5975 inert MSD

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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*

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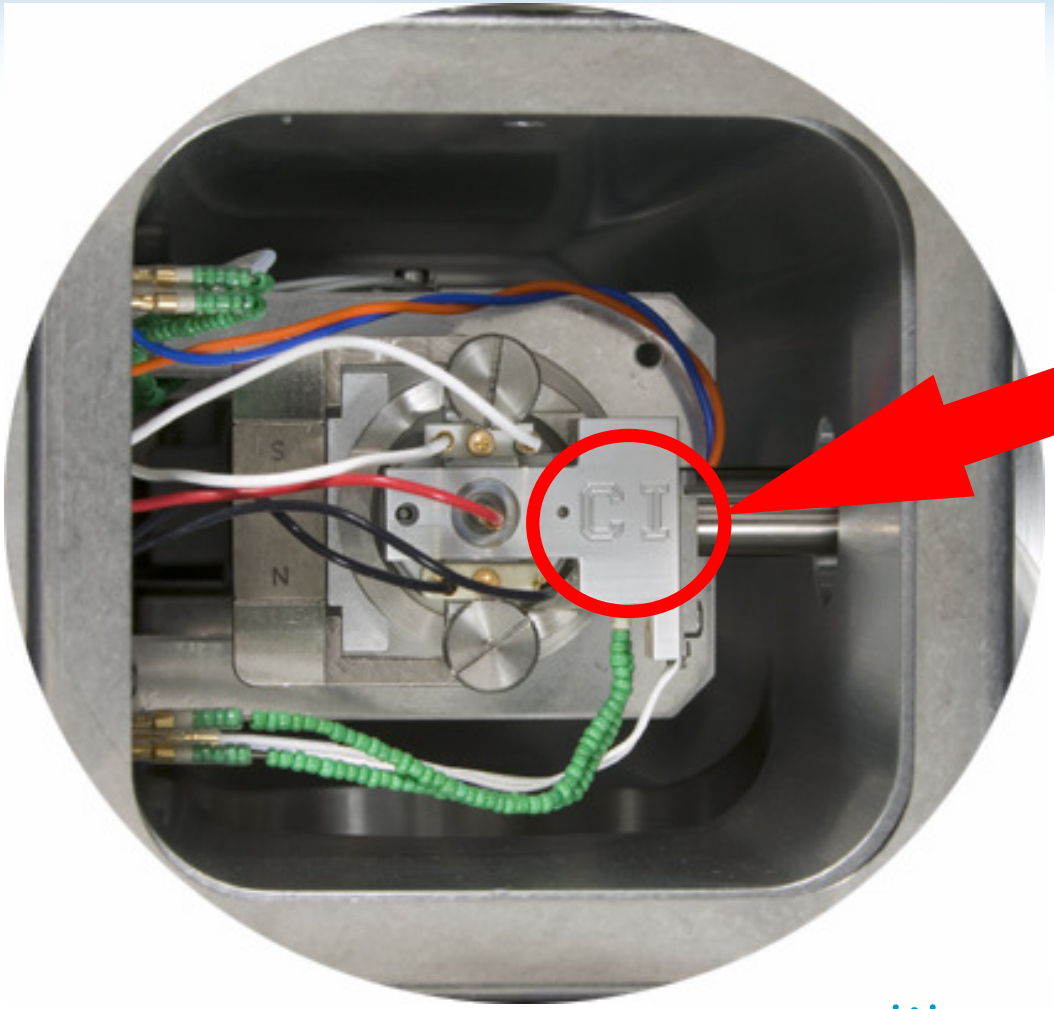
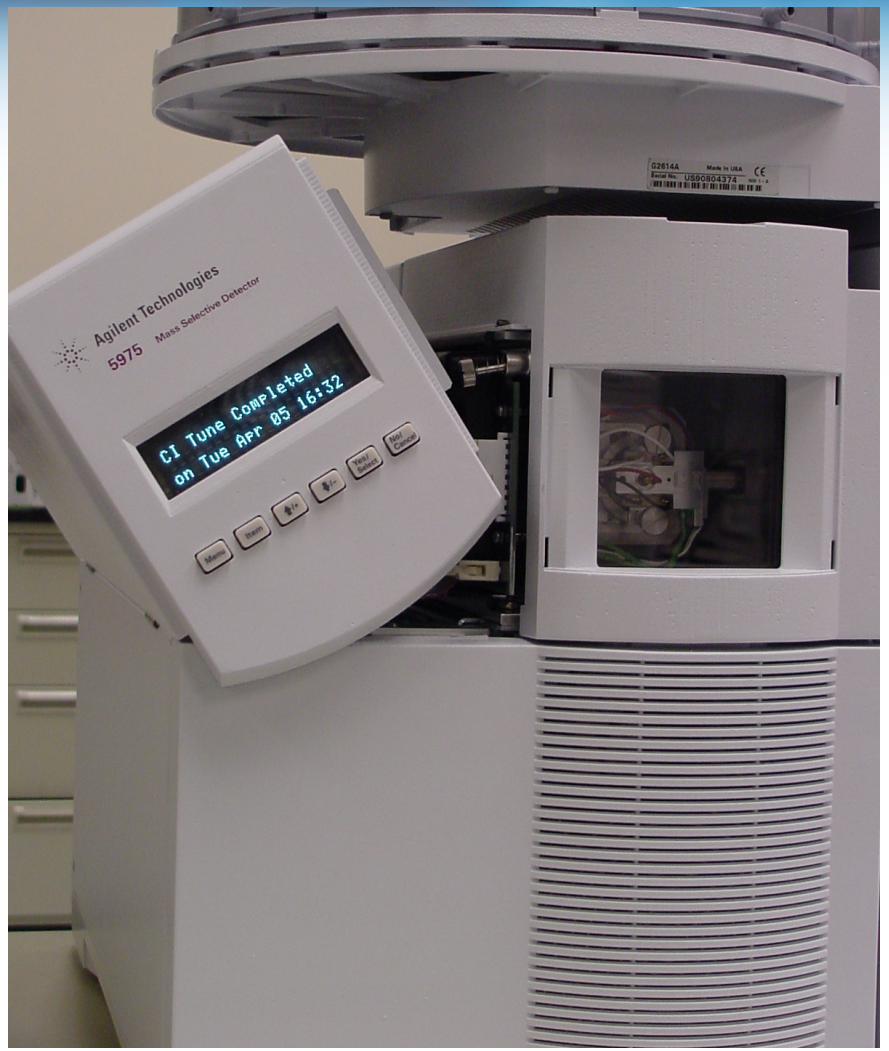
Functional Front Window



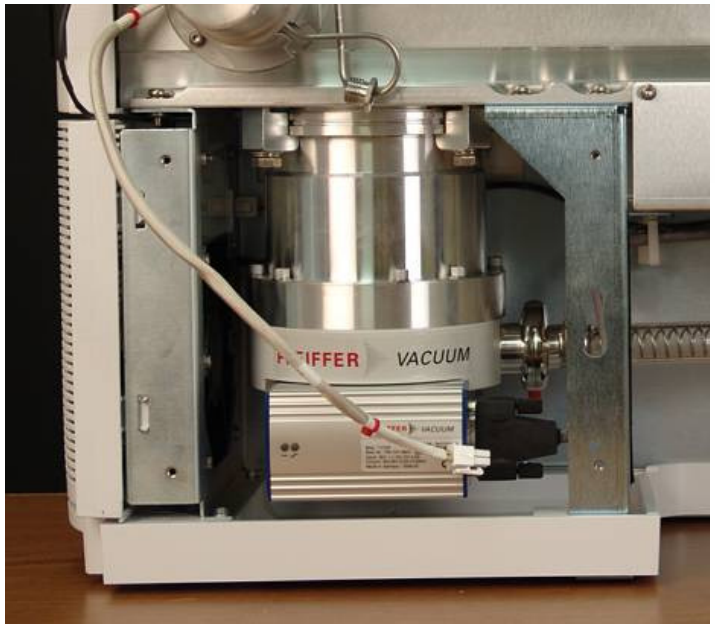
- *Wire connections*
- *Filament operation*
- *Column insertion*
- *CI Source identification*

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 m^3/hour mechanical pump (67% more capacity)

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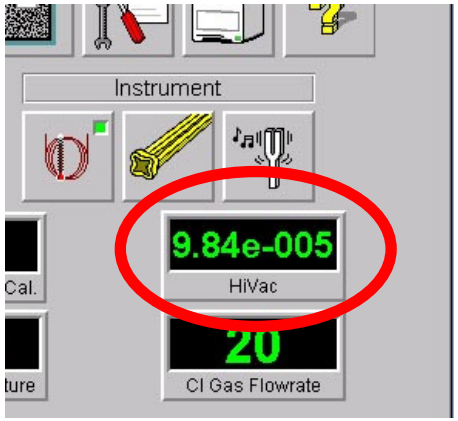
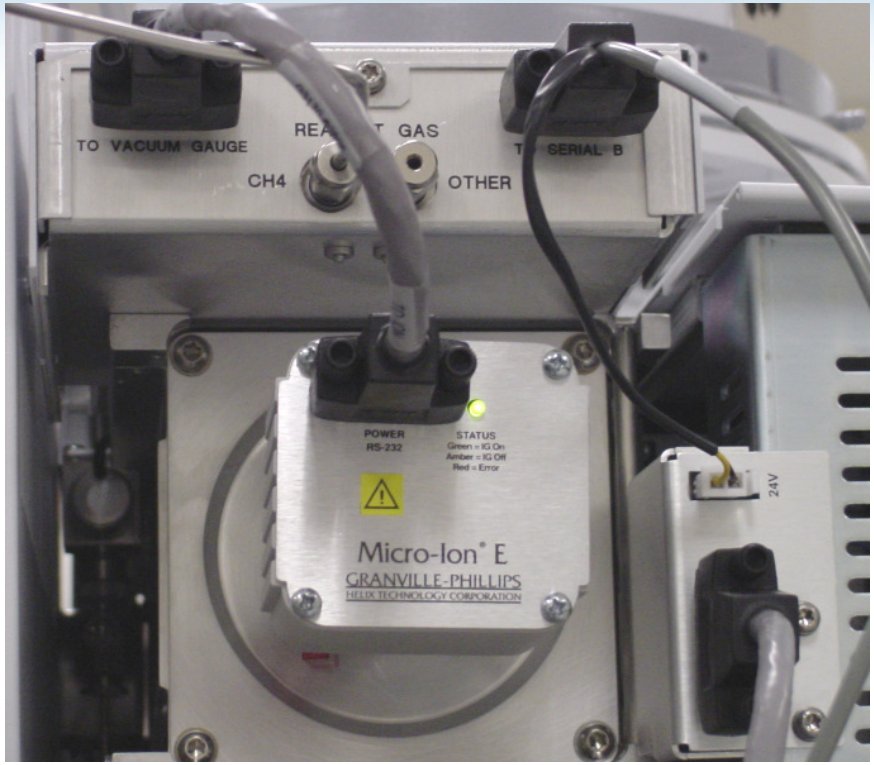
Integrated Ion Gauge/Controller

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



Software display



G3397A – optional gauge/controller

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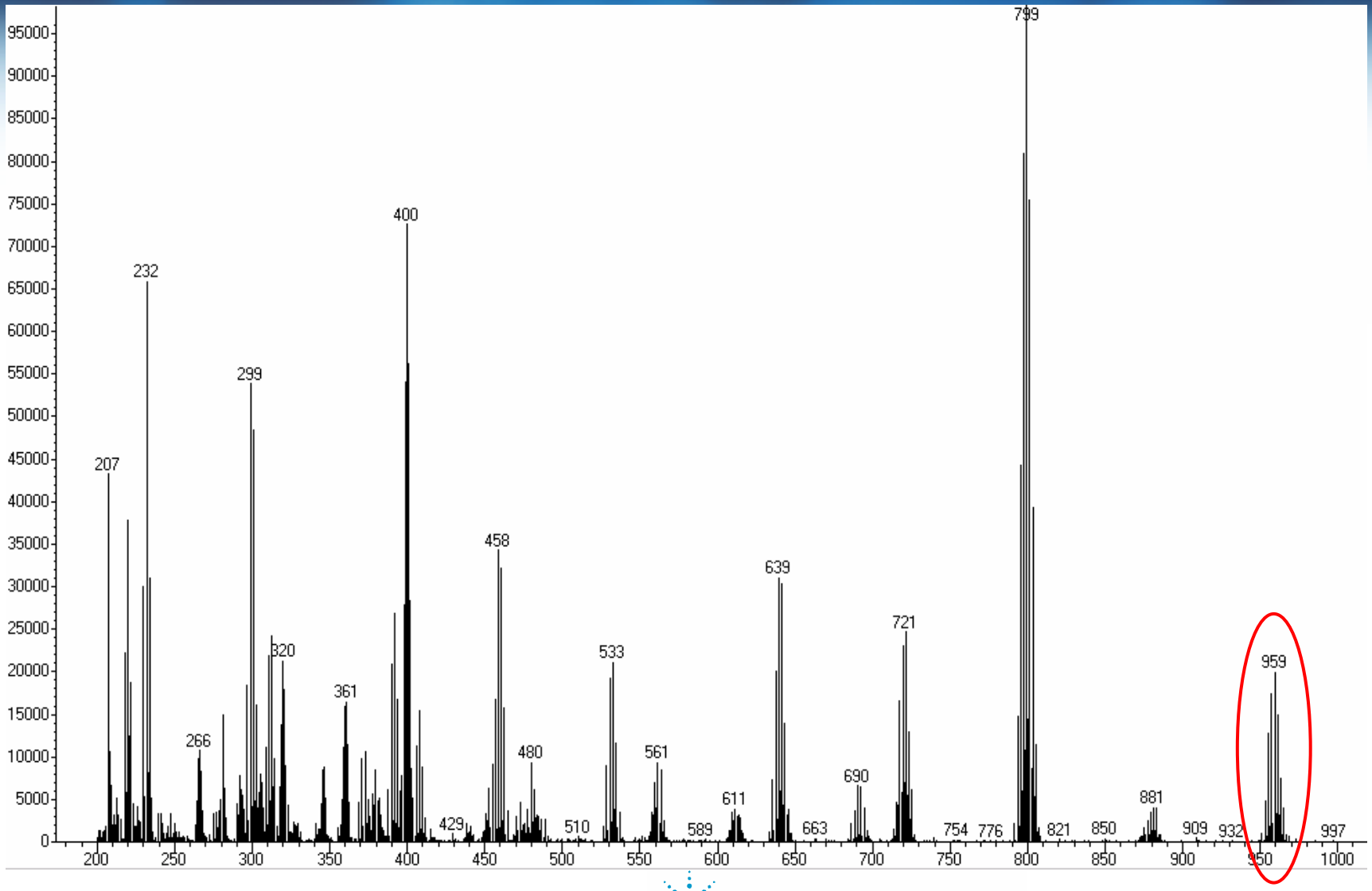
Extended Mass Range

- ***1050 m/z for 5975 inert MSD***
  - Quadrupole modified
  - New electronics
- ***800 m/z for <u>all</u> 5973 MSDs***

(Software upgrade does not enable 1050 m/z)

Extended Mass Range – PBDE 209



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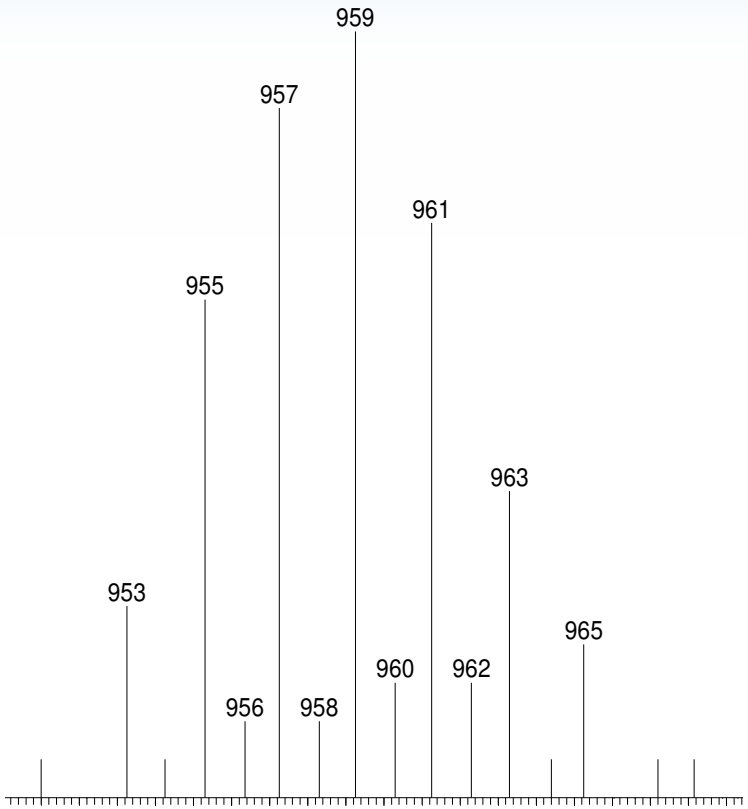
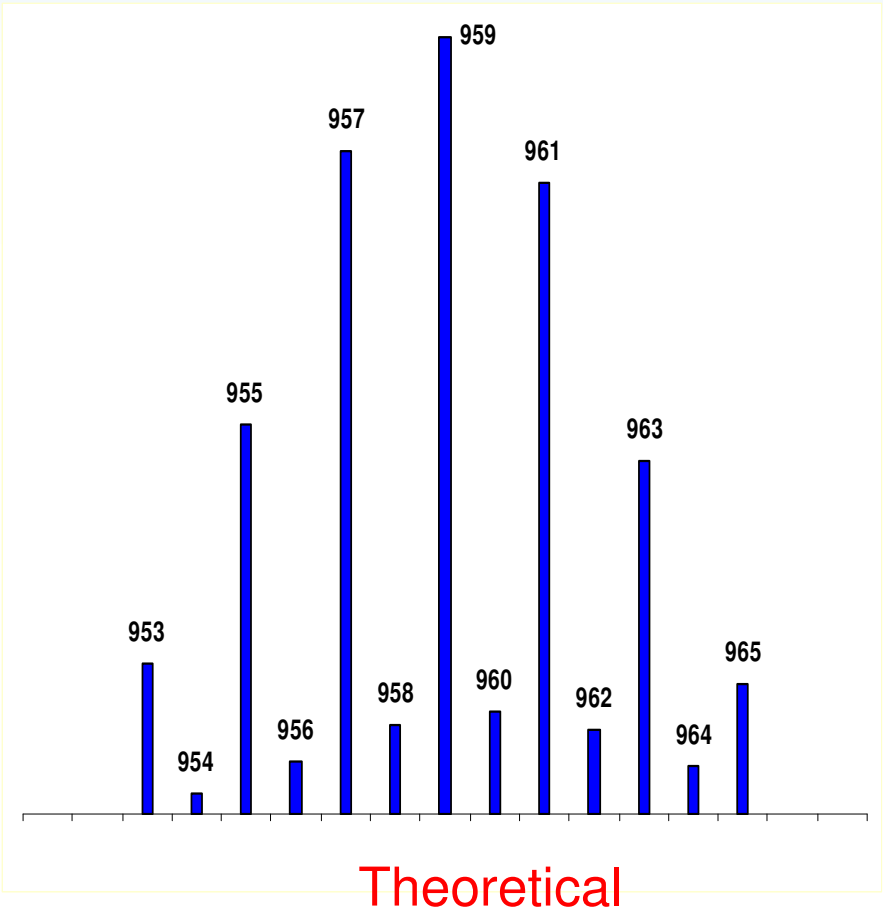
Extended Mass Range – PBDE 209



5975 inert MSD



Theoretical

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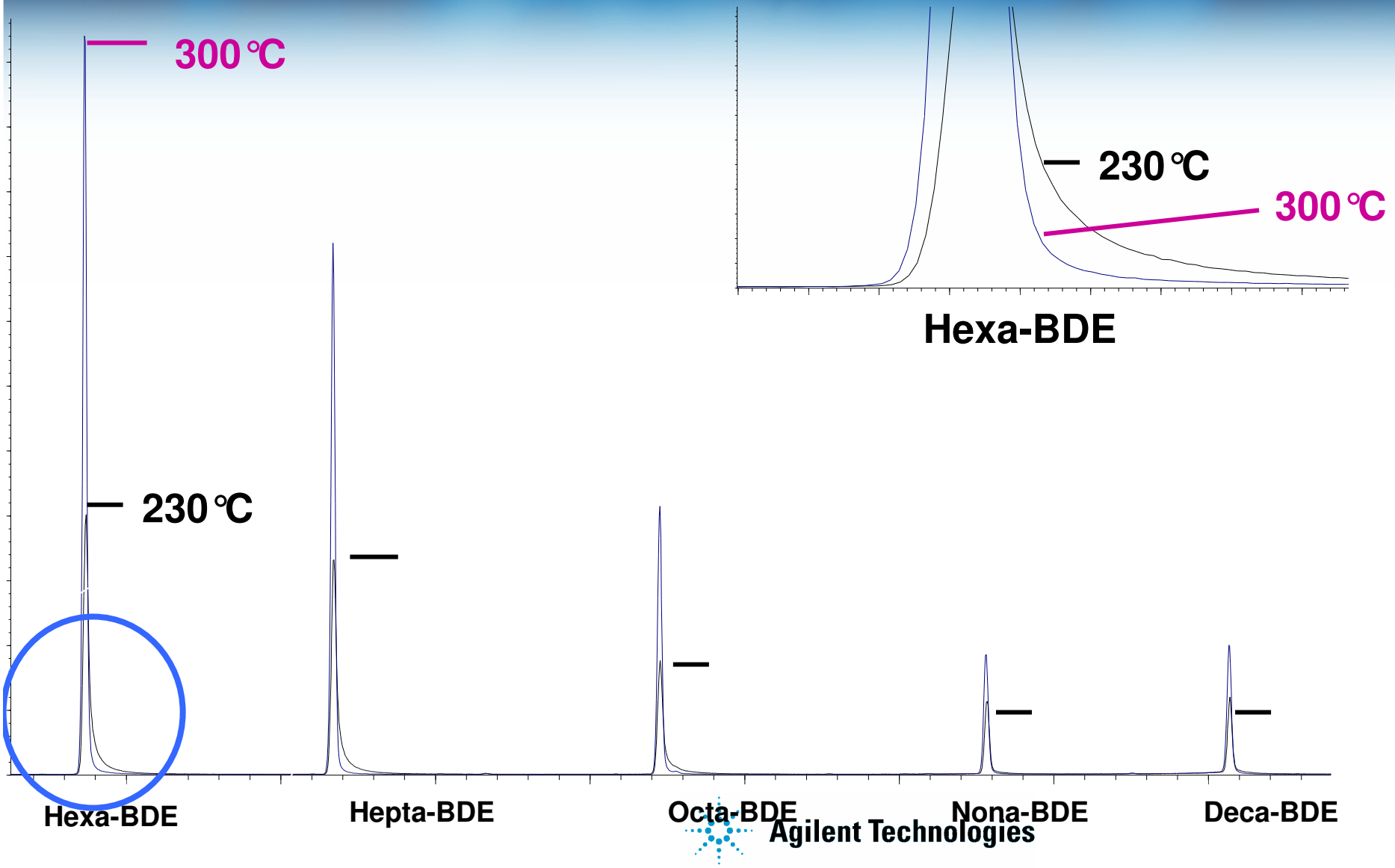
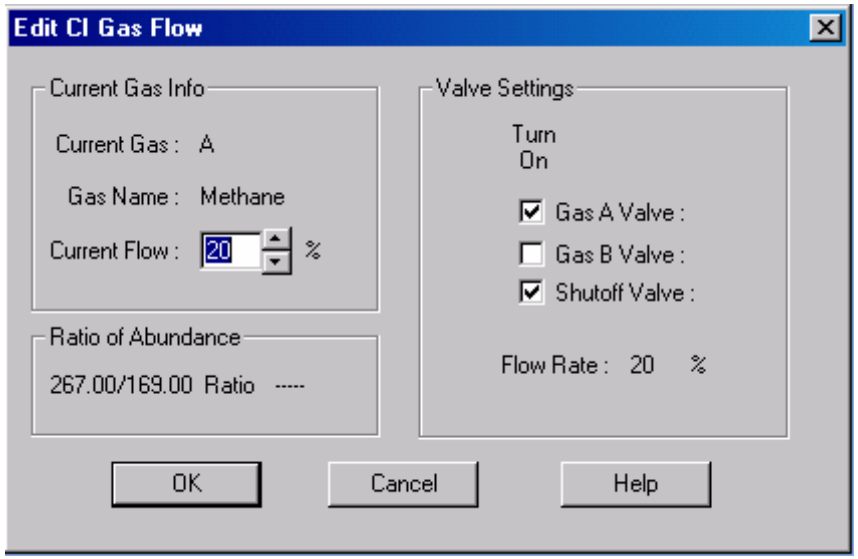
Comparing Source Temperatures – 230 °C vs 300 °C



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

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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

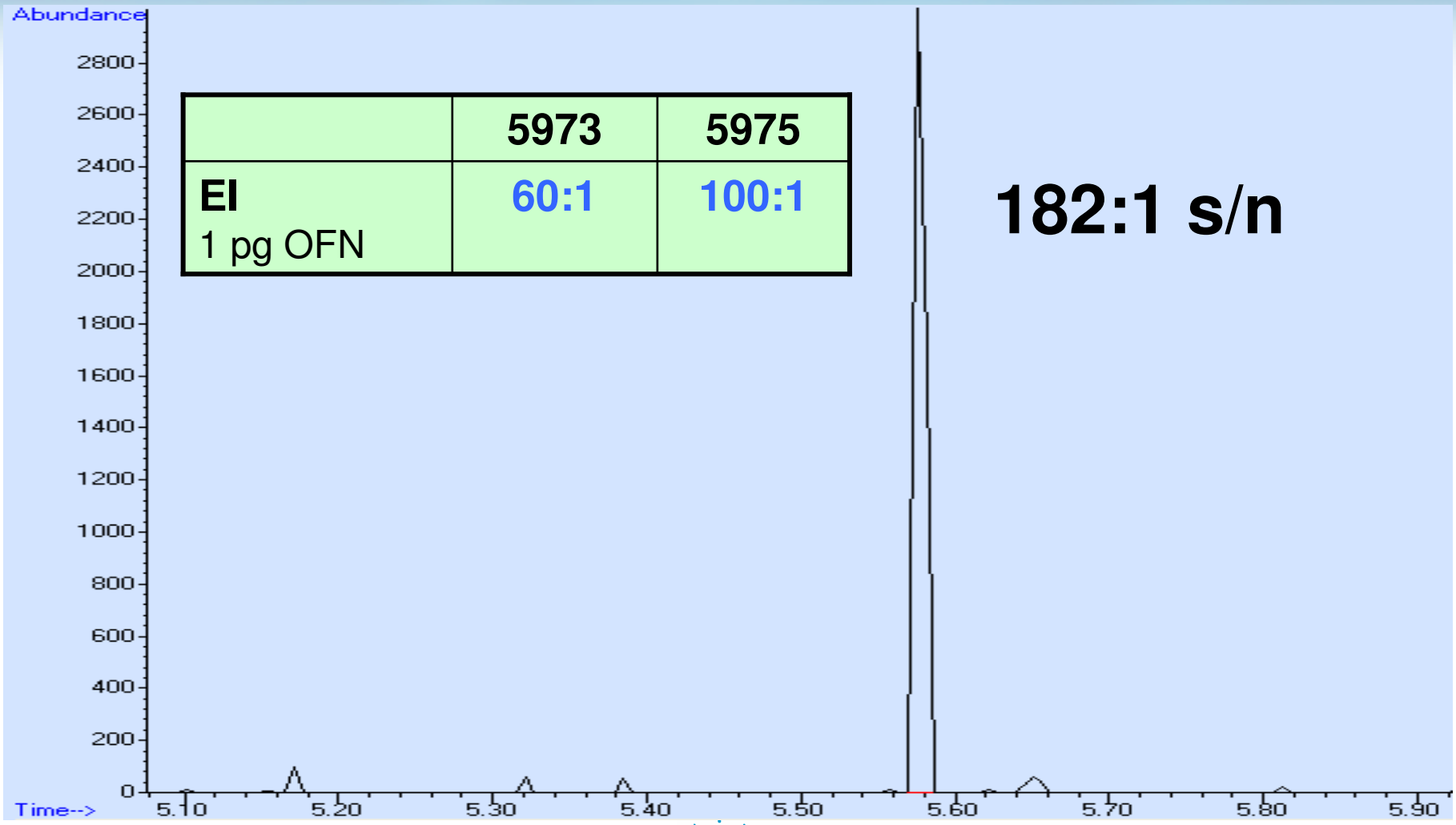
Automated EI with CI Source

Setup steps:

1. ***Tune instrument in PCI – create PCICH4.u***
2. ***Auto create EI tune file – create ei-cisource.u***
3. ***Tune instrument in NCI – NCICH4.u***
4. ***Assign tune file with method and run in sequence***

New Sensitivity Specifications – EI Scan

	5973	5975
EI 1 pg OFN	60:1	100:1



182:1 s/n

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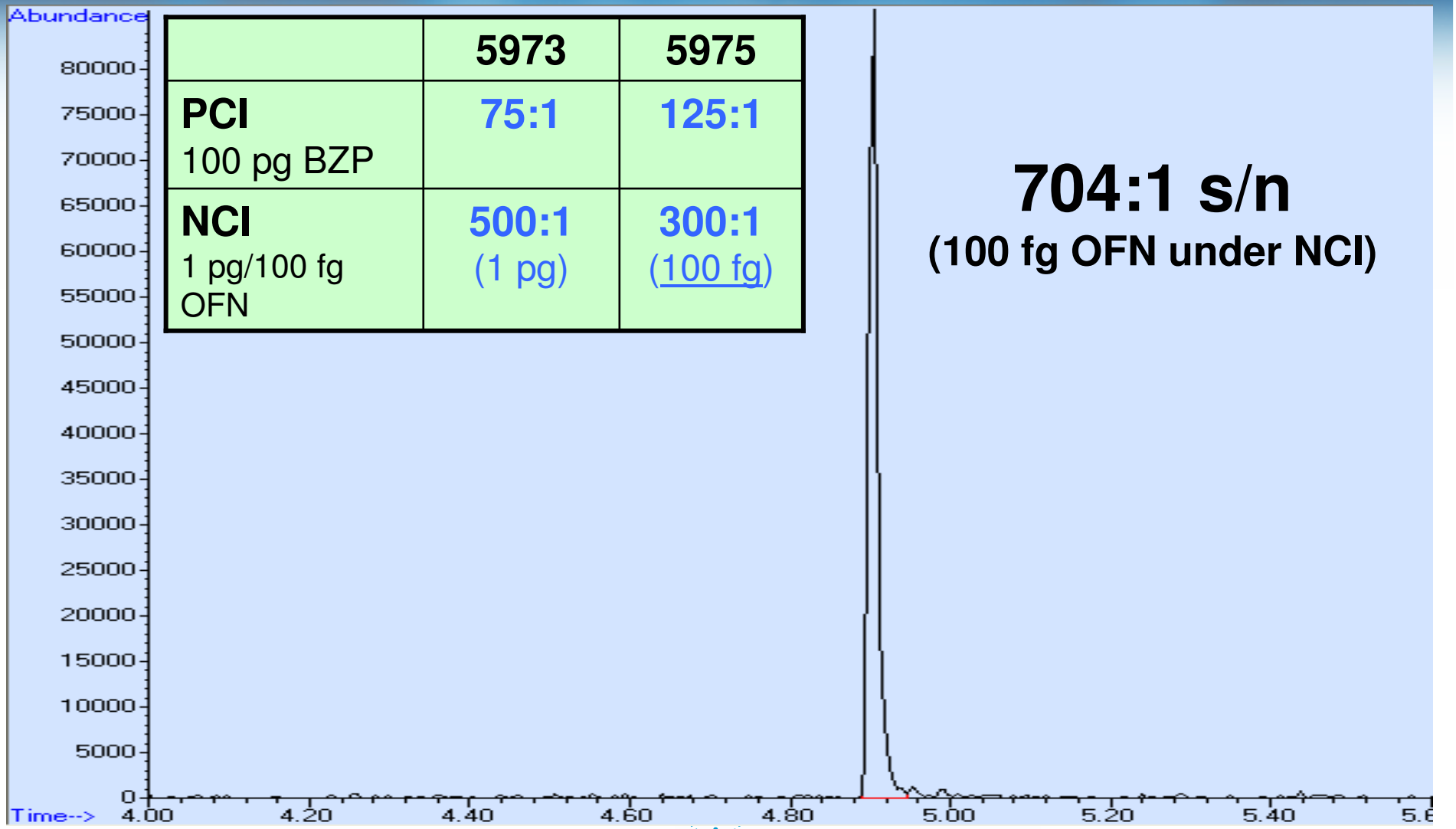
New Sensitivity Specifications – CI Scan

	5973	5975
PCI 100 pg BZP	75:1	125:1
NCI 1 pg/100 fg OFN	500:1 (1 pg)	300:1 (100 fg)



704:1 s/n
(100 fg OFN under NCI)

6850 GC Control via ChemStation

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

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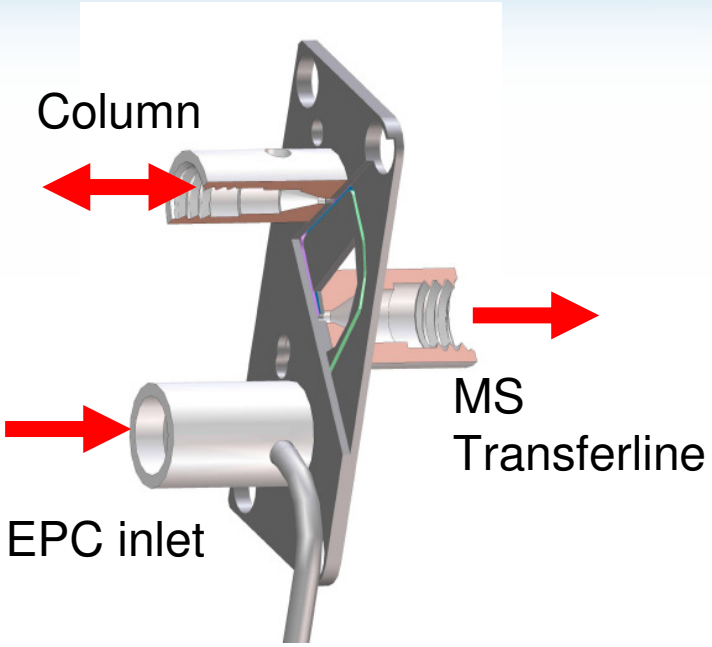
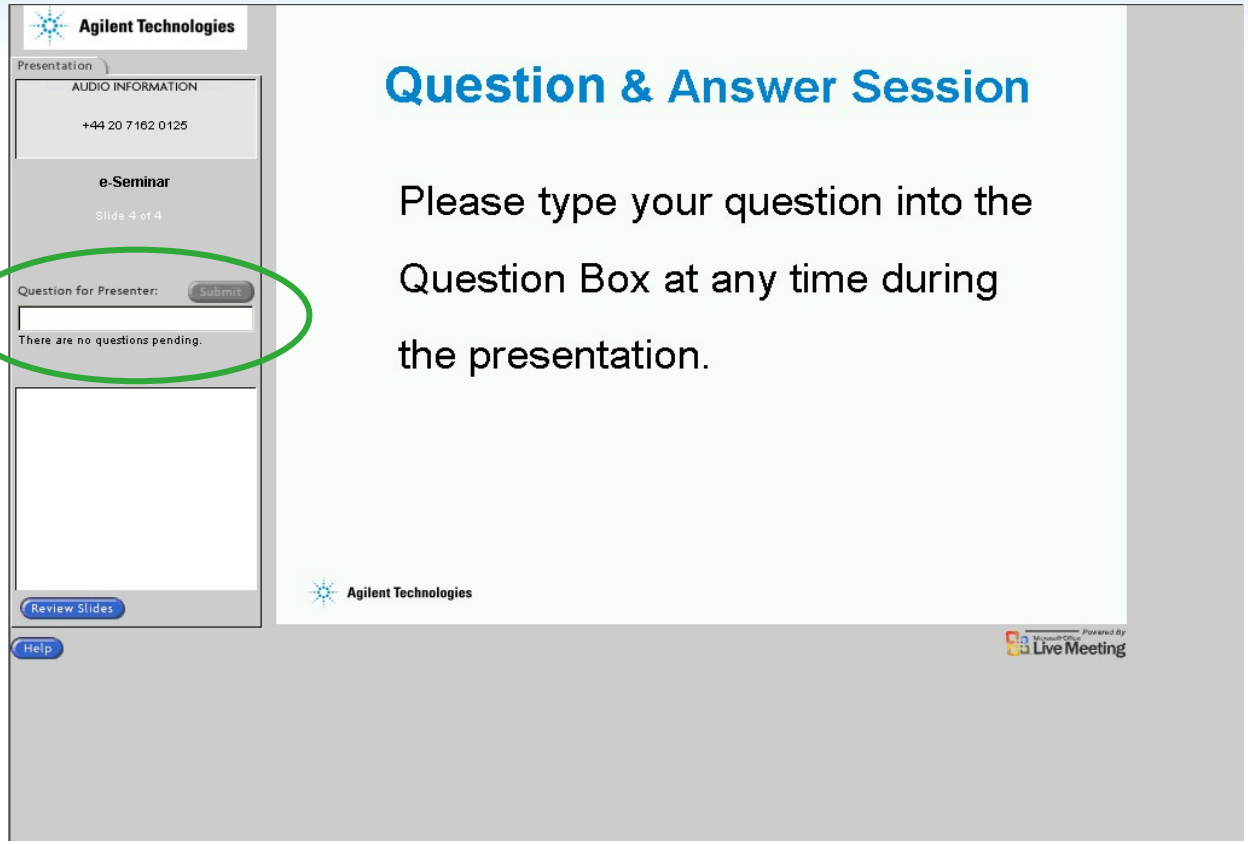
QuickSwap MSD interface

- ***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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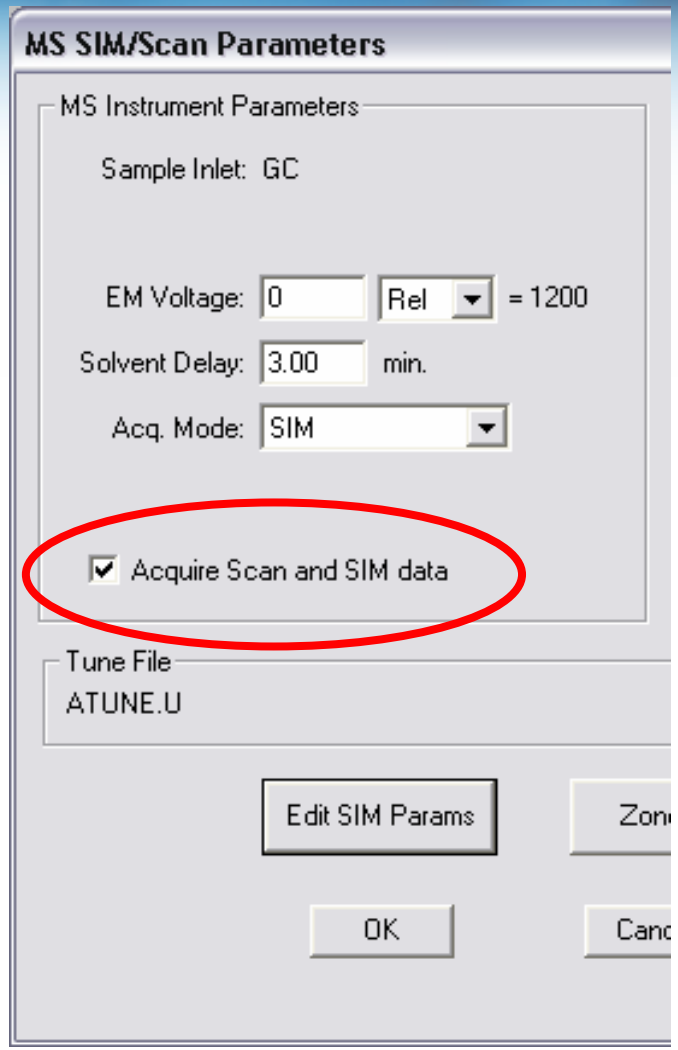
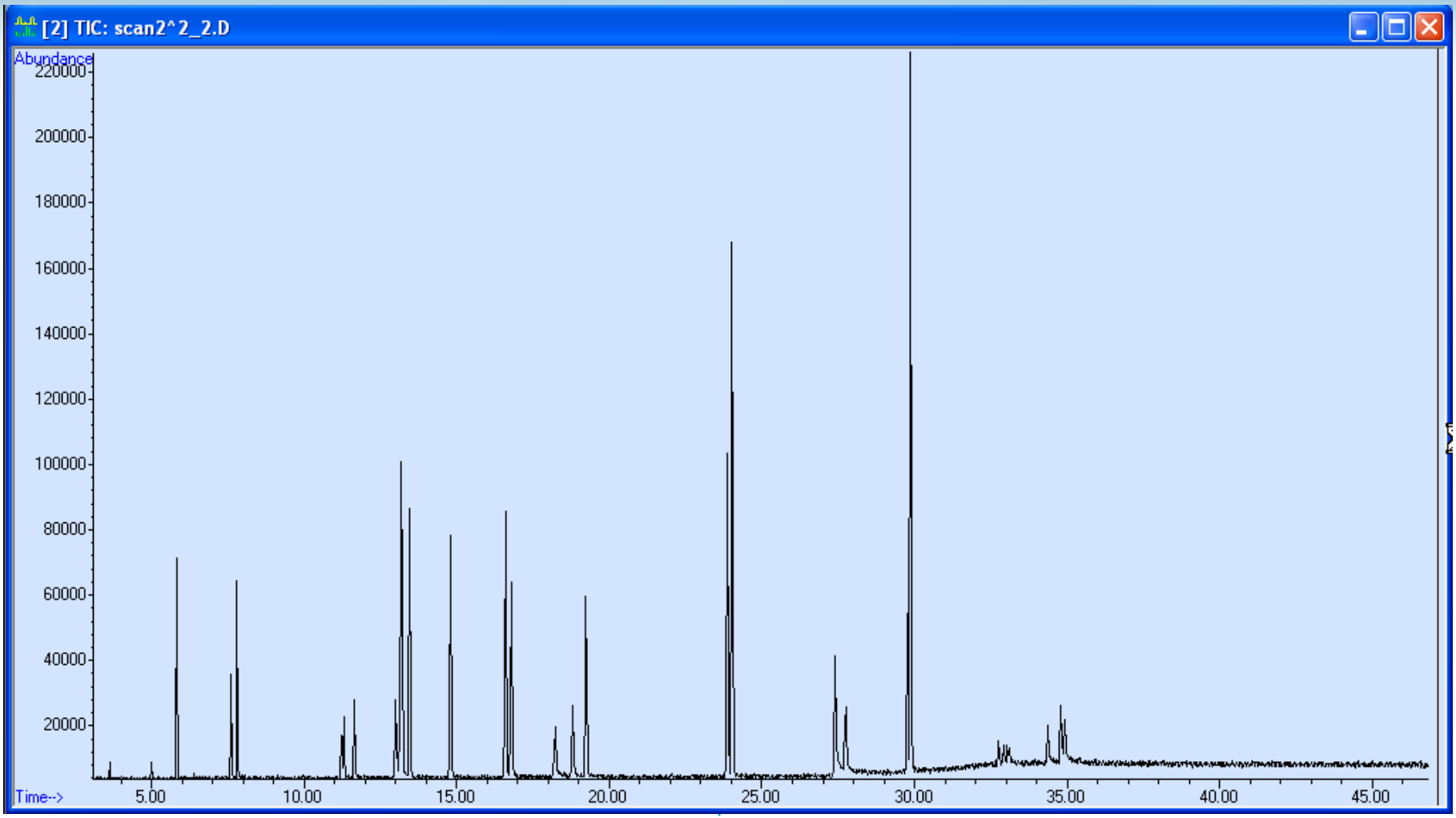
AutoSIM Setup for SIM/Scan

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



Inject Standard

5975 eMethod ChemStation Summary



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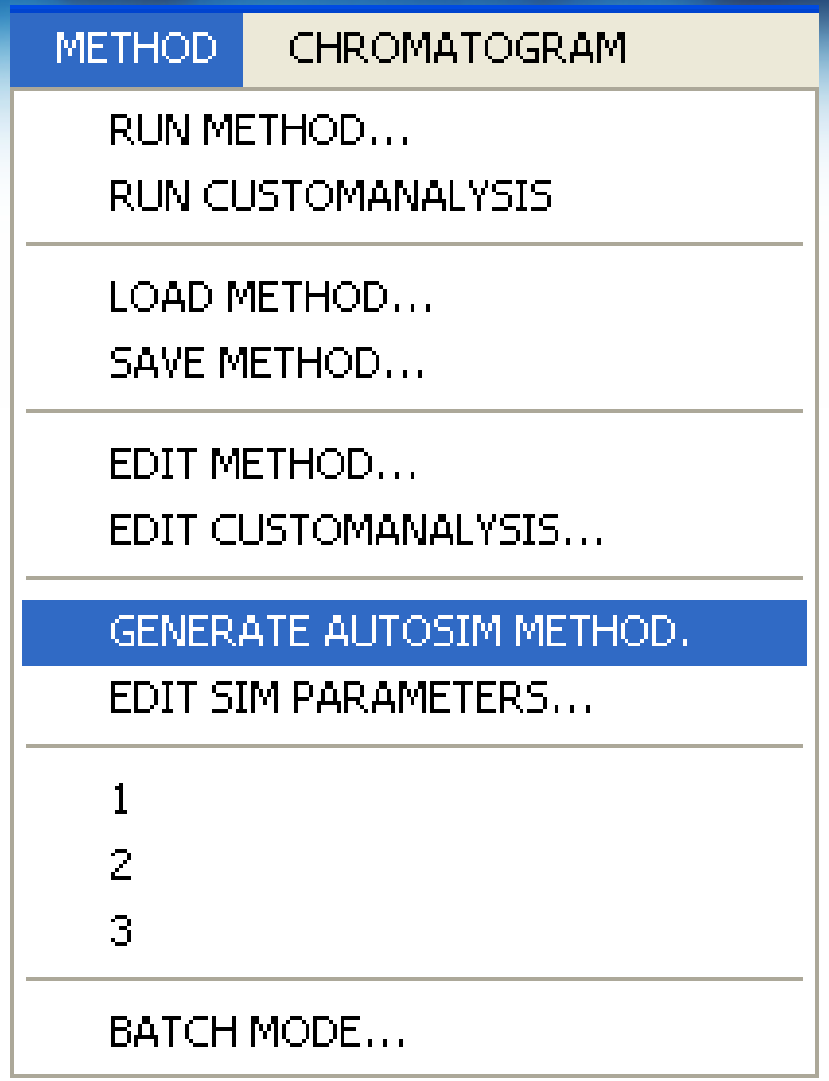
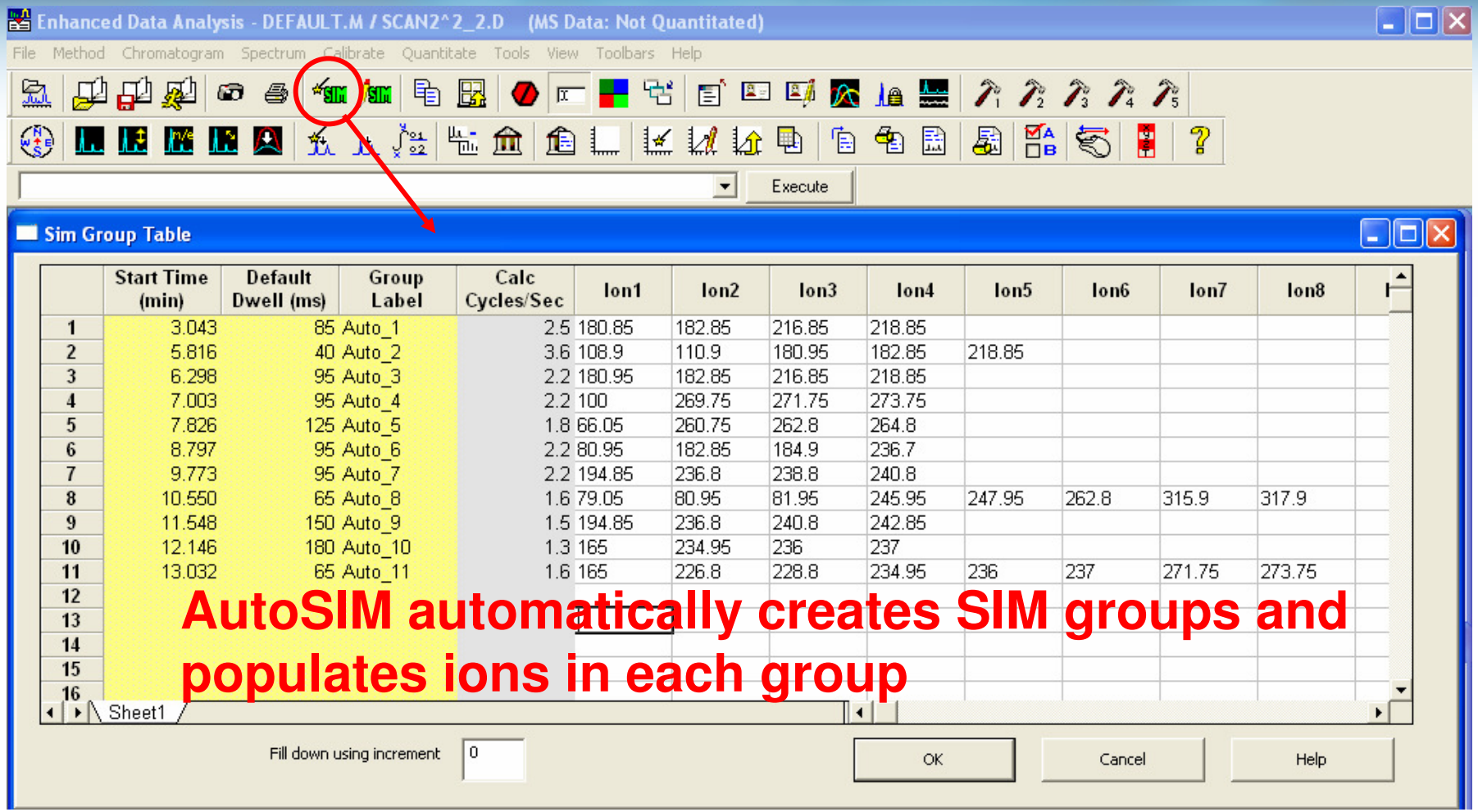
Run AutoSIM

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



Edit SIM Method



	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												

AutoSIM automatically creates SIM groups and populates ions in each group

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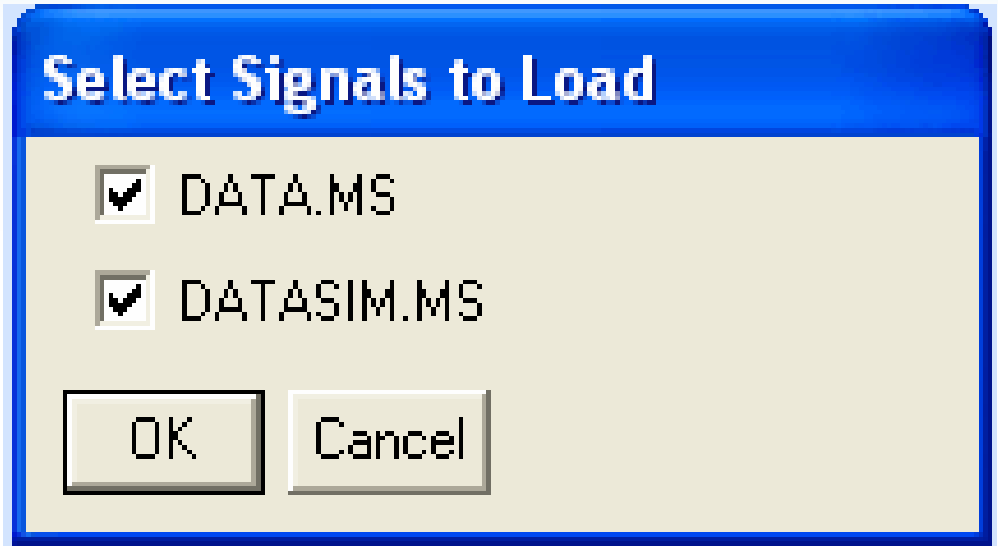
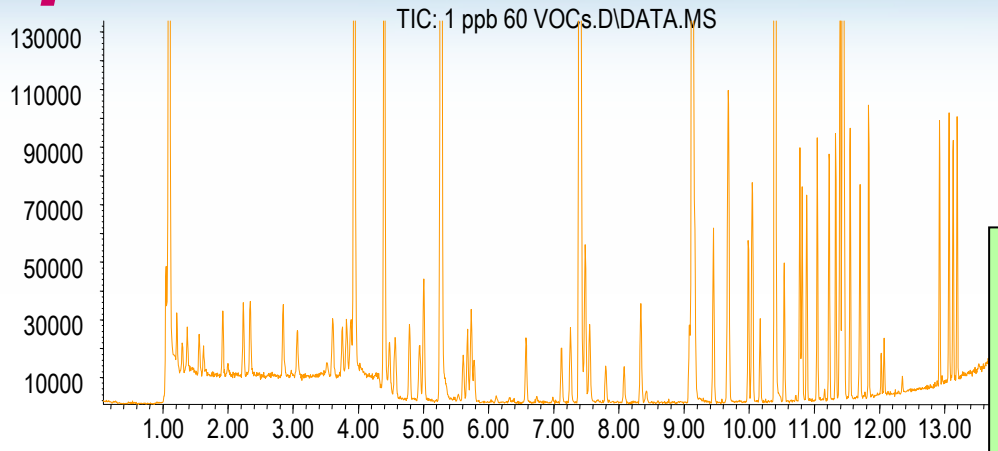
Set Up Synchronous SIM/Scan

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

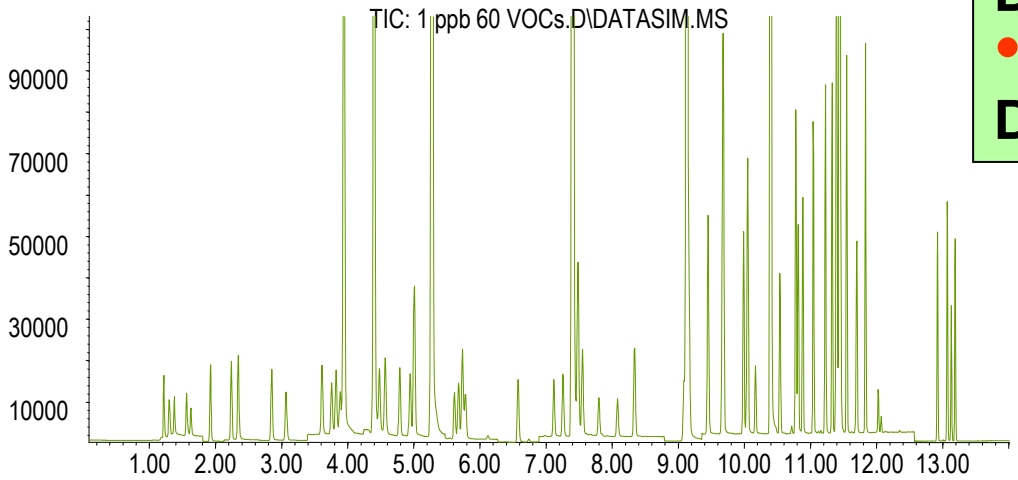


Scan and SIM Chromatograms from SIM/Scan Analysis of 60 VOCs at 1 ppb Each

Scan



SIM



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

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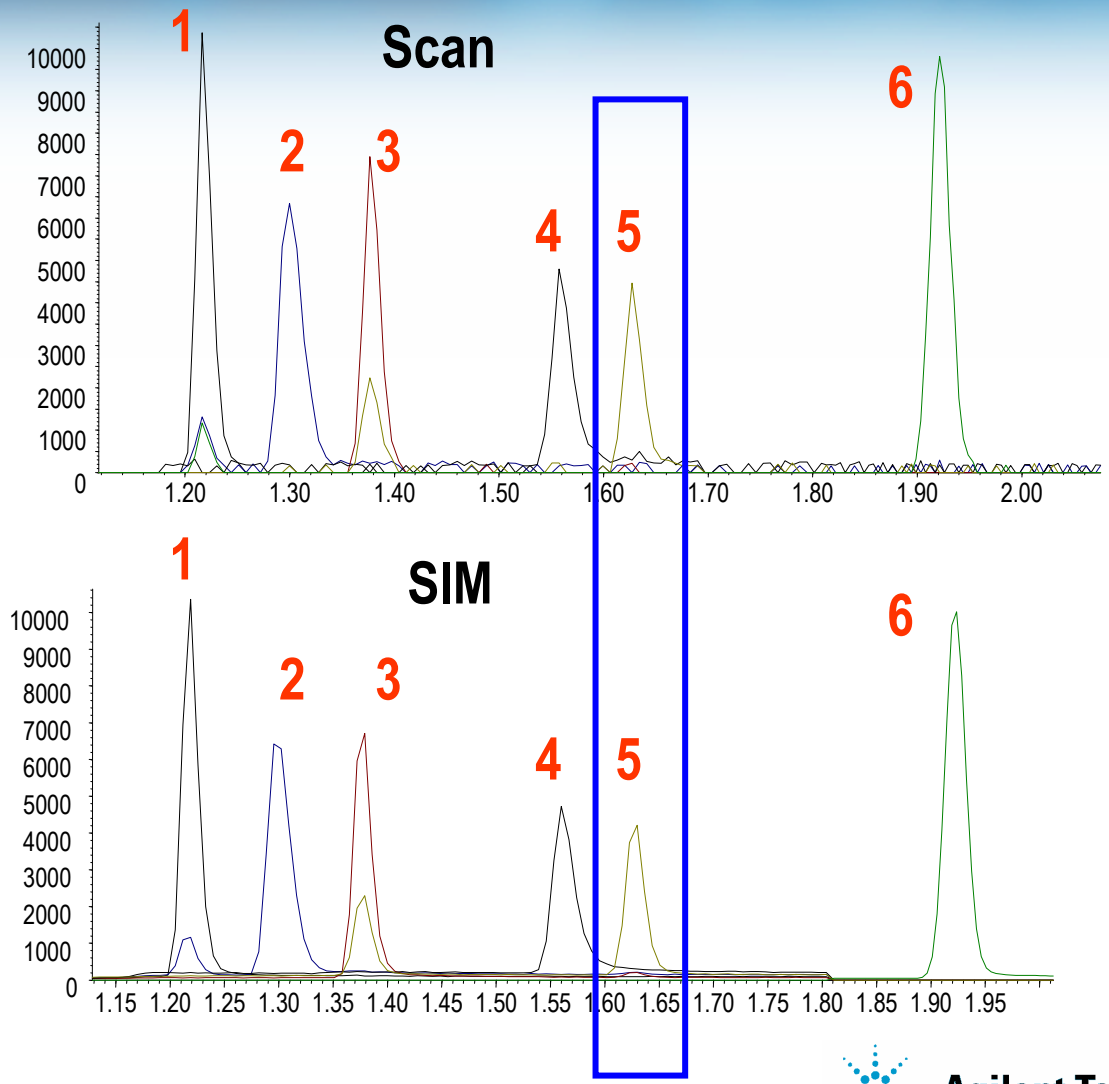
Synchronous SIM/Scan Analysis of VOC Target Gases at 1 ppb each



VOC Gases (1 ppb each)

1. Dichlorodifluoromethane
2. Chloromethane
3. Vinyl chloride
4. Bromomethane
5. **Ethyl chloride**
6. Trichlorofluoromethane

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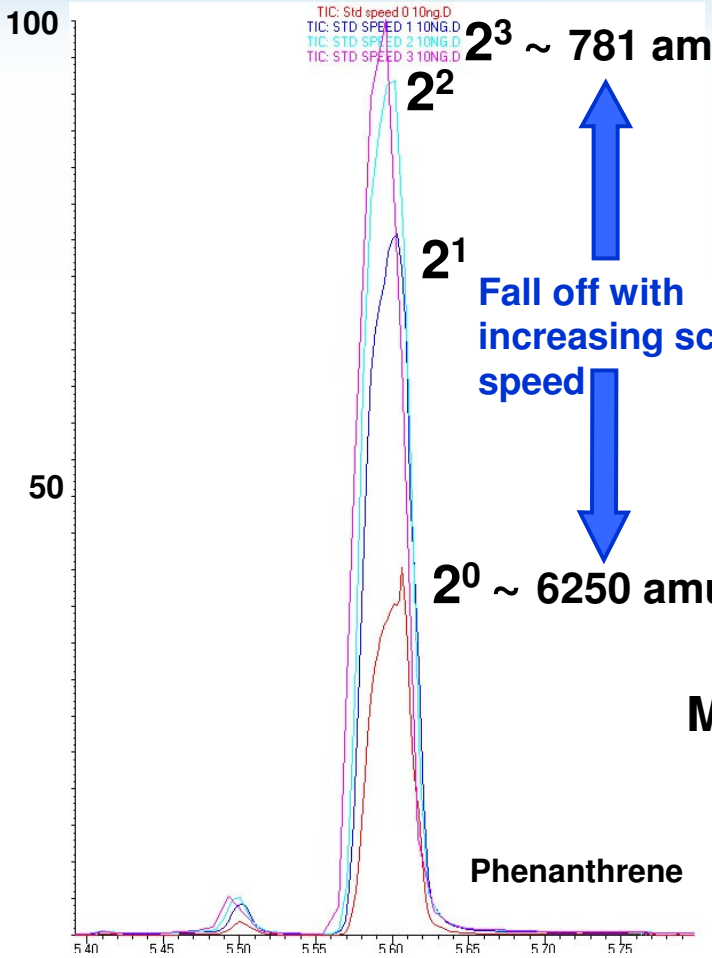
SIM/Scan and Scan-Only Sensitivity Comparison: 5-mL Purge of 1 ppb Ethyl Chloride (a Low Responding Gas)

	RMS S/N	Peak/Peak S/N
SIM (SIM/Scan)	749	254
Scan (SIM/Scan)	75	20
Scan (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



2^3 ~ 781 amu/sec

2^2

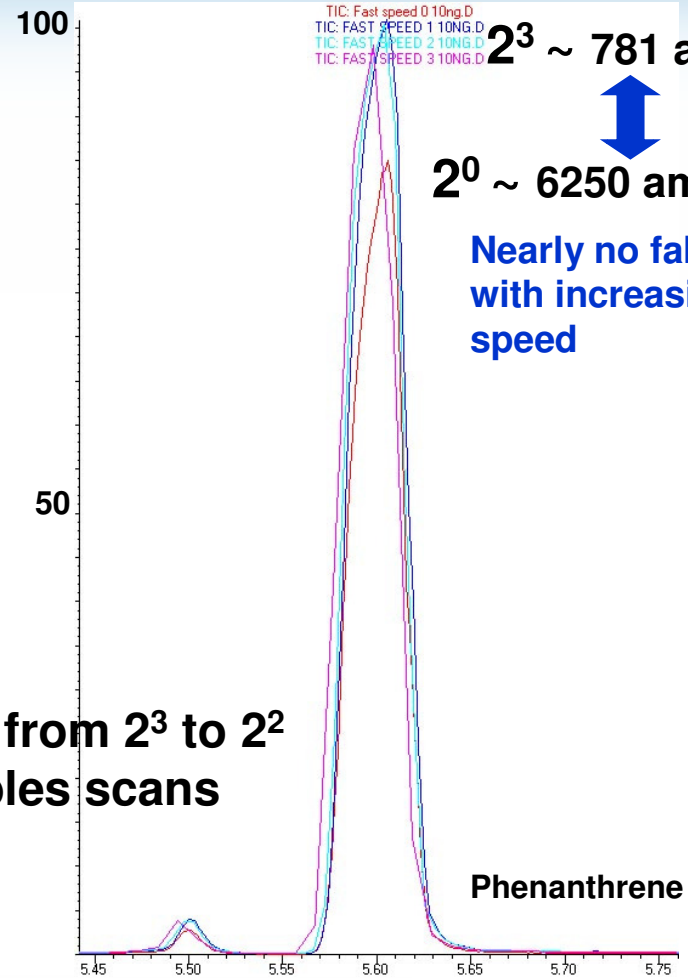
2^1

Fall off with increasing scan speed

2^0 ~ 6250 amu/sec

Phenanthrene

Performance Electronics



2^3 ~ 781 amu/sec

2^1 2^2

2^0 ~ 6250 amu/sec

Nearly no fall off with increasing scan speed

Phenanthrene

Moving from 2^3 to 2^2 doubles scans

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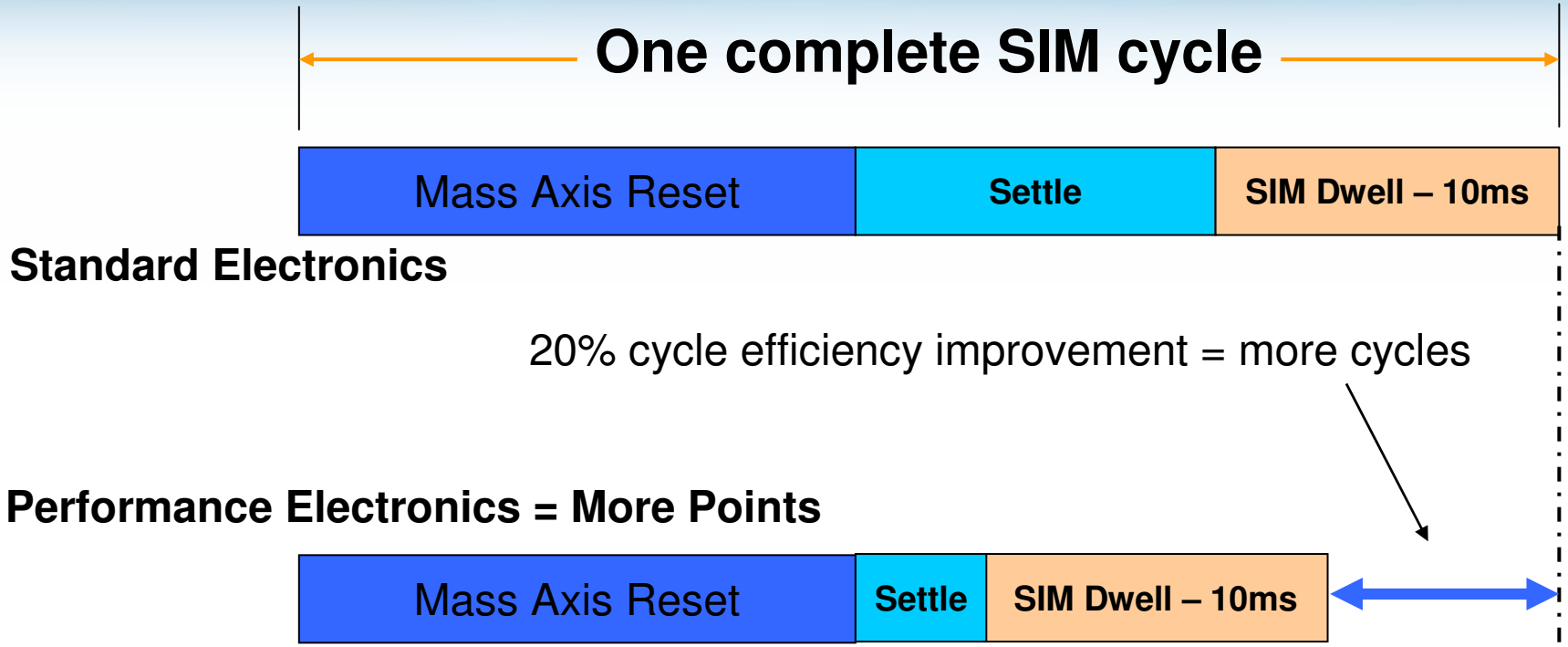
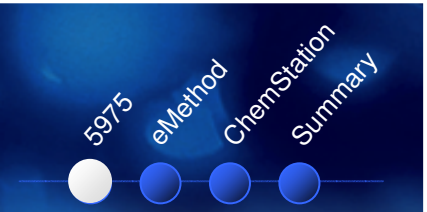
Why Our SIM/scan is So Good



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***

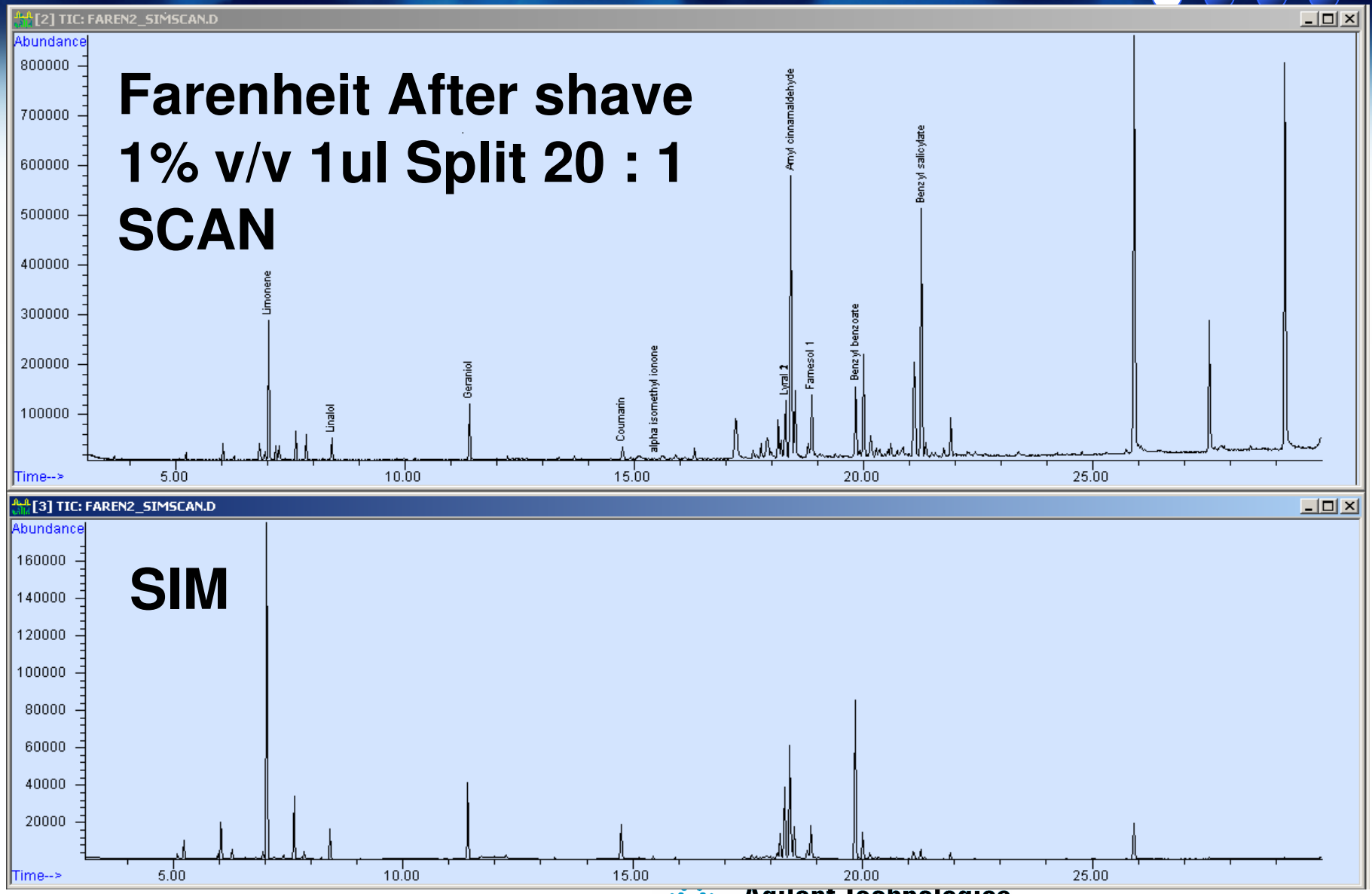
  - SIM table built with AUTOSIM

  - 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



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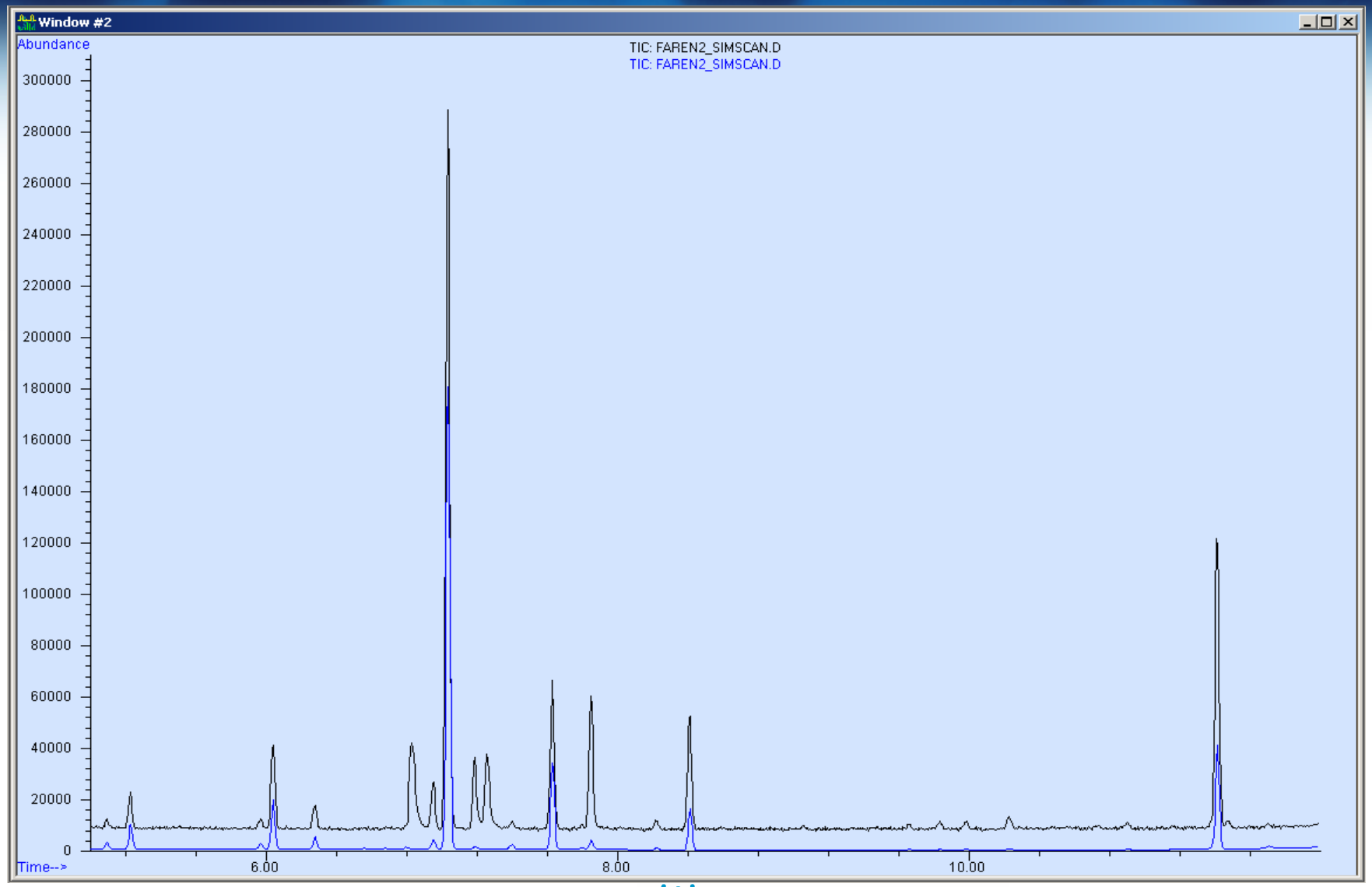
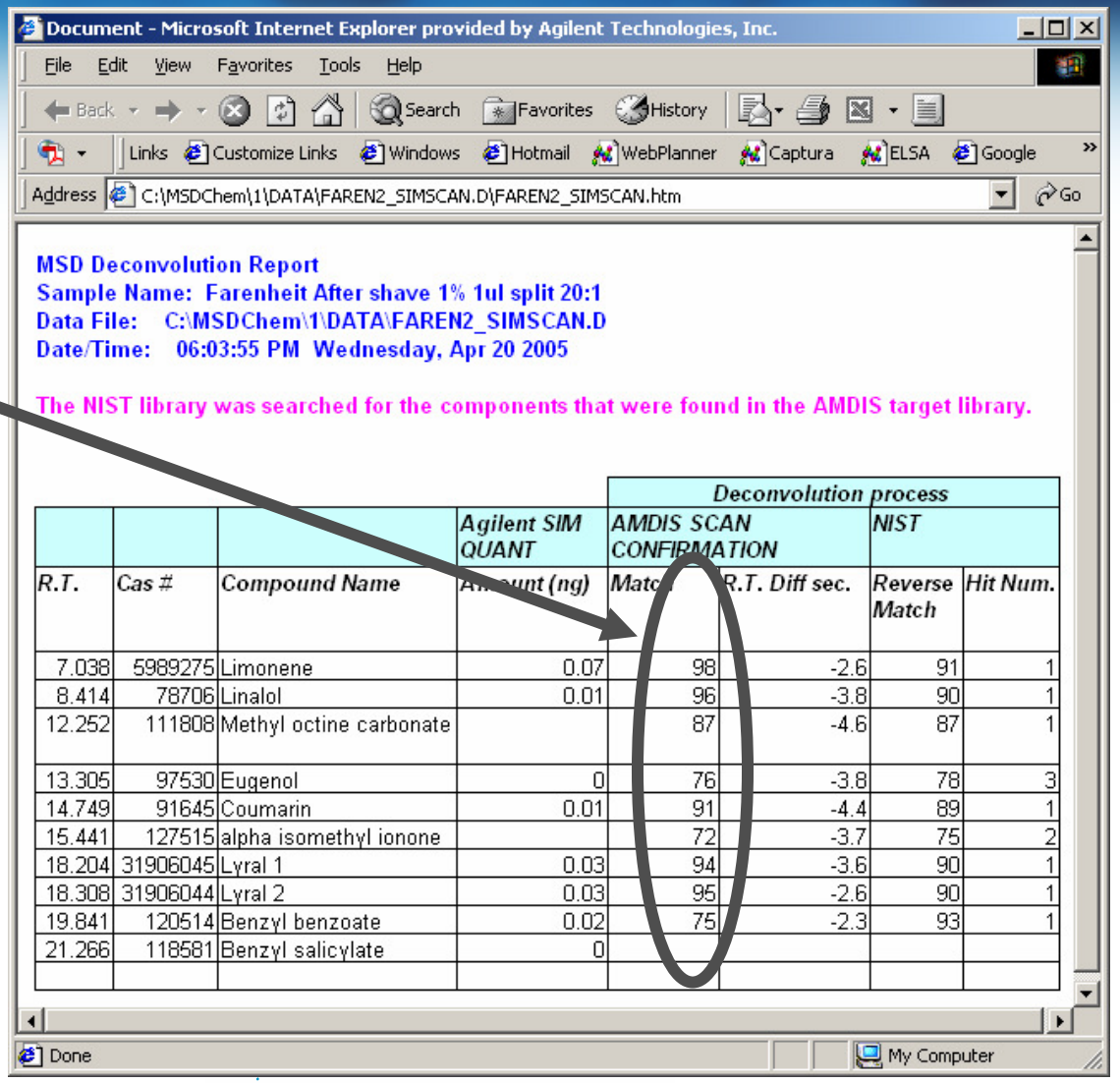
Allergens Overlaid SIM/Scan



Allergens SIM/Scan analysis and deconvolution with DRS

Match Factors

72 to 98



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Address C:\MSDChem\1\DATA\FAREN2_SIMSCAN.D\FAREN2_SIMSCAN.htm Go

MSD Deconvolution Report
Sample Name: Farenheit After shave 1% 1ul split 20:1
Data File: C:\MSDChem\1\DATA\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.

				Deconvolution process			
			Agilent SIM QUANT	AMDIS SCAN CONFIRMATION		NIST	
R.T.	Cas #	Compound Name	Amount (ng)	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	Lyral 1	0.03	94	-3.6	90	1
18.308	31906044	Lyral 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				

Done My Computer

With courtesy of Chris Sandy and J-F Garnier

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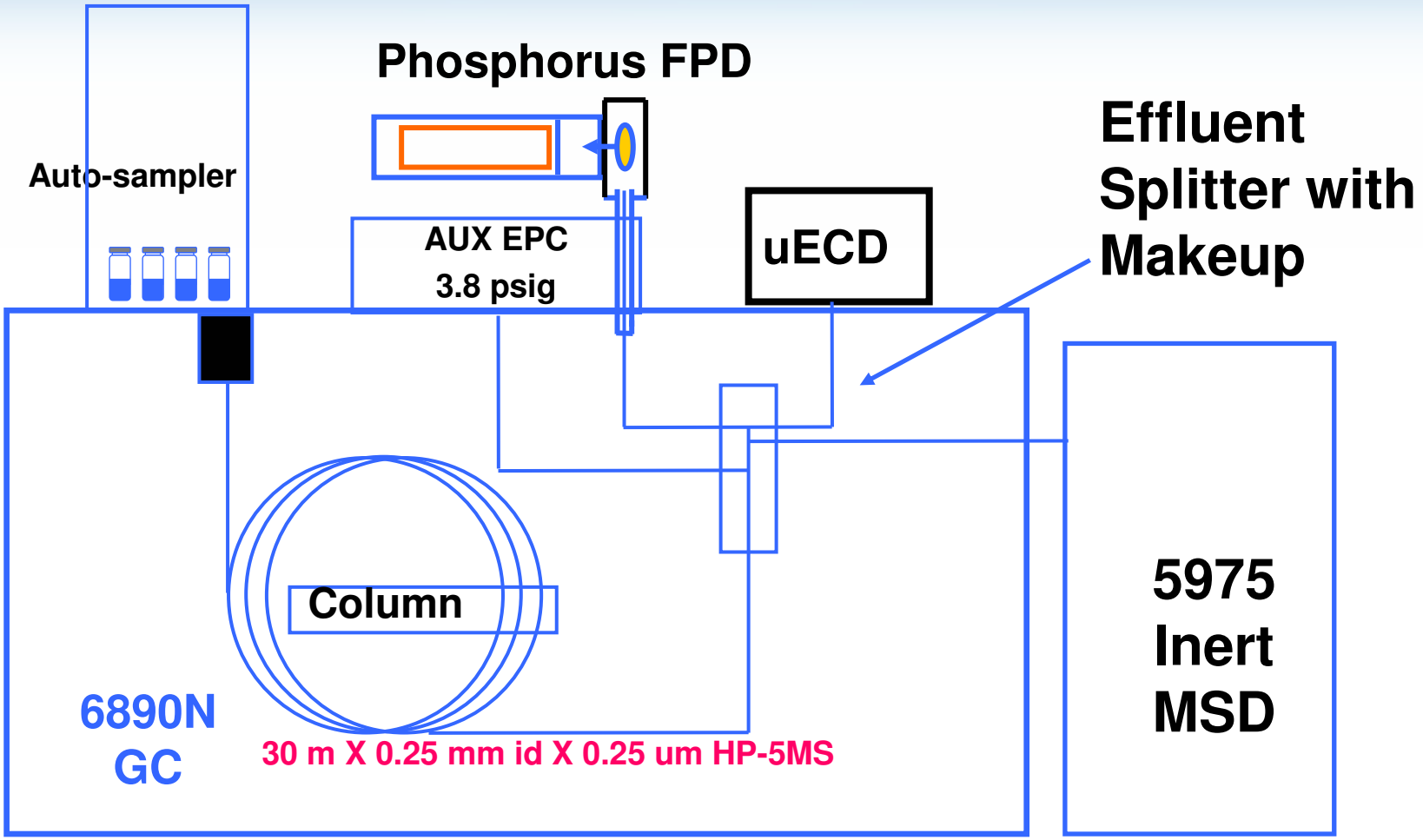
6890N/5975 inert Pesticide Analysis with 3-Way Splitter

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



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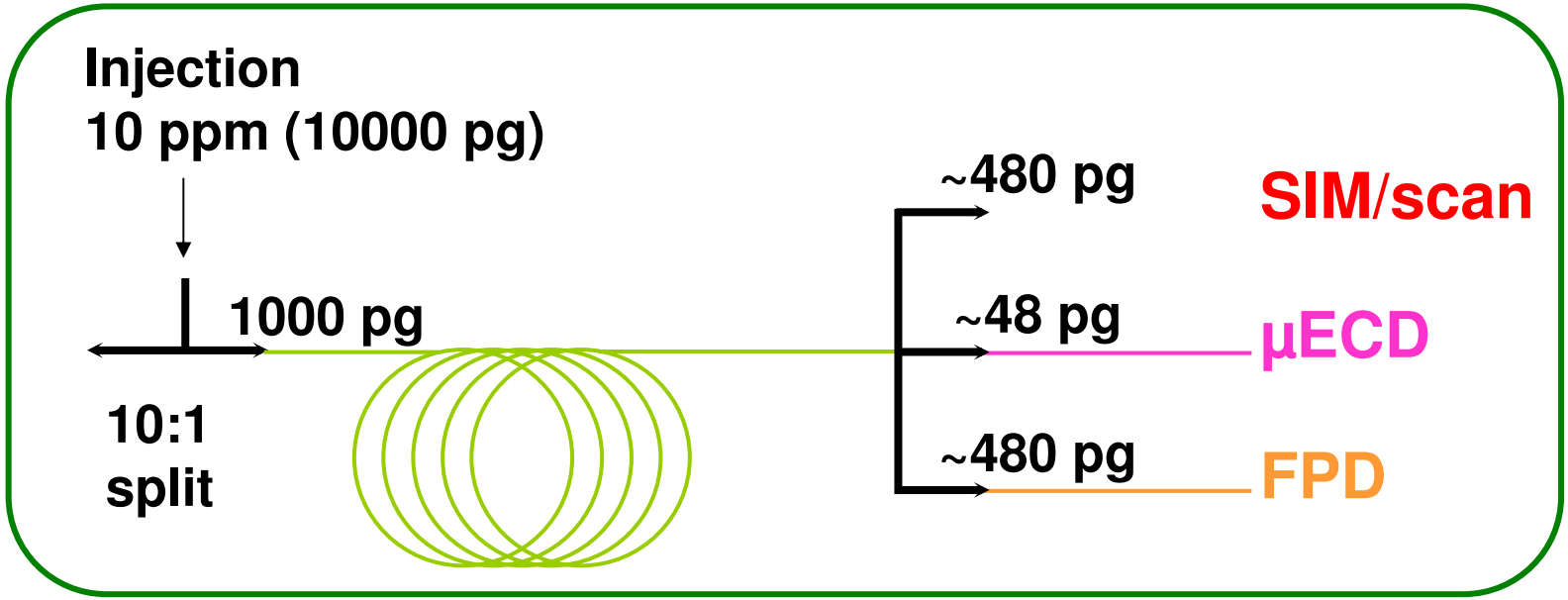
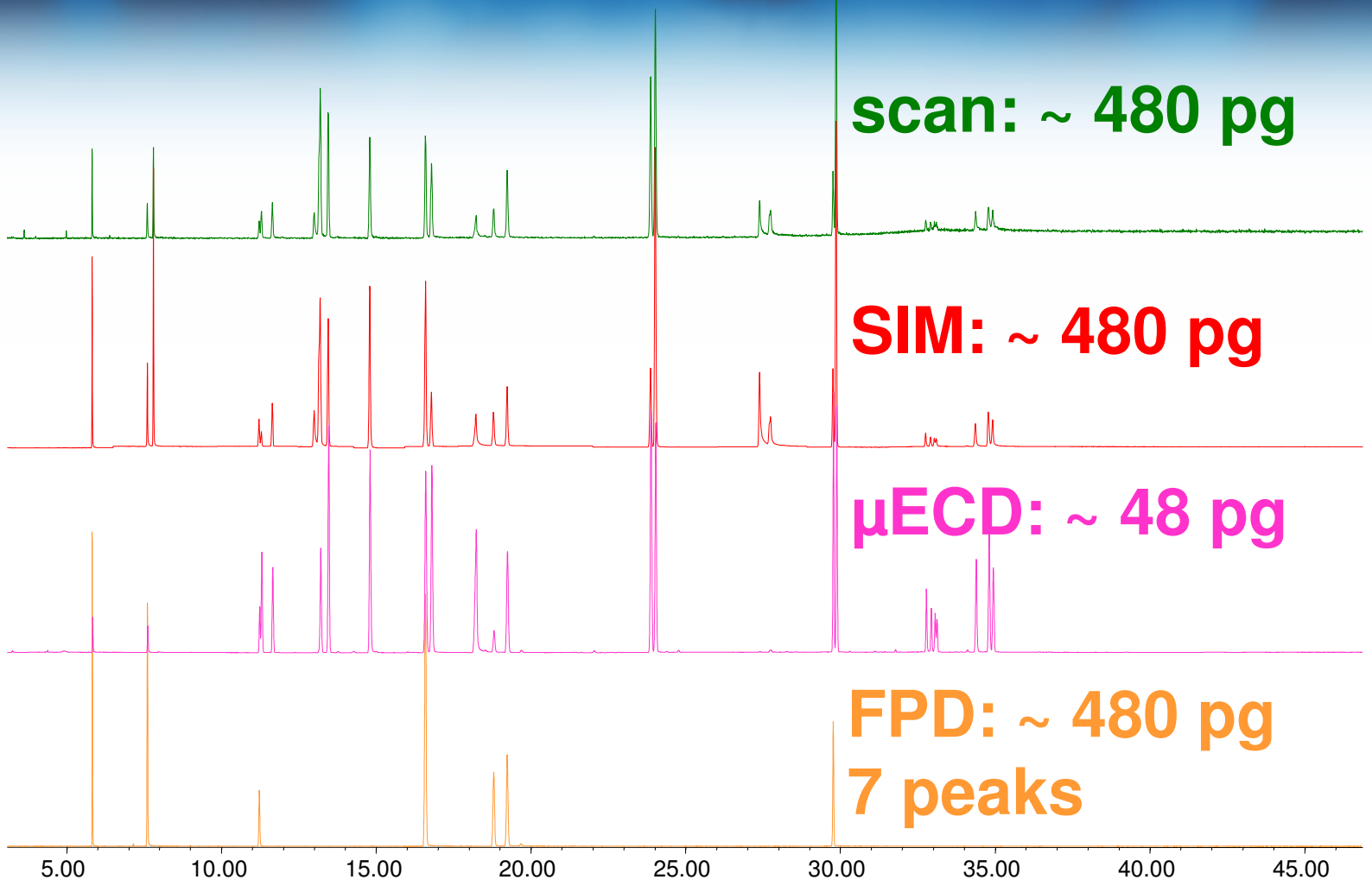
1-injection-4-signal System

- *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:µECD = 10:10:1*



Kai Meng, Bruce Quimby, M Szelewski
Agilent Technologies

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



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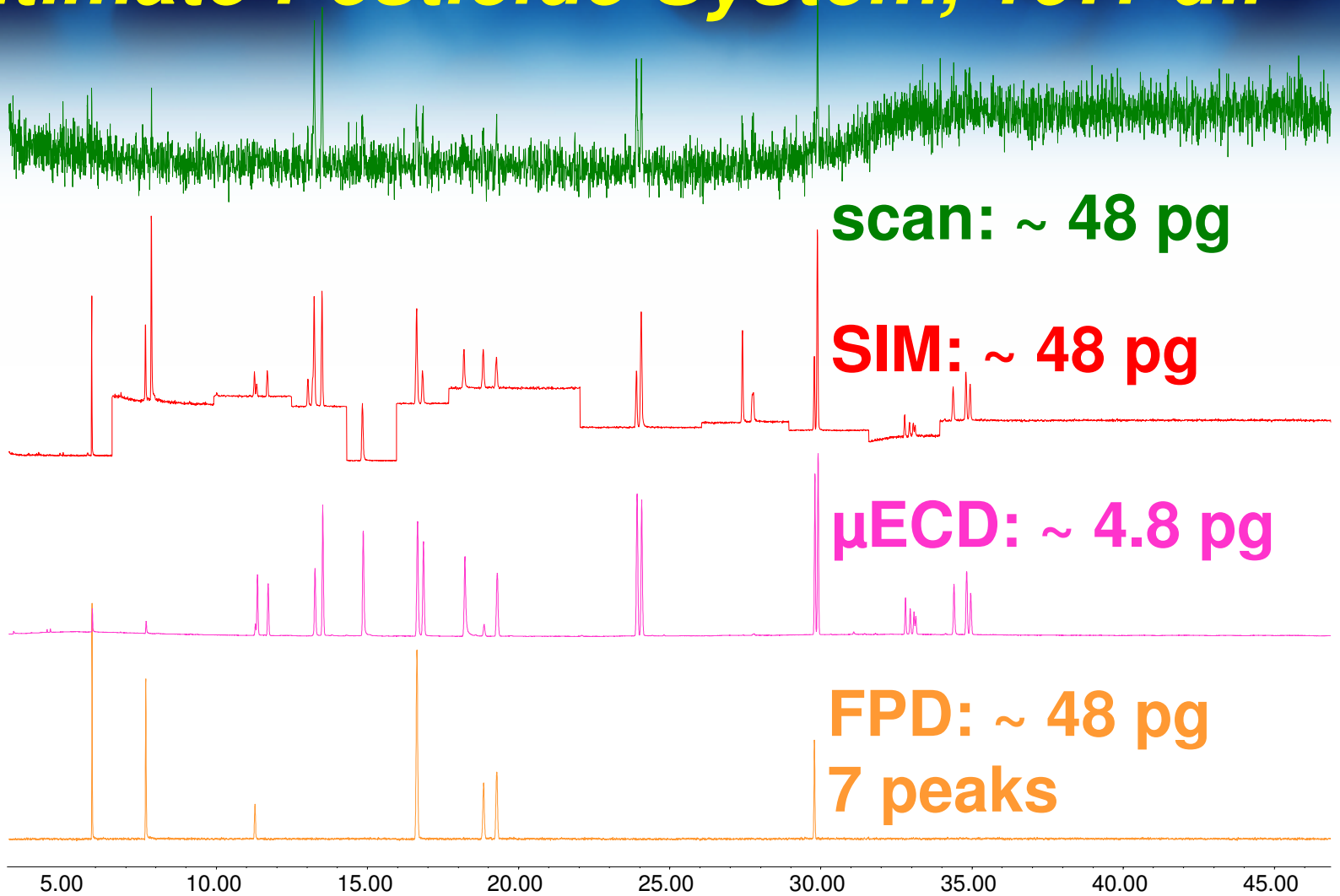
5975 SIM/scan + 3-way splitter
Ultimate Pesticide System, 10:1 dil

5975 eMethod ChemStation Summary



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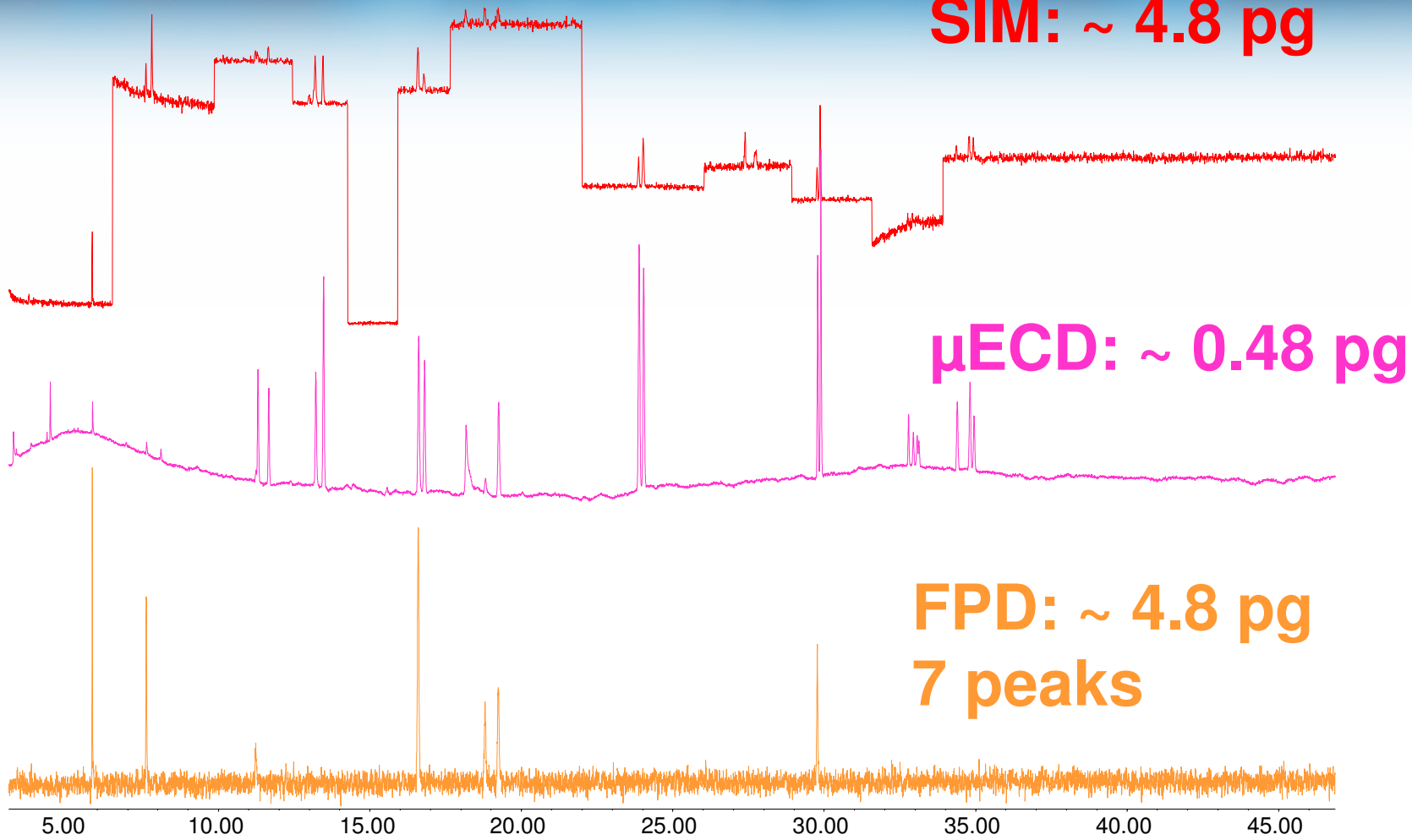
5975 SIM/scan + 3-way splitter
Ultimate Pesticide System, 100:1 dil

5975 eMethod ChemStation Summary



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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*

Introduction to eMethods and MSD Chemstation

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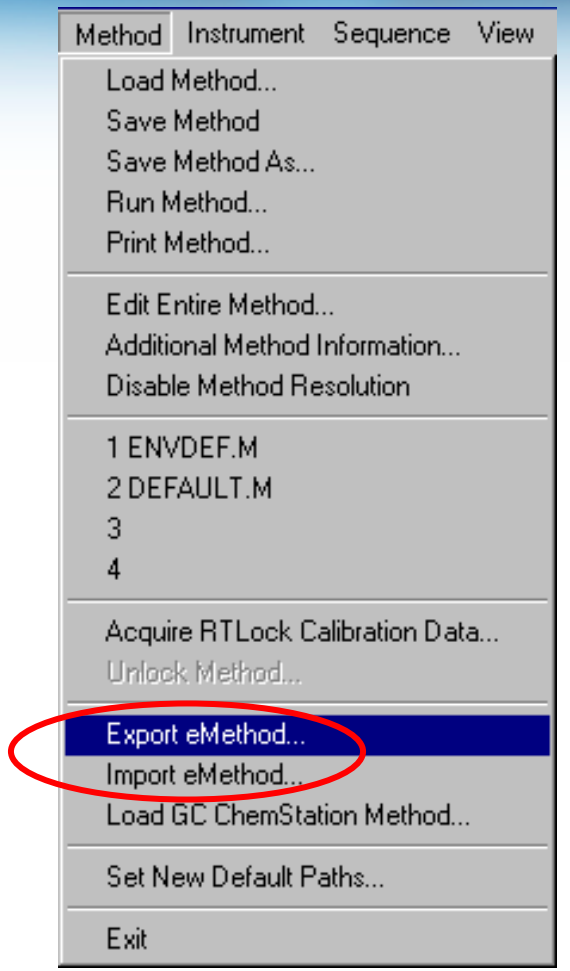
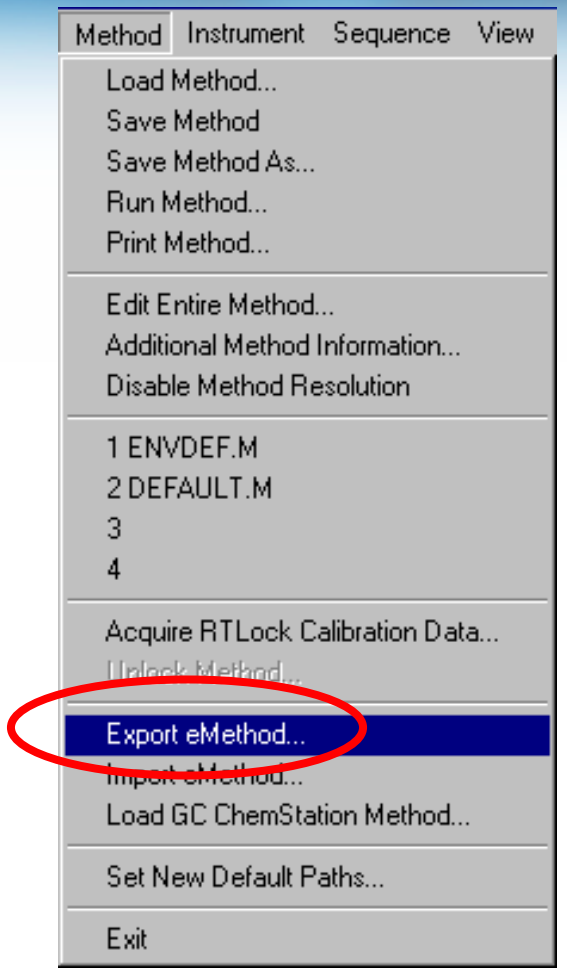
What are eMethods?

- ***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

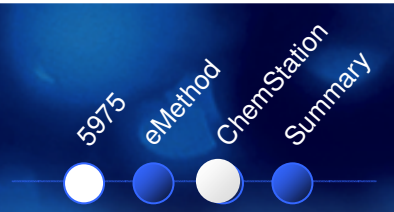


eMethod Benefits

- *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

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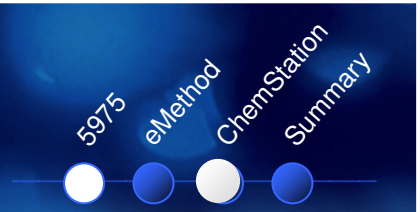
Instrument Control Enhancements



- *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*

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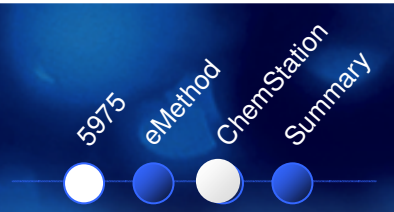
Data Analysis Enhancements

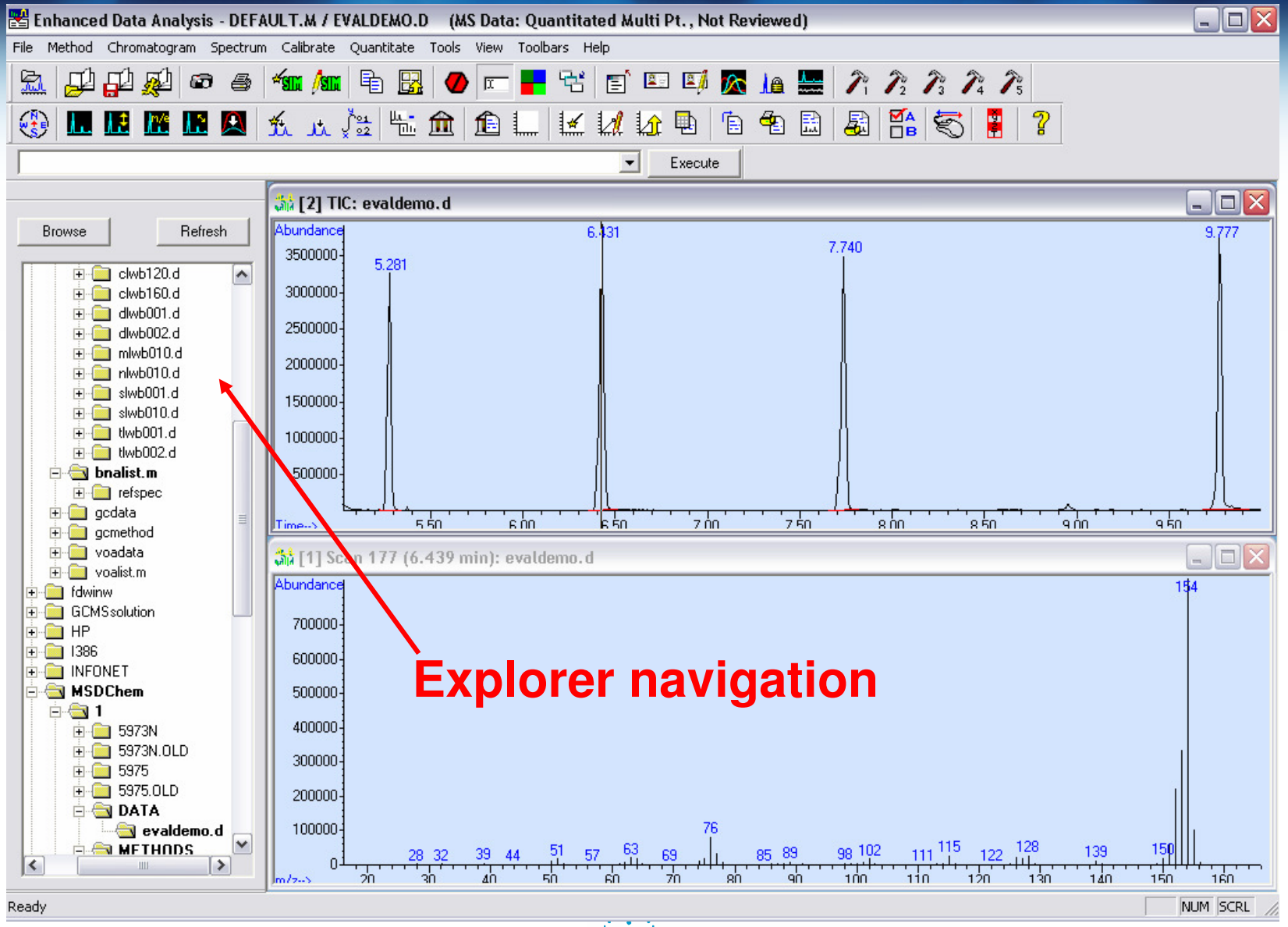


- *Explorer-style navigation tool*
- *Interactive editing of Integration Parameters*
- *Switchable right mouse click functions*
- *Spreadsheet-like SIM Parameters Table*
- *Icons for custom tools, DA options, variable watch*
- *Toolbar on/off capabiity*
- *Selectable DA color themes*

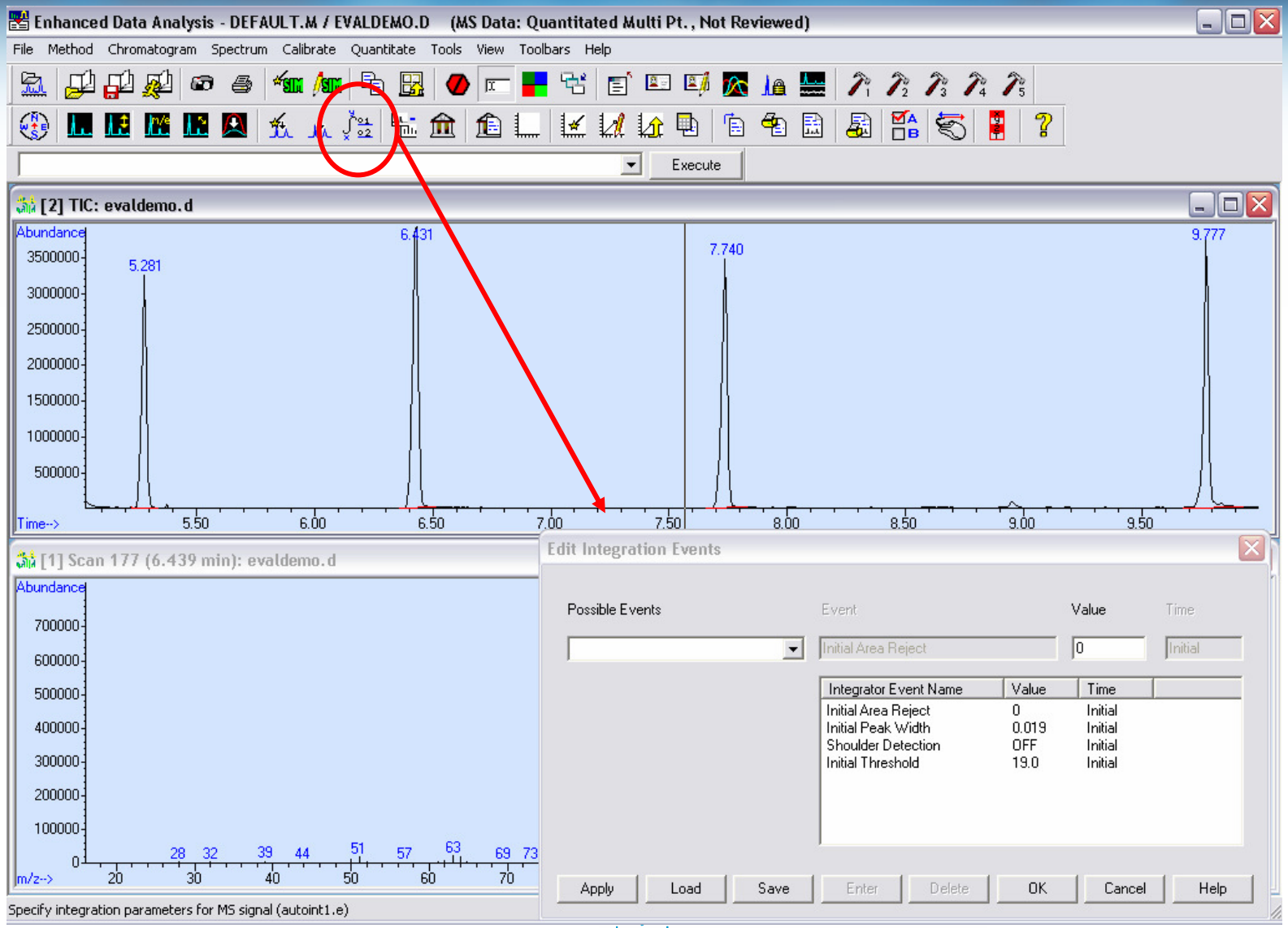
Data Analysis Enhancements

- ***QEdit functionality is improved:***
  - Separate window for Baseline Display
  - Generating reports directly from QEdit
  - Custom configuring X-axis

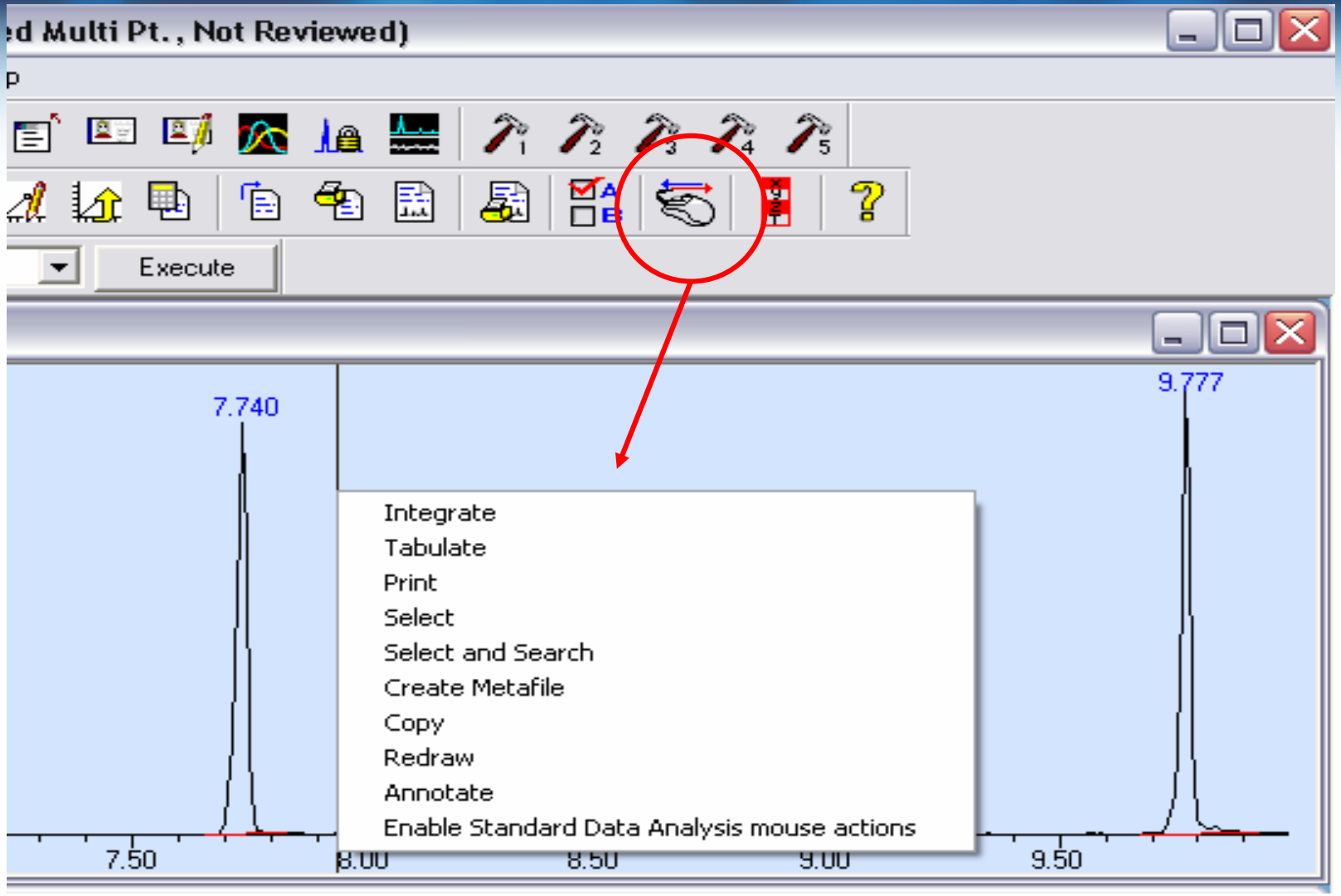
Explorer Navigation



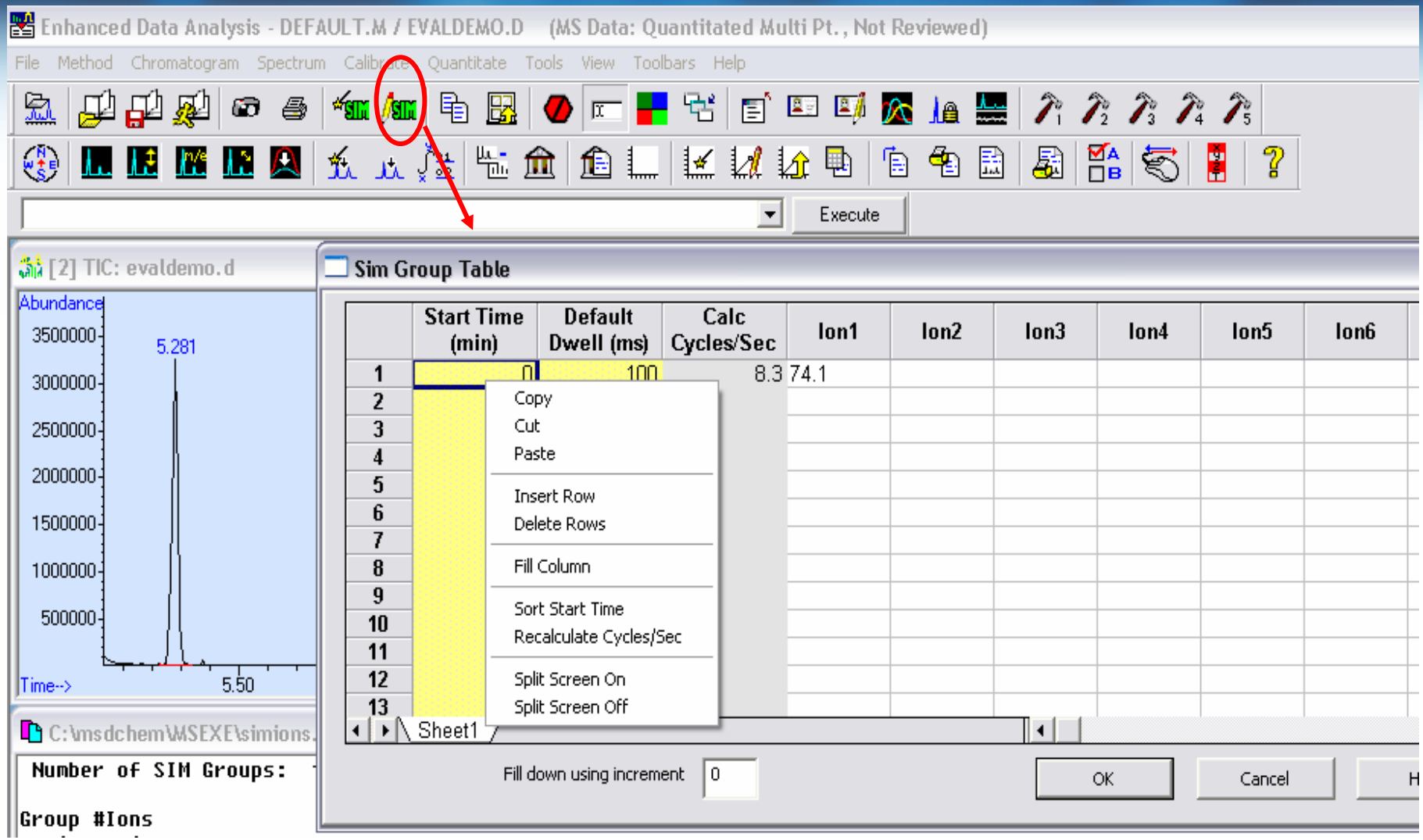
Interactive Edit Integration



Right Click Features



SIM Parameter Table



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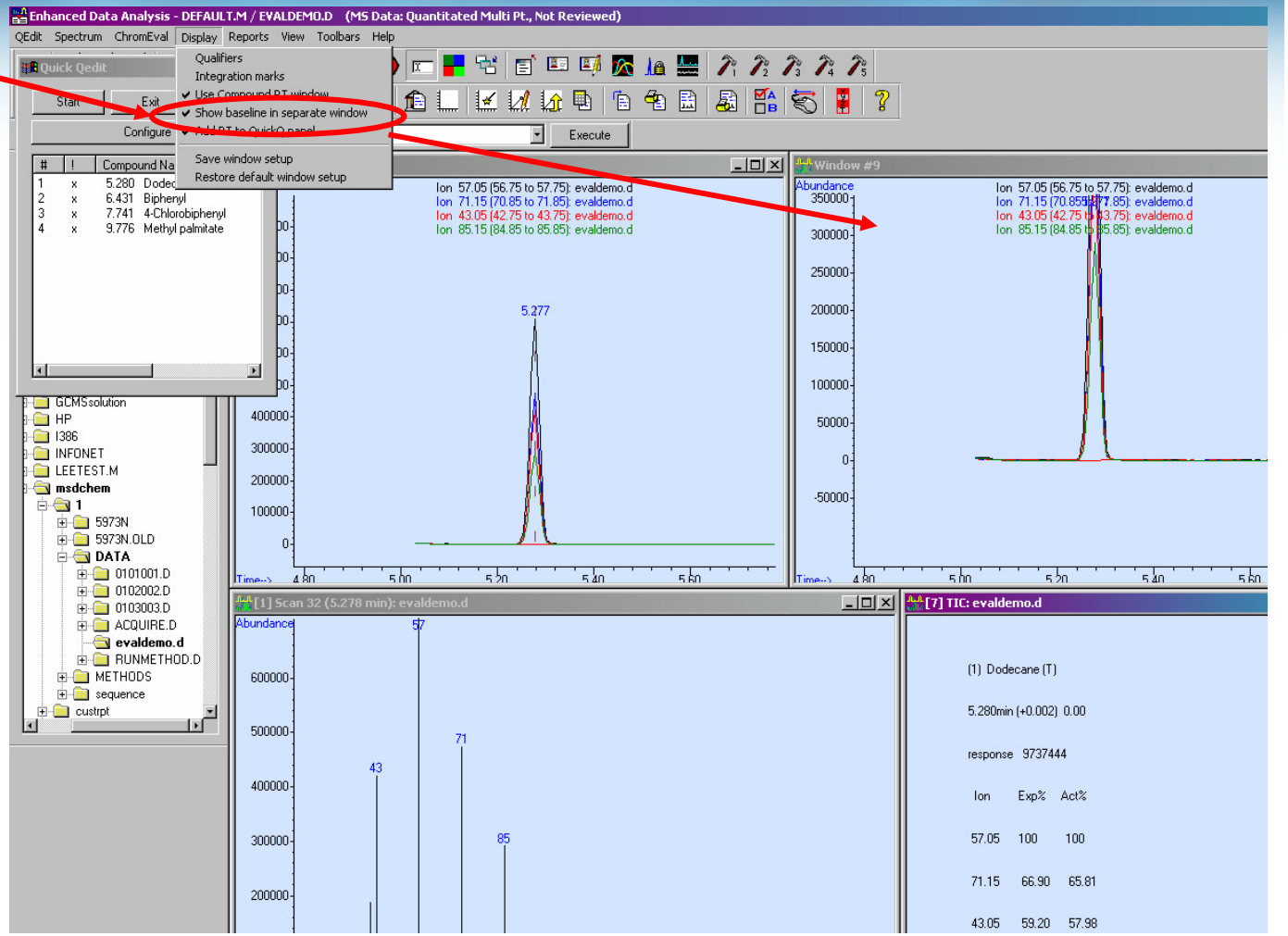
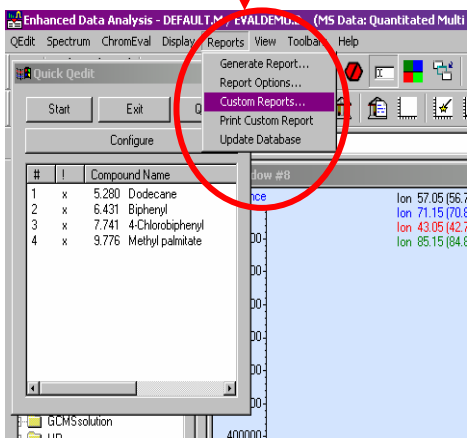
QEdit

Baseline Display



Reports



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Library Options

- *NIST05*
- *Wiley 7th ed*

NEW

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

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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Recht herzlichen Dank für Ihre Teilnahme an unserem E-Seminar.

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