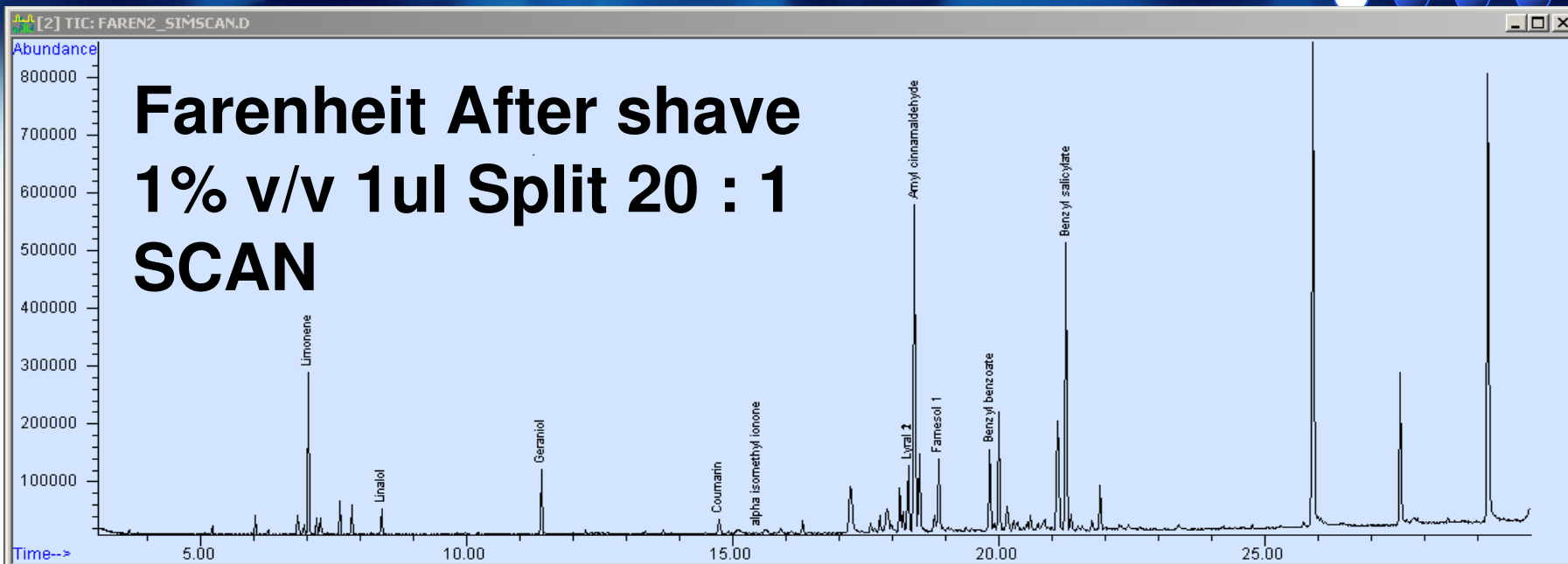
- **Allergens analysis: Proposed 5975 method, 26 Targets
SIM/Scan mode**

- **SIM table built with AUTOSIM**
- **Quant with SIM target ion**
- **Confirmation by DRS with Scan data**

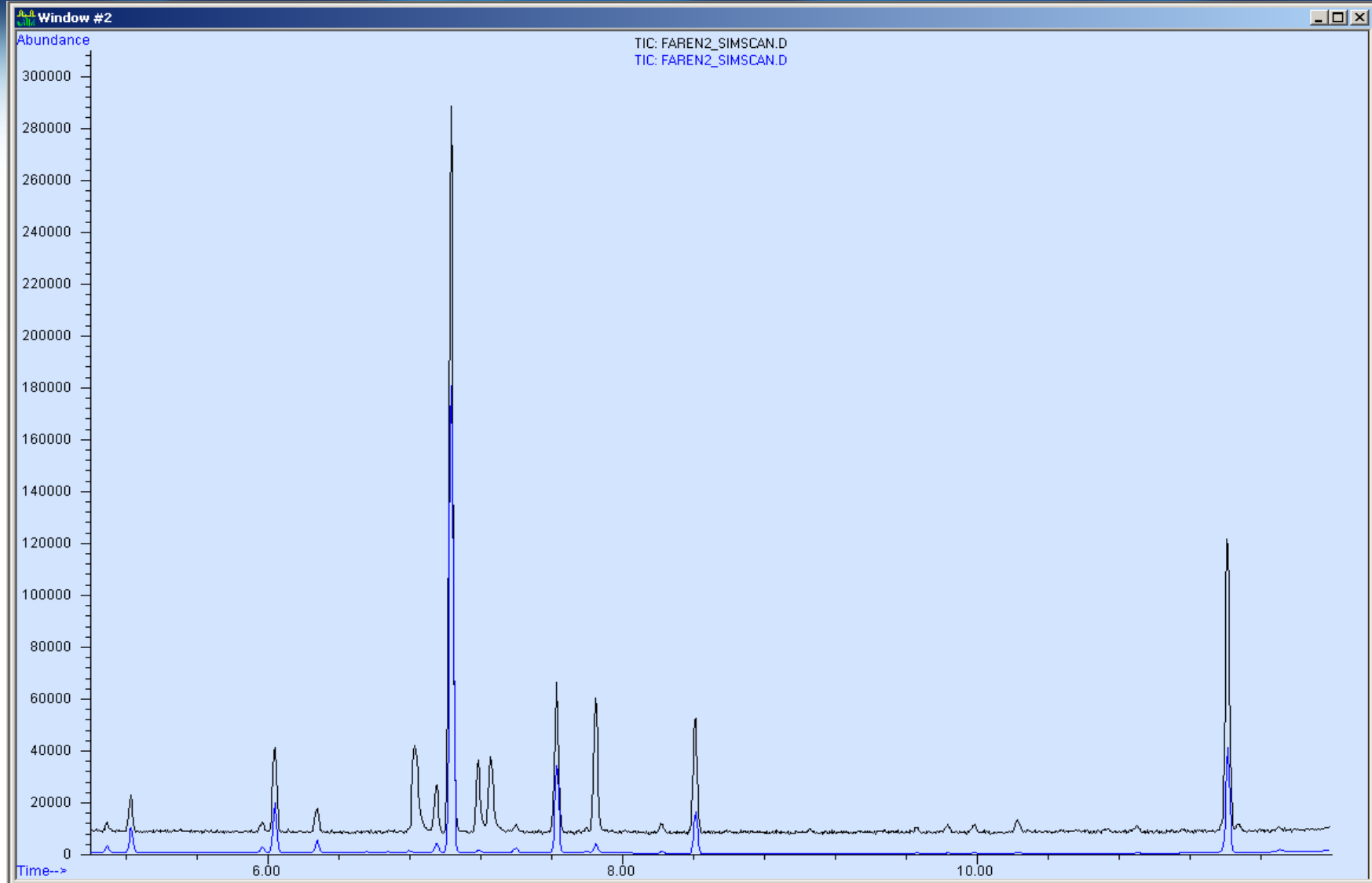
- **Pesticides analysis with microfluidics technology for
flexible GC and GC/MS analysis**



Allergens analysis in SIM/Scan



Allergens Overlaid SIM/Scan



Allergens SIM/Scan analysis and deconvolution with DRS

Match Factors

72 to 98

MSD Deconvolution Report
Sample Name: Farenheit After shave 1% 1ul split 20:1
Data File: C:\MSDCHEM\1\DATA\FAREN2_SIMSCAN.D\FAREN2_SIMSCAN.D
Date/Time: 06:03:55 PM Wednesday, Apr 20 2005

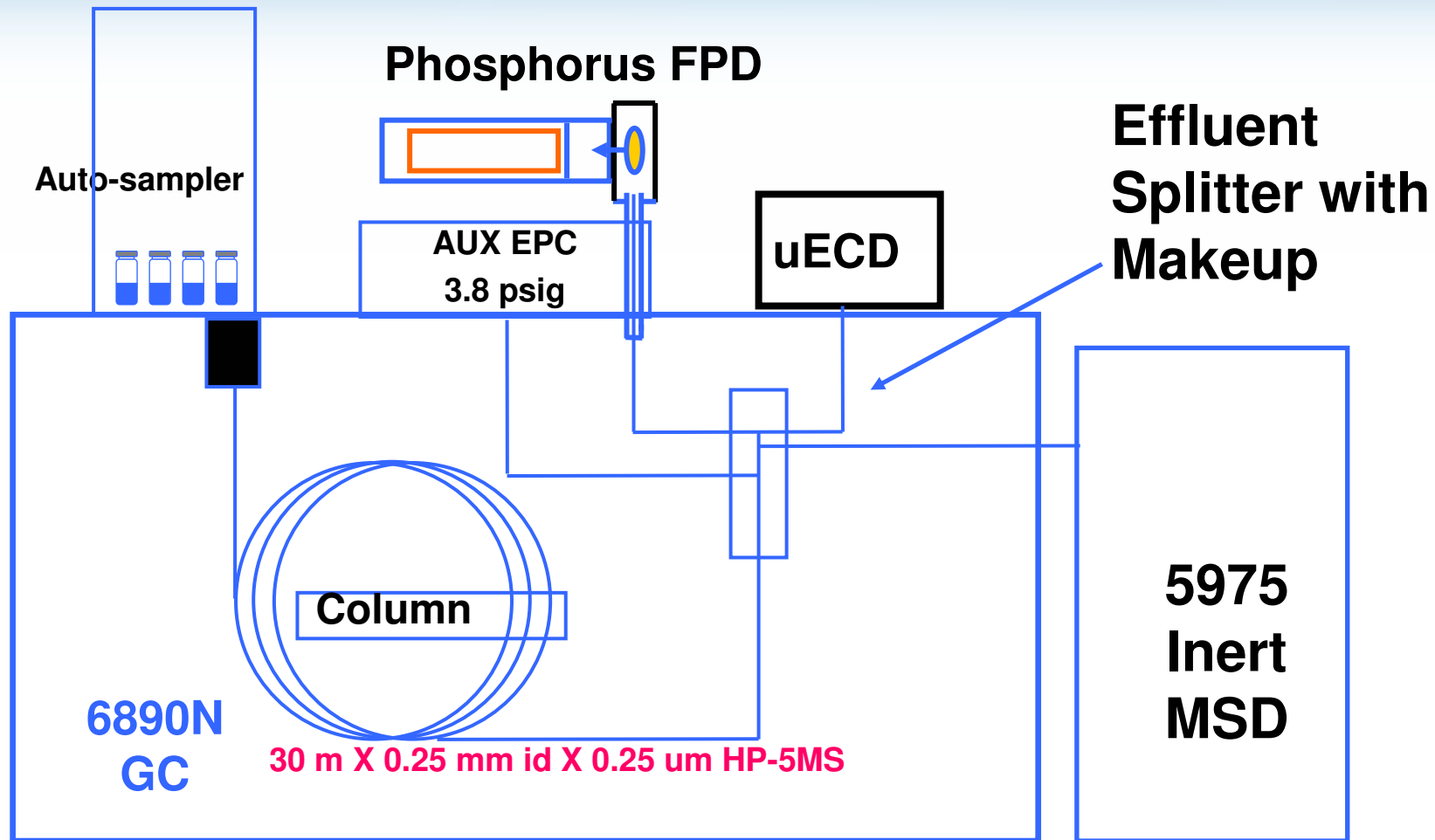
The NIST library was searched for the components that were found in the AMDIS target library.

R.T.	Cas #	Compound Name	Agilent SIM QUANT Amount (ng)	Deconvolution process			
				AMDIS SCAN CONFIRMATION Match	R.T. Diff sec.	Reverse Match	Hit Num.
7.038	5989275	Limonene	0.07	98	-2.6	91	1
8.414	78706	Linalol	0.01	96	-3.8	90	1
12.252	111808	Methyl octine carbonate		87	-4.6	87	1
13.305	97530	Eugenol	0	76	-3.8	78	3
14.749	91645	Coumarin	0.01	91	-4.4	89	1
15.441	127515	alpha isomethyl ionone		72	-3.7	75	2
18.204	31906045	Lyril 1	0.03	94	-3.6	90	1
18.308	31906044	Lyril 2	0.03	95	-2.6	90	1
19.841	120514	Benzyl benzoate	0.02	75	-2.3	93	1
21.266	118581	Benzyl salicylate	0				

With courtesy of Chris Sandy and J-F Garnier

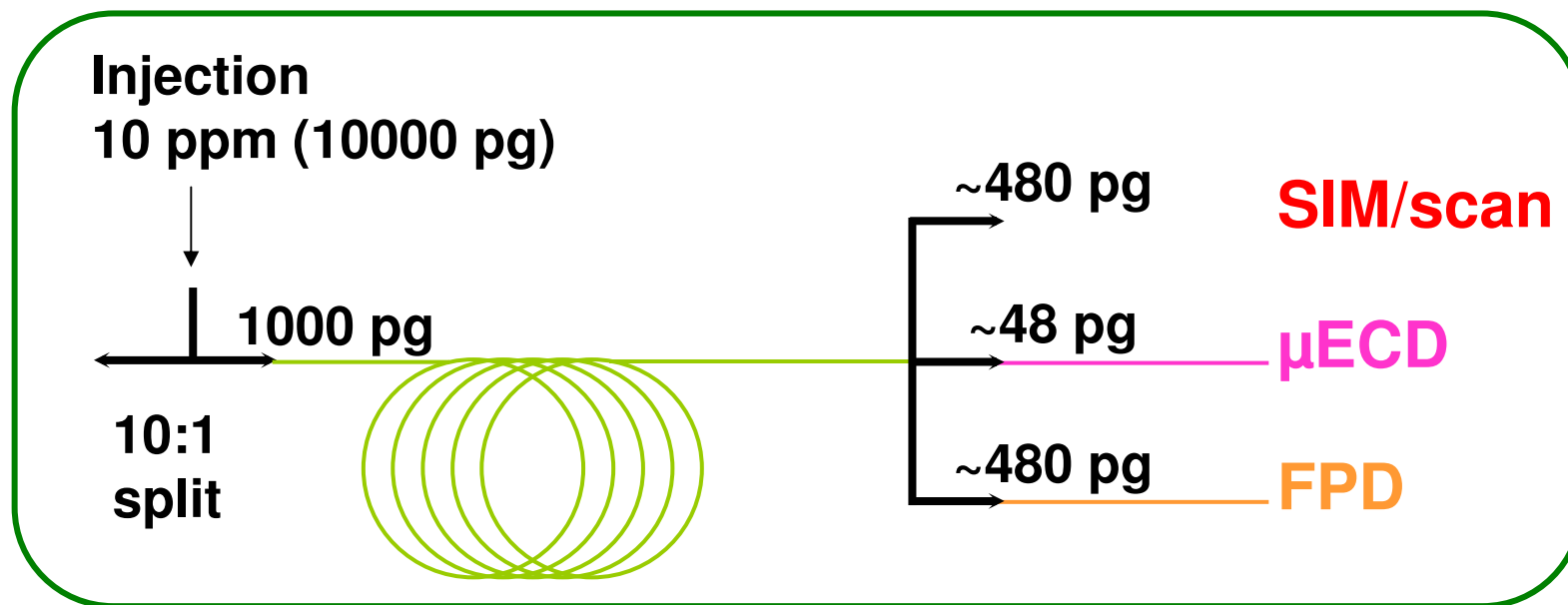
6890N/5975 inert Pesticide Analysis with 3-Way Splitter

Method with 10:10:1 split FPD:MSD:ECD

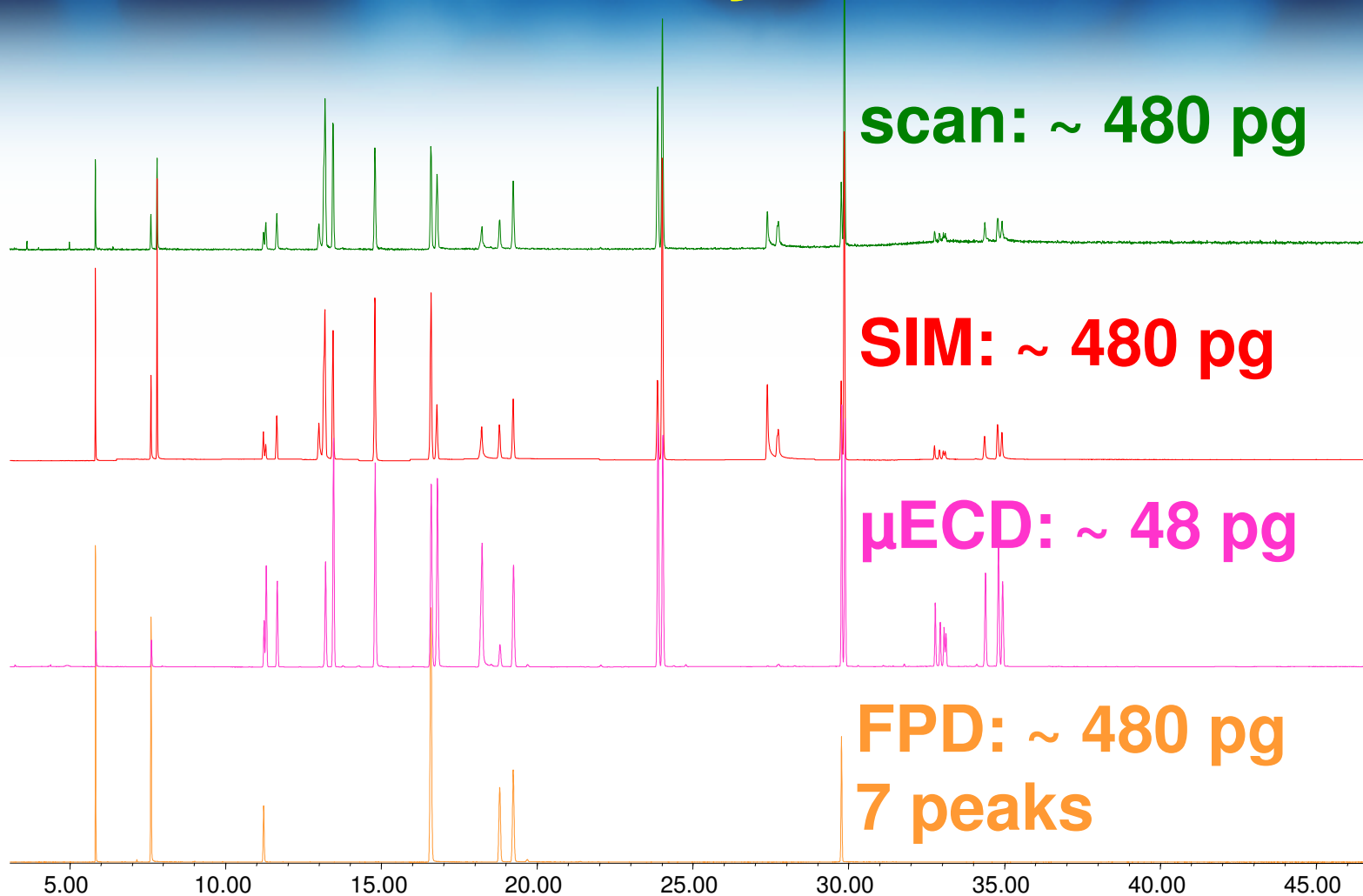


1-injection-4-signal System

- 5975, RTLocked, 30x0.25x0.25 HP-5MS
- Samples: pesticide mix at 10, 1, and 0.1 ppm
- Injection: 10:1 split
- At the end of the column, eluent flow is split 3 ways:
 $MSD:FPD:\mu ECD = 10:10:1$

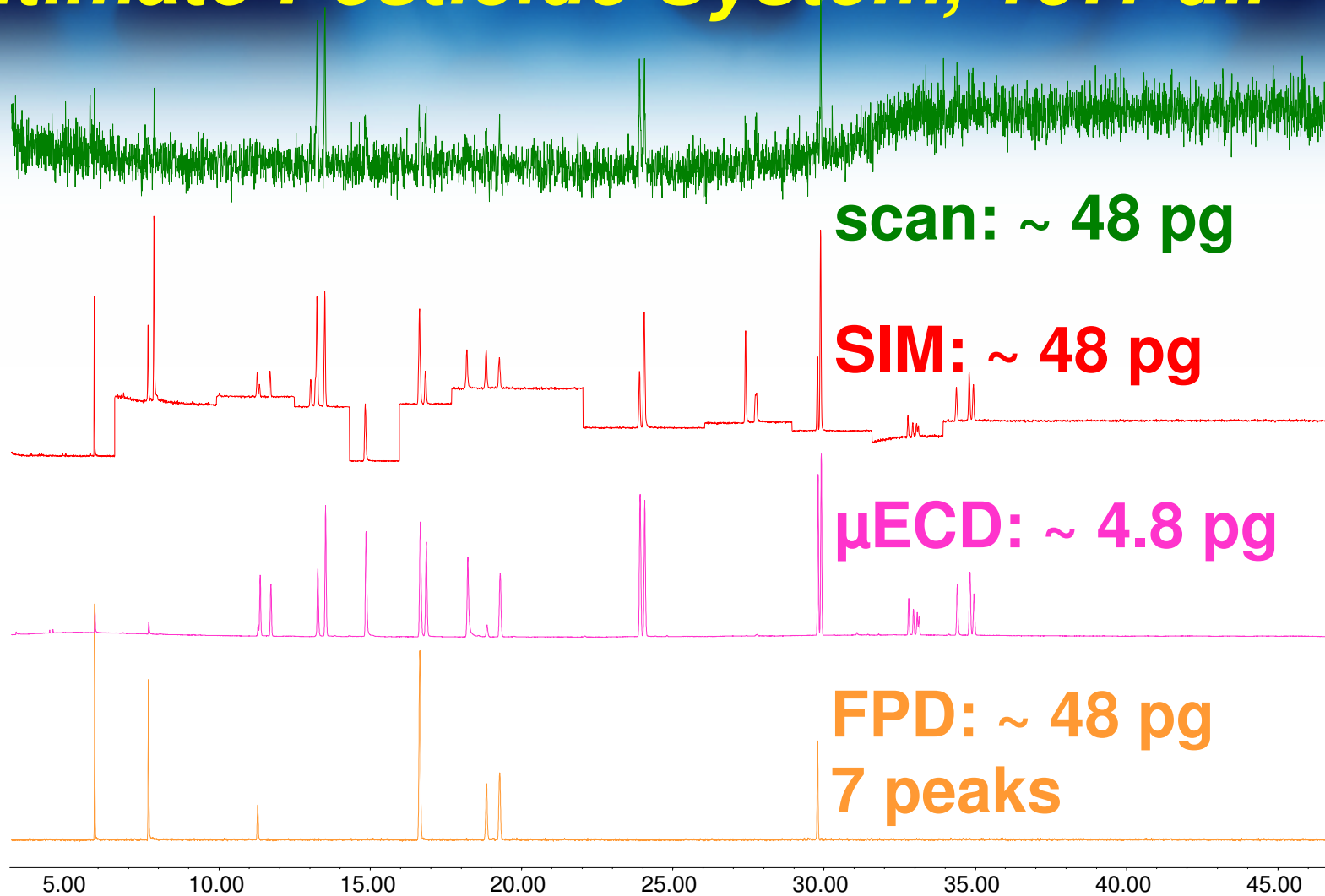


5975 SIM/scan + 3-way splitter Ultimate Pesticide System



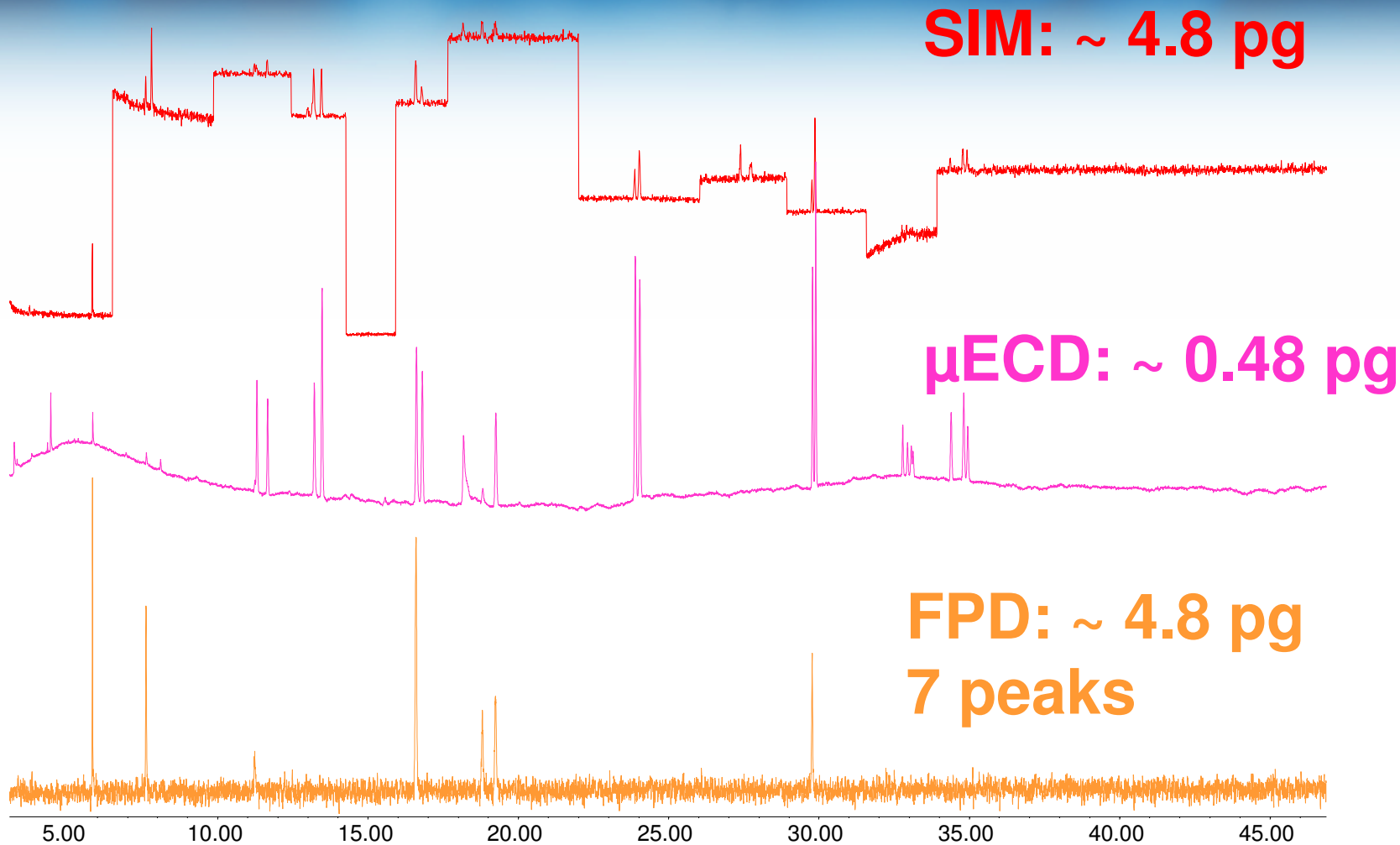
5975 SIM/scan + 3-way splitter Ultimate Pesticide System, 10:1 dil

5975 eMethod ChemStation Summary

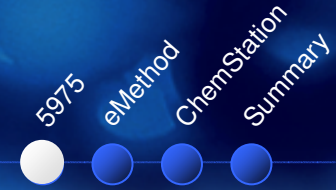


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5975 SIM/scan + 3-way splitter Ultimate Pesticide System, 100:1 dil



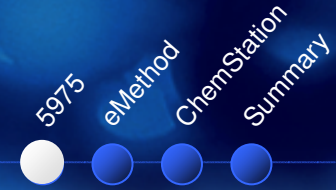
Synchronous SIM/Scan – Summary



- ***Great for target analysis and identifying unknowns***
 - SIM data for quantitation
 - Scan data for confirmation of unknowns
- ***SIM/Scan is an alternative to MS/MS***
 - MS/MS does not produce library searchable spectra
- ***Our SIM/Scan delivers real performance – is not just a spec***



Agilent MSD Unique Features



- ***Inert Ion source***
- ***Hyperbolic quad***
- ***Quad temp***
- ***CI system***
- ***Analyzer modularity***



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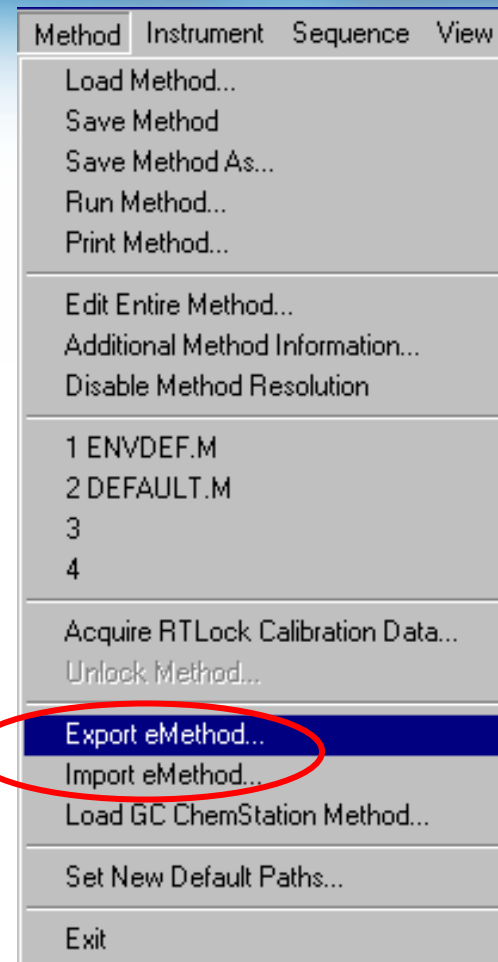
Introduction to eMethods and MSD Chemstation



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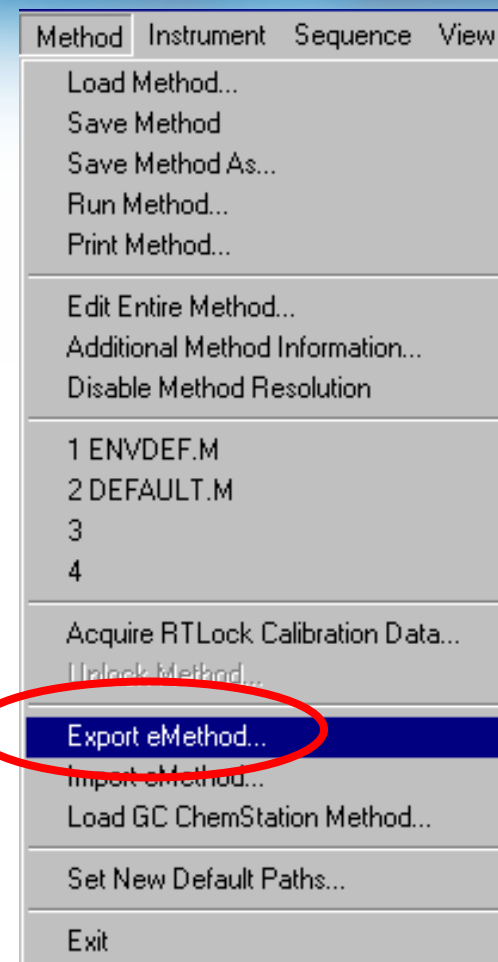
What are eMethods?

- ***eMethods is short for Electronic Methods.***
- ***Can now package existing GC/MSD methods***
 - Export them to other 5973 MSDs
 - Export them to 5975 inert MSDs

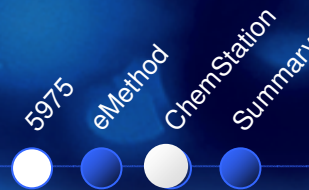


eMethod Benefits

- **Fast setup of new 5975 inert MSD**
- **Method sharing between 5973 and 5975 MSDs**
- **Download apps from website and import entire method into MSD ChemStation**



MSD ChemStation Software



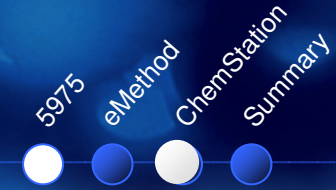
- ***Two GC/MS per ChemStation***
- ***GC and GC/MS control***
- ***Retention time locking***
- ***Custom reports***
- ***eMethods***
- ***Four configurations***
 - Enhanced mode
 - EnviroQuant
 - DrugQuant
 - Reformulated Gas

Most popular GC/MS software in the world



Agilent Technologies

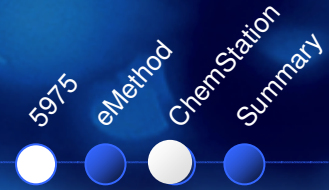
Instrument Control Enhancements



- ***Combined Top/Instrument Control Screen***
- ***New icons for quick access to tune, EMF and print***
- ***Configurable sequence table***
- ***More right mouse click functions in editing sequences***
- ***Printing selected sections of method and sequence***
- ***Import of GC ChemStation method parameters (excluding 5890 GC)***
- ***Display of IP address(s) of GC and MSD instruments***



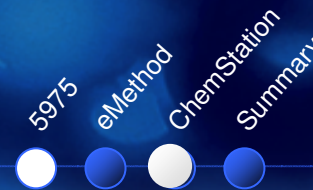
Data Analysis Enhancements



- ***Explorer-style navigation tool***
- ***Interactive editing of Integration Parameters***
- ***Switchable right mouse click functions***
- ***Spreadsheet-like SIM Parameters Table***
- ***Icons for custom tools, DA options, variable watch***
- ***Toolbar on/off capability***
- ***Selectable DA color themes***



Data Analysis Enhancements



- ***QEdit functionality is improved:***

- Separate window for Baseline Display
- Generating reports directly from QEdit
- Custom configuring X-axis



Explorer Navigation

The screenshot displays the ChemStation software interface. At the top, the title bar reads "Enhanced Data Analysis - DEFAULT.M / EVALDEMO.D (MS Data: Quantitated Multi Pt., Not Reviewed)". Below the title bar is a menu bar with options: File, Method, Chromatogram, Spectrum, Calibrate, Quantitate, Tools, View, Toolbars, Help. A toolbar with various icons is located below the menu bar. A central toolbar contains an "Execute" button.

The main workspace is divided into three panels:

- Left Panel (File Explorer):** A tree view showing a directory structure. The "bna1ist.m" folder is selected. A red arrow points from the text "Explorer navigation" to this panel.
- Top Right Panel:** A Total Ion Chromatogram (TIC) plot titled "[2] TIC: evaldemo.d". The y-axis is labeled "Abundance" and ranges from 0 to 3,500,000. The x-axis is labeled "Time-->" and ranges from 5.50 to 9.50 minutes. Four peaks are labeled with their retention times: 5.281, 6.431, 7.740, and 9.777.
- Bottom Right Panel:** A mass spectrum plot titled "[1] Scan 177 (6.439 min): evaldemo.d". The y-axis is labeled "Abundance" and ranges from 0 to 700,000. The x-axis is labeled "m/z-->" and ranges from 20 to 160. The base peak is at m/z 154. Other labeled peaks include 28, 32, 39, 44, 51, 57, 63, 69, 76, 85, 89, 98, 102, 111, 115, 122, 128, 139, and 150.

At the bottom of the window, the status bar shows "Ready" and "NUM SCRL".

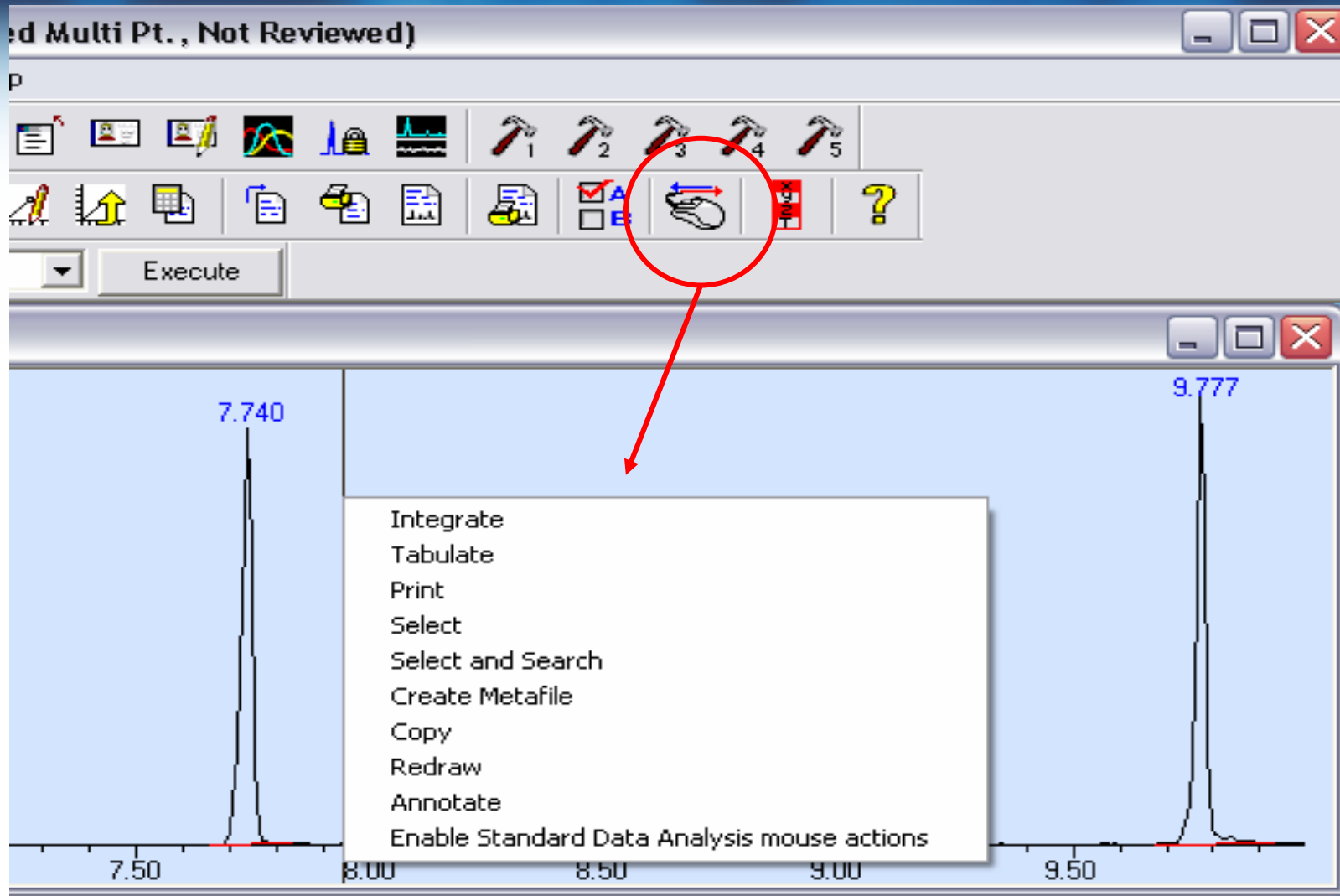
Interactive Edit Integration

The screenshot displays the 'Enhanced Data Analysis' software interface. The main window shows a Total Ion Chromatogram (TIC) for 'evaldemo.d' with peaks labeled at retention times 5.281, 6.431, 7.740, and 9.777. A red circle highlights the 'Edit Integration' icon in the toolbar, with a red arrow pointing to the 'Edit Integration Events' dialog box. The dialog box shows the 'Possible Events' dropdown set to 'Initial Area Reject' and a table of integration parameters.

Integrator Event Name	Value	Time
Initial Area Reject	0	Initial
Initial Peak Width	0.019	Initial
Shoulder Detection	OFF	Initial
Initial Threshold	19.0	Initial

Specify integration parameters for MS signal (autoint1.e)

Right Click Features



SIM Parameter Table

Enhanced Data Analysis - DEFAULT.M / EVALDEMO.D (MS Data: Quantitated Multi Pt., Not Reviewed)

File Method Chromatogram Spectrum Calibrate Quantitate Tools View Toolbars Help

Execute

[2] TIC: evaldemo.d

Abundance

3500000

3000000

2500000

2000000

1500000

1000000

500000

5.281

Time--> 5.50

C:\msdchem\MSEXEX\simions

Number of SIM Groups:

Group #Ions

Sim Group Table

	Start Time (min)	Default Dwell (ms)	Calc Cycles/Sec	Ion1	Ion2	Ion3	Ion4	Ion5	Ion6
1	0	100	8.3 74.1						
2									
3									
4									
5									
6									
7									
8									
9									
10									
11									
12									
13									

Sheet1

Fill down using increment 0

OK Cancel

Baseline Display

The screenshot shows the QEdit software interface with the 'Reports' menu open. The 'Show baseline in separate window' option is checked. The main window displays a chromatogram with a peak at 5.277 minutes. The 'Reports' menu is also open, showing options like 'Generate Report...', 'Report Options...', 'Custom Reports...', 'Print Custom Report', and 'Update Database'. The 'Custom Reports...' option is highlighted.

#	!	Compound Name	Ion	Retention Time
1	x	Dodecane	57.05	56.75 to 57.75
2	x	Biphenyl	71.15	70.85 to 71.85
3	x	4-Chlorobiphenyl	43.05	42.75 to 43.75
4	x	Methyl palmitate	85.15	84.85 to 85.85

Chromatogram Data:

Retention Time (min)	Abundance
5.277	~350,000

Mass Spectrum Data:

Retention Time (min)	Abundance
43	~400,000
57	~600,000
71	~450,000
85	~300,000

Report Data:

Retention Time (min)	Response	Ion	Exp%	Act%
5.280	9737444	57.05	100	100
71.15		71.15	66.90	65.81
43.05		43.05	59.20	57.98

Reports

The screenshot shows the QEdit software interface with the 'Reports' menu open. The 'Custom Reports...' option is highlighted. The main window displays a chromatogram with a peak at 5.277 minutes. The 'Reports' menu is also open, showing options like 'Generate Report...', 'Report Options...', 'Custom Reports...', 'Print Custom Report', and 'Update Database'.

#	!	Compound Name	Ion	Retention Time
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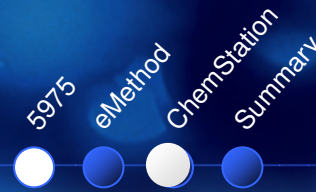
Library Options

- ***NIST05***
- ***Wiley 7th ed***
- ***Stan pesticide***
- ***Pfleger/Maurer/Weber MS Drug Library, 3rd ed***
- ***NIST Chemical Structures Library***

NEW



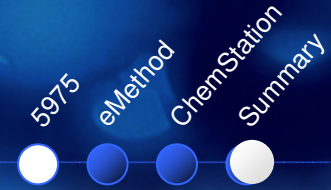
Other Software Options



- ***Deconvolution Reporting Software***
- ***Security ChemStation***
- ***Headspace software***
- ***RTL Pesticide Database : FAMES, Flavors, Volatiles Organics, Organotin derivatives, PCB congeners, Forensic toxicology***



GC/MS Configurations



- **5973N** *EI with diffusion pump*
- **5975 inert** *EI with standard turbo pump*
- **5975 inert** *EI with performance turbo pump*
- **5975 XL** *EI/PCI/NCI with performance turbo pump*

All systems available with choice of either 6850 or 6890 GCs

Summary

- ***Better reliability and quality***
- ***Enhanced performance***
 - eMethods
 - AutoSIM and SIM/scan
 - Higher mass range
 - AutoCI
 - Sensitivity
 - Software improvements



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www.agilent.com/chem

***Oder registrieren Sie sich für E-Notes
um regelmäßige Informationen zu erhalten.***

