

Can Your Mass Spec Data System Do This?

- Powerful Capabilities of Varian MS Workstation 6.91

by:

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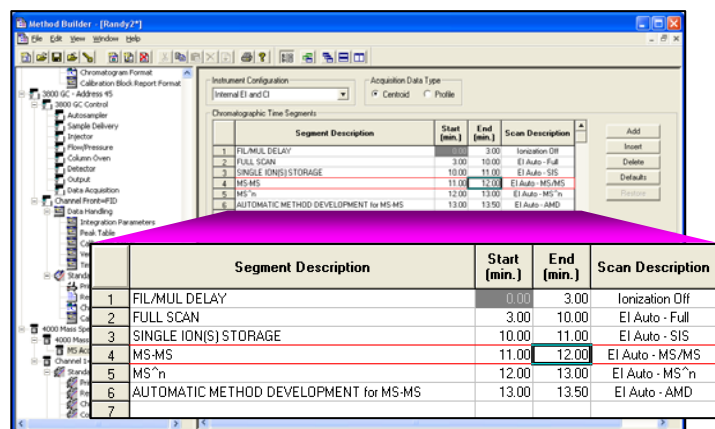
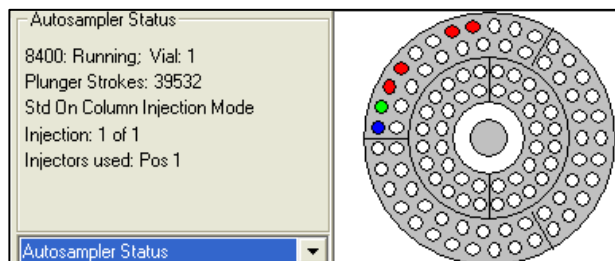
June 2, 2008

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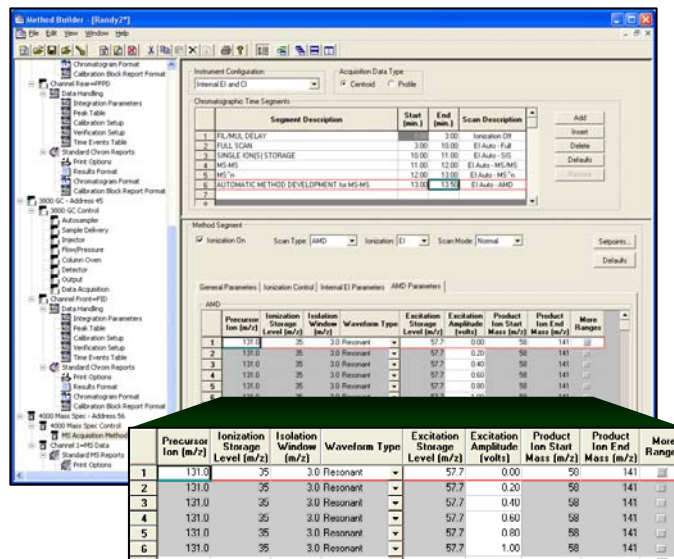
Mass spectrometry generates huge data sets of points in three dimensions of time vs mass versus intensity. These must be massaged and distilled into a simple report of analytes found and their concentrations. Getting there can be a journey, especially to assure that the results are accurate and complete. Varian has simplified the process through MS Workstation, and yet permits enough flexibility and adaptability to handle very complicated experiments and assurances that the answers are valid. This monograph illustrates some of the powerful capabilities available in Varian MS Workstation toward these goals.

Operator Interface

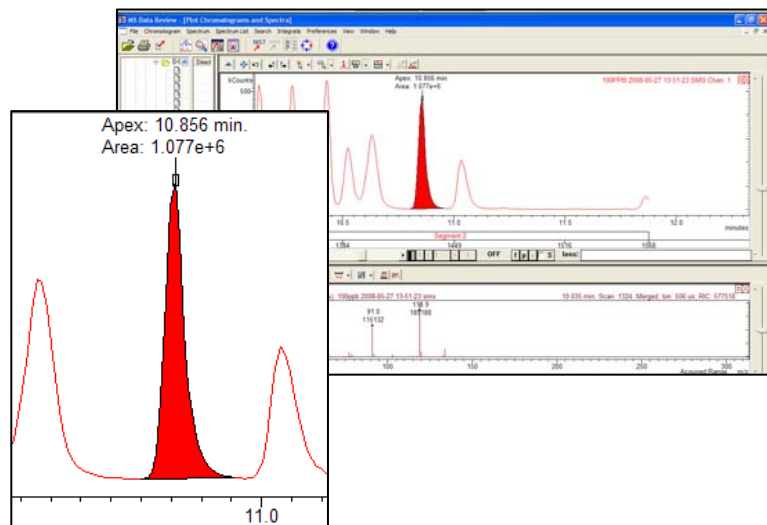
1. **Colorful AutoSampler™ Display** - **green** is active vial, **blue** vials have been completed and **red** are waiting to be run. Click on middle of carousel to get the active SampleList. Click on any vial to inject that single sample.



2. **Readily convert between Full Scan, Single Ion(s) Monitoring, MS-MS, MSⁿ and Chemical Ionization** in one chromatographic run.

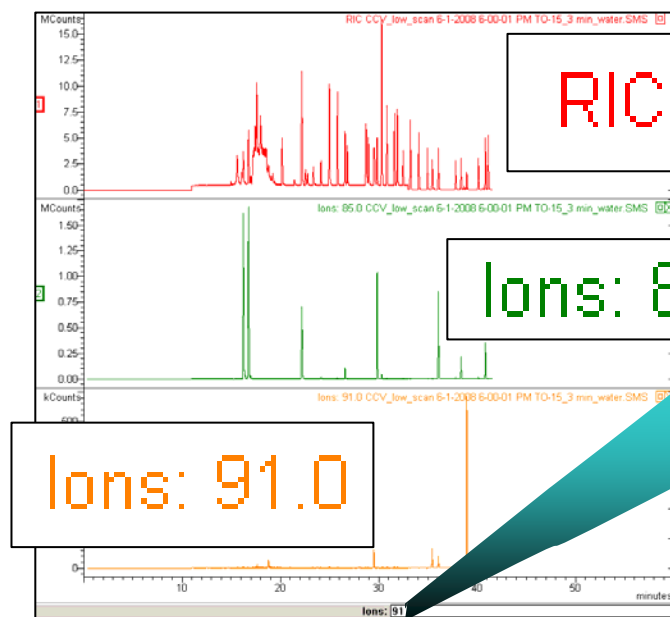
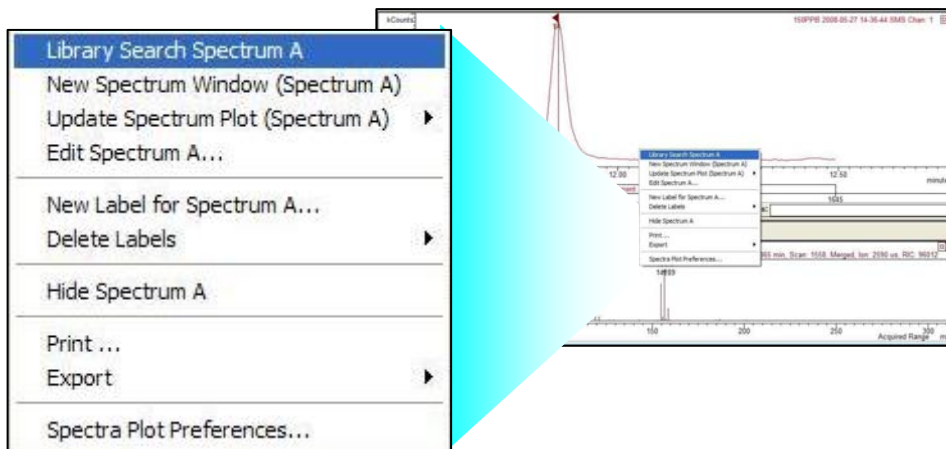


3. **Automatic Method Development for MS-MS**, to find optimum settings.

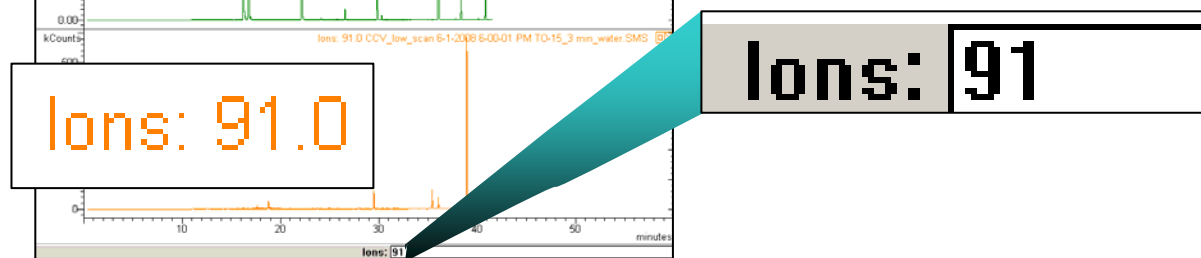


4. **Compute areas on live chromatogram.**

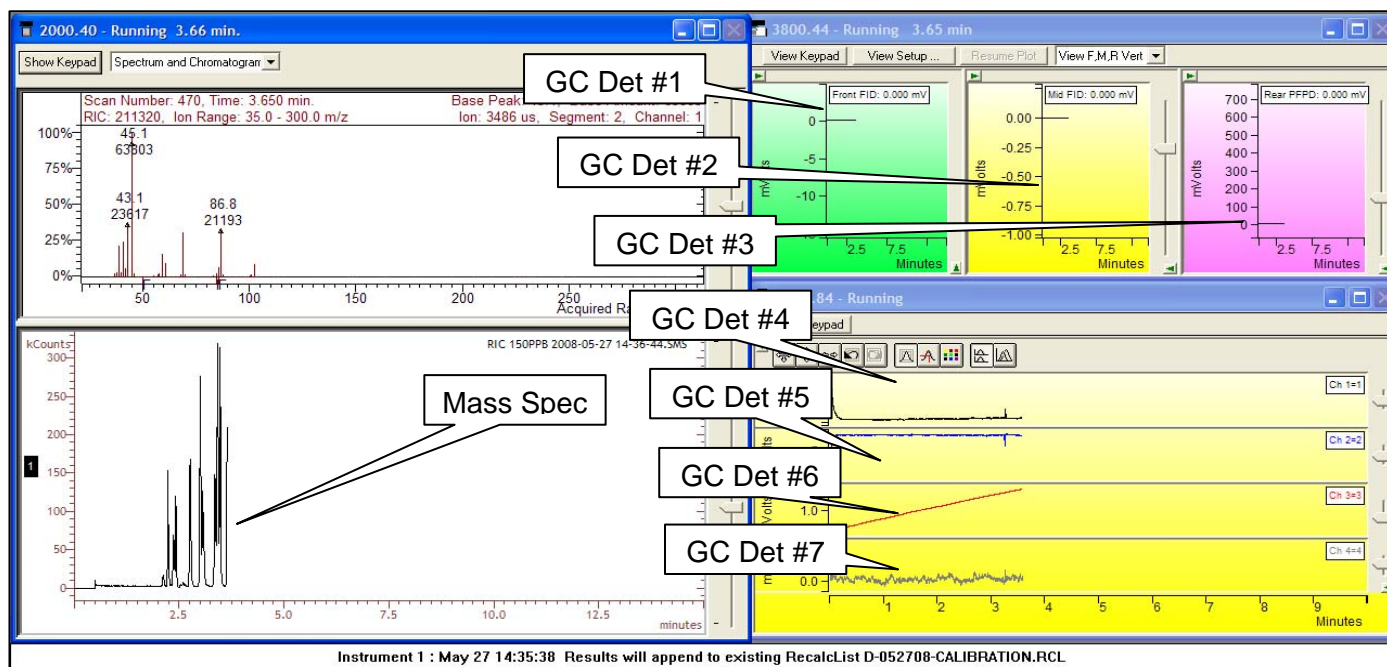
5. Library search live chromatogram readily.



6. Monitor single ions (or ion groups) in live chromatogram with System Control [with Varian 240, 4000, 1200 and 300 series MS only].



7. Simultaneously collect MS data, plus runs from up to 7 [sic] GC detectors with single method and single workstation



8. **Green light – Red light status** of GC thermal zones.

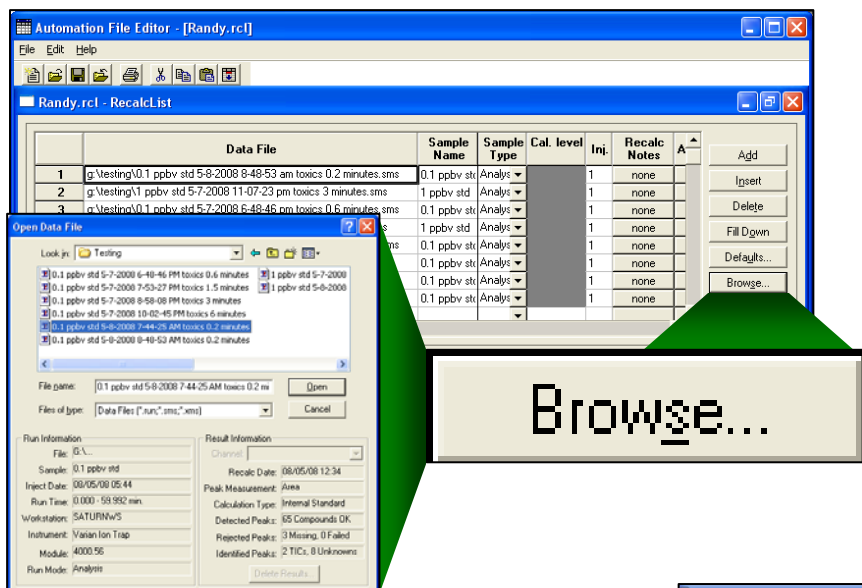
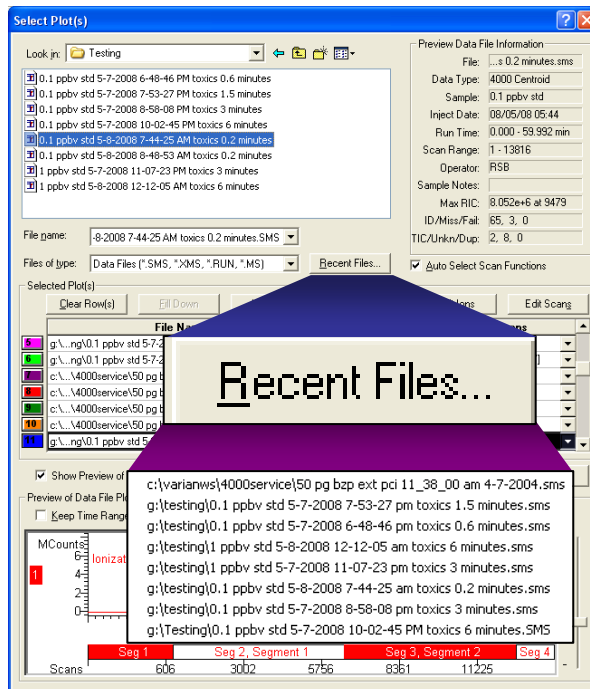
9. **Quick access to details of thermal zone** by clicking on zone label.

10. **Open data files/ methods/SampleLists/ sequences/RecalcLists** directly by double-clicking in Windows Explorer.

11. **Tool Bar** for easy access to any operation and recent run files and methods.

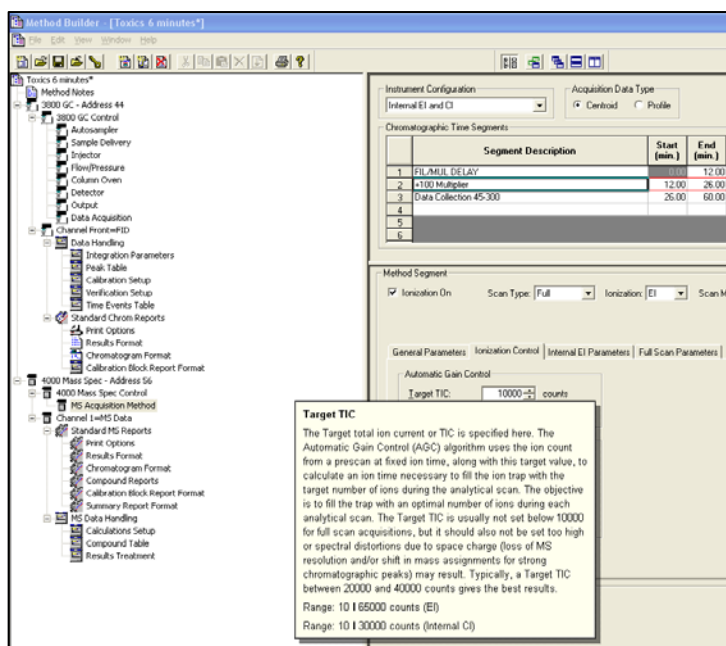
12. **Delete icons in Tool Bar** to simplify operations.

13. Recent Files button allows fast recovery of recent activities.



14. Browse button in many screens ensures proper path for desired file.

15. Get immediate Help with entry by right-clicking on most parameter-entry prompts to display detailed explanation.



16. Copy [ctrl C] and Paste [ctrl V] peak table details into Excel or Word.

The screenshot illustrates the process of copying peak table data from Method Builder to Microsoft Excel. On the left, the Method Builder window displays a table with the following data:

	RT	IS	Compound ID
1	16.019		Propylene
2	16.152		Dichlorodifluoromethane
3	16.672		1,2-Dichlorotetrafluoroethane
4	16.885		Chloromethane
5	17.336		Vinyl chloride
6	17.491		1,3-Butadiene
7	18.673		Bromomethane
8	19.109		Chloroethane
9	20.054		Trichlorofluoromethane
10	21.329		Ethanol
11	22.041		1,1-Dichloroethene
12	22.054		1,1,2-Trichlorotrifluoroethane
13	22.534		Acetone
14	22.660		Carbon disulfide
15	23.284		2-Propanol
16	24.016		Methylene Chloride
17	24.869		methyl-t-butyl ether
18	24.870		trans-1,2-dichloroethene
19	25.692		n-Hexane
20	26.456		1,1-Dichloroethane
21	26.699		Vinyl acetate
22	28.587		cis-1,2-Dichloroethene
23	28.656		2-Butanone

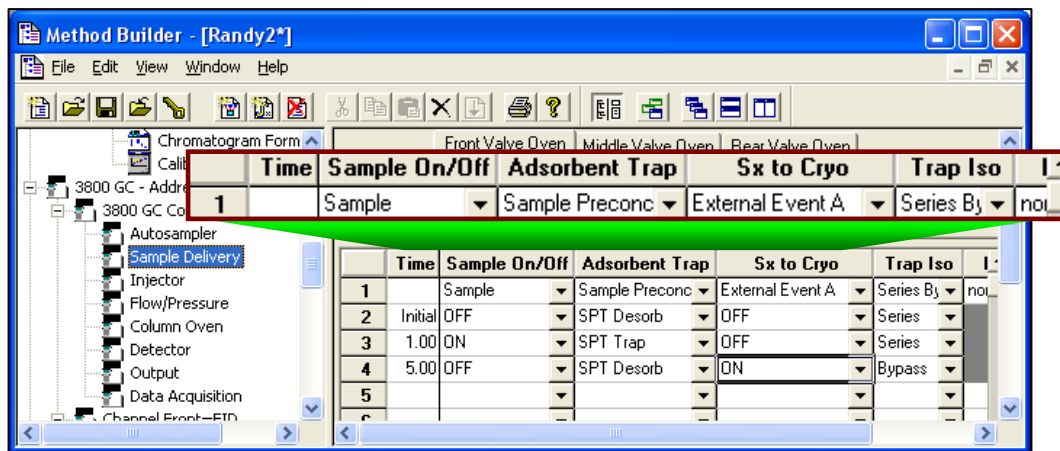
On the right, the Microsoft Excel window shows this data pasted into a spreadsheet. The columns are labeled RT, IS, Compound ID, and Quan Ion. The data is organized into rows corresponding to the peak numbers in the Method Builder window.

17. Relabeling headers for parameter entries by right-clicking on header to facilitate entries.

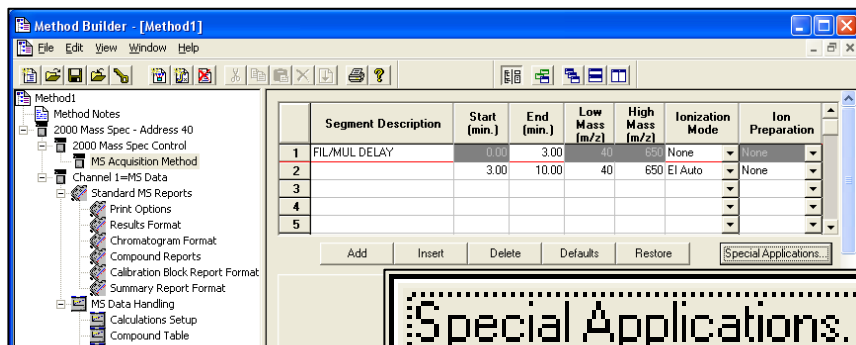
The screenshot shows the Automation File Editor window with a table containing parameter entries. The table has the following columns: Data File, Sample Name, dilution, weight, and MultiChar. A context menu is open over the 'Sample Name' header, providing options to relabel the header and reset columns to defaults.

	Data File	Sample Name	dilution	weight	MultiChar
1	g:\testing\0.1 ppbv std 5-7-2008 8-58-08 pm toxics 3 minutes.sms	0.1 ppbv std	10	0.972	none
2	g:\testing\0.1 ppbv std 5-7-2008 8-58-08 pm toxics 3 minutes.sms	0.1 ppbv std	10	0.728	none
3	g:\testing\0.1 ppbv std 5-7-2008 8-58-08 pm toxics 3 minutes.sms	0.1 ppbv std	10	0.976	none
4	g:\testing\0.1 ppbv std 5-7-2008 8-58-08 pm toxics 3 minutes.sms	0.1 ppbv std	10	0.957	none
5	g:\testing\0.1 ppbv std 5-7-2008 8-58-08 pm toxics 3 minutes.sms	0.1 ppbv std	10	0.957	none
6	g:\testing\0.1 ppbv std 5-7-2008 8-58-08 pm toxics 3 minutes.sms	0.1 ppbv std	10	0.728	none
7	g:\testing\0.1 ppbv std 5-7-2008 8-58-08 pm toxics 3 minutes.sms	0.1 ppbv std	10	0.976	none
8	g:\testing\0.1 ppbv std 5-7-2008 8-58-08 pm toxics 3 minutes.sms	0.1 ppbv std	10	0.957	none

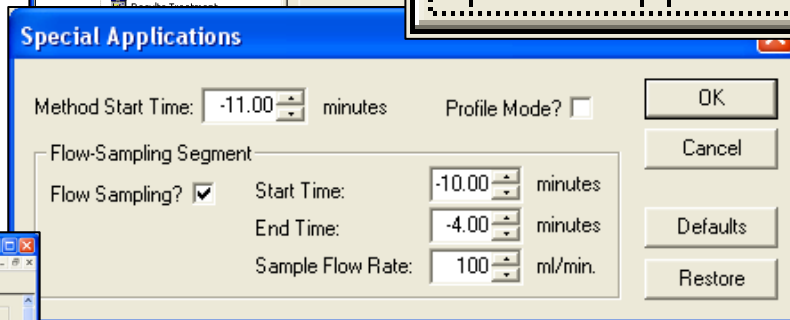
18. **Function-labeling for valve operations by right-clicking on header for clearer operations.**



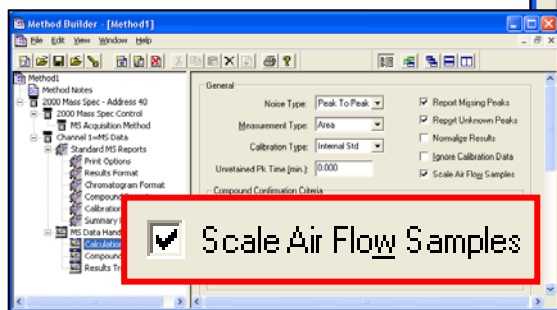
19. **User-selectable delay in start of MS data collection, for sample processing prior to injection. [2000 and 2200 only]**



20. **Method control of mass flow controller for air sample loading and documentation of volume in report. [2000 and 2200 only]**



21. **Correction to results for air sample volume loaded. [2000 and 2200 only]**



22. **Auto Start at specific clock time** – For example, the instrument can be set to perform a complete calibration sequence at 3 am, before work shift begins. Calibrations can be performed more often and still keep productivity up.

	Sample Name	Sample Type	Cal. level	Inj.	AutoLink	Rack
1		Autolink			WAIT 3:	
2	Aroclor 1221		1	1	none	1
3	Aroclor 1016		1	1	none	1
4	Aroclor 1231		1	1	none	1
5	Aroclor 1242		1	1	none	1
6	Aroclor 1248		1	1	none	1

AutoLink Parameters

Command

WAIT 3:

Data Review

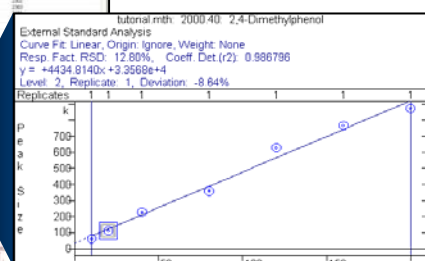
23. Single screen for data review of multiple data files for peak processing, graphically adjusting peaks, fine tuning calibration curves, calibration updates, and method adjustments. Peak summary display can be sorted by any header, such as Peak Name. Changes here generate updated information for all displays and are stored in data file and reports.

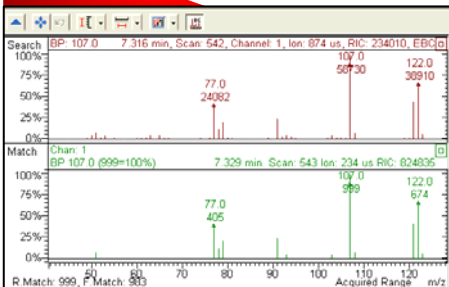
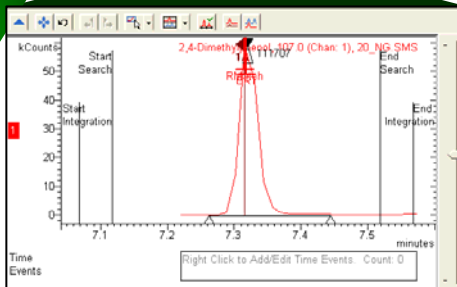
Data File	RT ...	Peak Name	S...	Result T...	Area	Amt/RF
120_NG.SMS	7.982	1,2,4-Trichlorobenzene		Identified	253271	2111
10_NG.SMS	7.984	1,2,4-Trichlorobenzene		Identified	27145	2715
20_NG.SMS	7.985	1,2,4-Trichlorobenzene		Identified	45621	2281
40_NG.SMS	7.992	1,2,4-Trichlorobenzene		Identified	96647	2416
50NG_CCC.SMS	7.993	1,2,4-Trichlorobenzene		Identified	144662	70.55
200_NG.SMS	7.996	1,2,4-Trichlorobenzene		Identified	361797	1809
80_NG.SMS	7.755	2,4-Dichlorophenol		Identified	150565	1882
160_NG.SMS	7.756	2,4-Dichlorophenol		Identified	365335	2221
120_NG.SMS	7.758	2,4-Dichlorophenol		Identified	276211	2302
10_NG.SMS	7.759	2,4-Dichlorophenol		Identified	23828	2383

Sample ID: ALLER/2000 **Operator:** EBE
Method: ALLER/2000 **Lab:** 08/02/15:17
Injection Type: AHA **Calibration Type:** External Standard
Injection Date: 08/02/15:17 **Sample No.:** 1
Injection Time: 08/02/15:17 **Method:** ALLER/2000

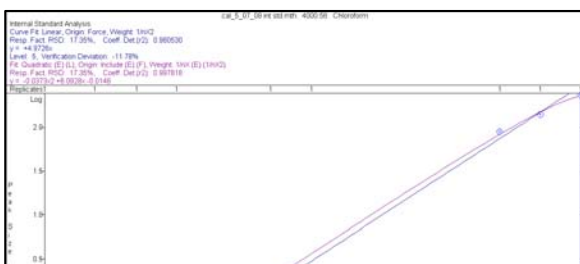
Compound Information:
Peak Name: 2,4-Dichlorophenol **Compound Name:** 2,4-Dichlorophenol **CAS Number:** 105-67-0 **MW:** 161.02

Integration:
Start: 7.316 min **End:** 7.324 min **Area:** 111707
Integration Type: Peak **Integration Method:** Peak **Integration Status:** Pass





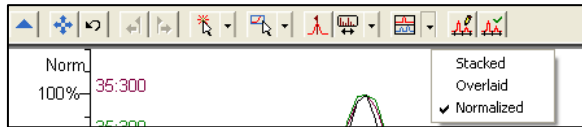
24. View and compare two curve fits and apply chosen one to method.



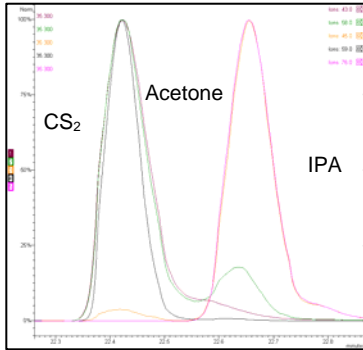
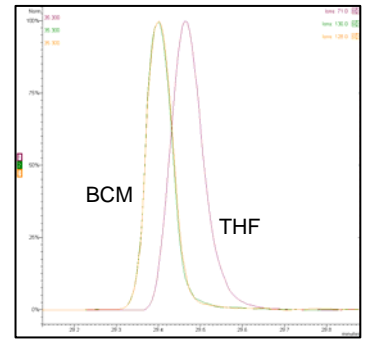
Overlay

	Overlay Curve 1	Overlay Curve 2
Curve Fit Type:	Linear	Quadratic
Origin Point:	Force	Force
Regression:	1/n^2	1/n

25. Normalize and overlay ion peaks to aid in sorting out identifications.



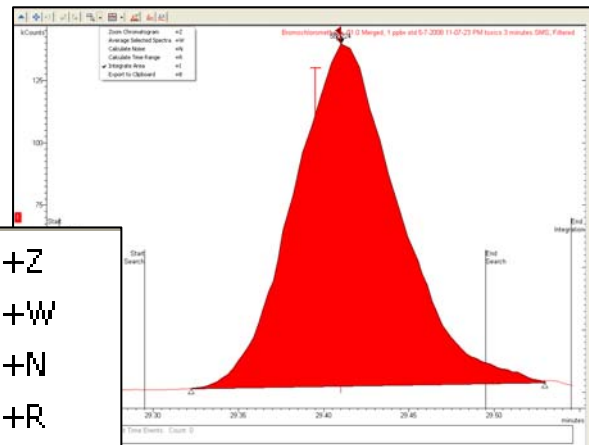
Confirmation of separation for Bromochloromethane and Tetrahydrofuran.



Demonstration of close elution of Carbon Disulfide and acetone, with separation from 2-Propanol.

26. Graphical assignment of baseline.

- Zoom Chromatogram +Z
- Average Selected Spectra +W
- Calculate Noise +N
- Calculate Time Range +R
- ✓ Integrate Area +I
- Export to Clipboard +B



Method Builder - [CAL_5_07_00 A]

Verification Results

Deviation Tolerance %: 30.0

Out Of Tolerance Action:

- Increment Error Count
- No Action
- Increment Error Count
- Terminate Sample List
- Halt Automation

27. Verification runs for easy check of quality control results. Deviations from anticipated concentrations are reported and if fails test, then a specified action can occur, including a halt to operations.

Calib Amt	Amt/RF	Dev%-Amt
0.530	0.585	10.306
0.520	0.513	-1.296
1.800	1.800	---
0.520	0.469	-9.865
0.520	0.580	10.306

Verification Deviation	+/- 30.00%	10.31%	Pass
------------------------	------------	--------	------

28. Easy graphical access to timed events for peak processing and adjust with mouse actions.

Peak No.	Retention Time (min)	Peak Name
35	35.300	2,4-Dichlorophenol
42	35.300	2,4-Dichlorophenol
52	35.300	2,4-Dichlorophenol
80	35.300	2,4-Dichlorophenol
102	35.300	2,4-Dichlorophenol
120	35.300	2,4-Dichlorophenol
140	35.300	2,4-Dichlorophenol
160	35.300	2,4-Dichlorophenol
180	35.300	2,4-Dichlorophenol
200	35.300	2,4-Dichlorophenol
220	35.300	2,4-Dichlorophenol
240	35.300	2,4-Dichlorophenol
260	35.300	2,4-Dichlorophenol
280	35.300	2,4-Dichlorophenol
300	35.300	2,4-Dichlorophenol
320	35.300	2,4-Dichlorophenol
340	35.300	2,4-Dichlorophenol
360	35.300	2,4-Dichlorophenol
380	35.300	2,4-Dichlorophenol
400	35.300	2,4-Dichlorophenol
420	35.300	2,4-Dichlorophenol
440	35.300	2,4-Dichlorophenol
460	35.300	2,4-Dichlorophenol
480	35.300	2,4-Dichlorophenol
500	35.300	2,4-Dichlorophenol
520	35.300	2,4-Dichlorophenol
540	35.300	2,4-Dichlorophenol
560	35.300	2,4-Dichlorophenol
580	35.300	2,4-Dichlorophenol
600	35.300	2,4-Dichlorophenol
620	35.300	2,4-Dichlorophenol
640	35.300	2,4-Dichlorophenol
660	35.300	2,4-Dichlorophenol
680	35.300	2,4-Dichlorophenol
700	35.300	2,4-Dichlorophenol
720	35.300	2,4-Dichlorophenol
740	35.300	2,4-Dichlorophenol
760	35.300	2,4-Dichlorophenol
780	35.300	2,4-Dichlorophenol
800	35.300	2,4-Dichlorophenol
820	35.300	2,4-Dichlorophenol
840	35.300	2,4-Dichlorophenol
860	35.300	2,4-Dichlorophenol
880	35.300	2,4-Dichlorophenol
900	35.300	2,4-Dichlorophenol
920	35.300	2,4-Dichlorophenol
940	35.300	2,4-Dichlorophenol
960	35.300	2,4-Dichlorophenol
980	35.300	2,4-Dichlorophenol
1000	35.300	2,4-Dichlorophenol

- WT: Add Width
- LI: Add Integration Inhibit
- SR: Add Solvent Reject
- GR: Add Group Peak
- VB: Add Valley Baseline
- FP: Add Forced Peak
- SP: Add Split Peak
- HF: Add Horizontal Forwards
- HB: Add Horizontal Backwards
- HM: Add Horizontal Minimum
- SN: Add Signal to Noise Ratio
- TP: Add Tangent Percent
- PR: Add Peak Reject

Edit Time Events

29. Export chromatogram or spectrum into .WMF Picture File and edit display for publication.

Print...
 Export
 Chromatogram Plot Preferences...
 Plot 1
 Chromatogram Pane
 Clipboard
 Picture File...

MCounts

35:300

3.0
2.5
2.0
1.5
1.0
0.5
0.0

25 26 27 28 29

minutes

3.0
2.0
1.0
0.0

26 28 30 32

minutes

Data Treatment

30. Calibration with "Average Response Factors".

(None, 1/n, 1/x, 1/nx, 1/x2, 1/nx2; preset = 1/nx2)

Selecting 1/x2 or 1/nx2 normalizes the relative contribution of each data point to the calibration curve based on the relative concentrations of the calibration levels, and the number of replicates at each level.

To do Average Response Factor Fit for the calibration curve, specify Curve Fit = Linear, Origin Point = Force, and Regression Weighing = 1/x2 or 1/nx2.

Filter Peak

Smoothing

Smooth Chromatogram

5 Point Smooth

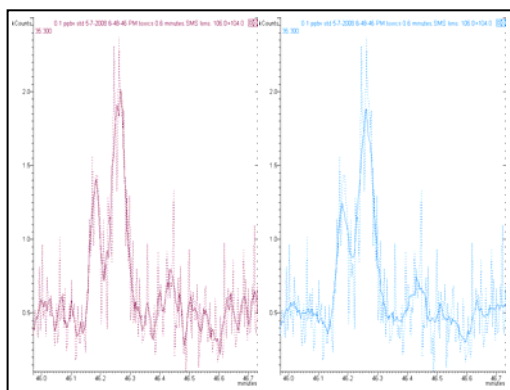
Smoothing Method

Mean

Savitsky Golay

Mean

Savitsky Golay



31. Data filtering by Savitsky-Golay [violet] or Mean (Boxcar) [sky blue], with SG maintaining peak acmes and nadirs, and Mean providing different suppression of noise.

Method Builder - [Randy2*]

Quant Ions:

43.0+71.0

32. Use of multiple ions for Quan ions to enhance peak size.

33. Tangent% parameter for peak skimming allows an automatic judgment based on the relative height of the rider peak to the height of the major peak; less manual intervention in area allocations is then required when relative peak sizes change.

Method Builder - [Toxics-300mL*]

Compound Attributes: 1.000 Crpd 1.000 RIC, CM Lnk

Quant Ions

Tangent %: 10

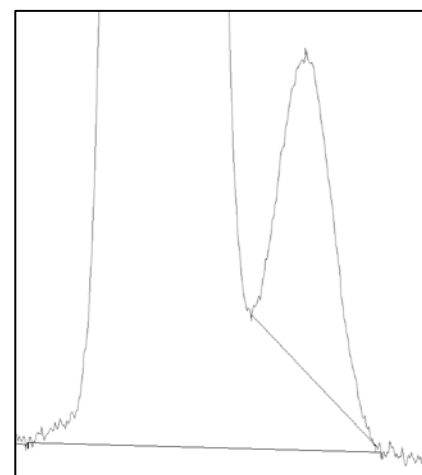
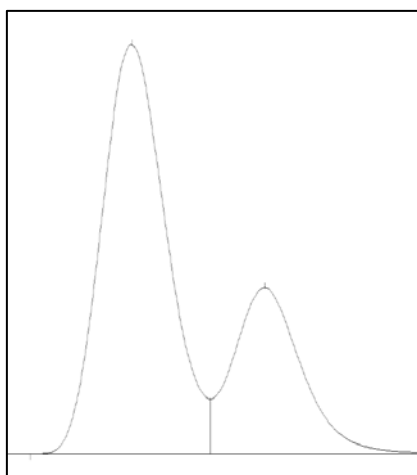
Peak Skimming

Tangent %: 10

Peak Size Reject (counts): 500

Peak S/N Threshold:

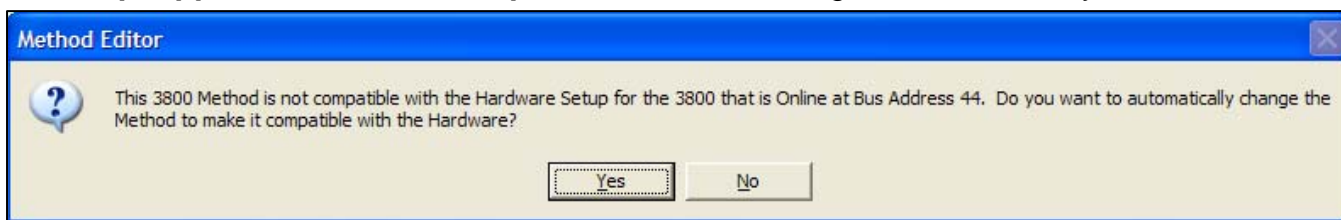
Filter Peak... Integrate



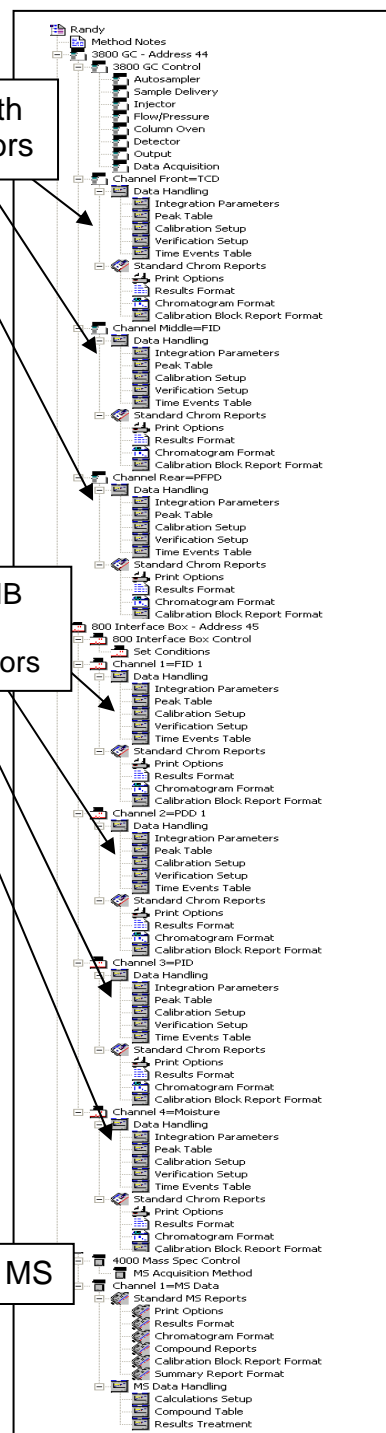
Method Construction

34. Methods can be activated on other similar instruments without changes, facilitating protocol transfers.

35. Prompt appears for choice to update method, if configuration on new system is different.



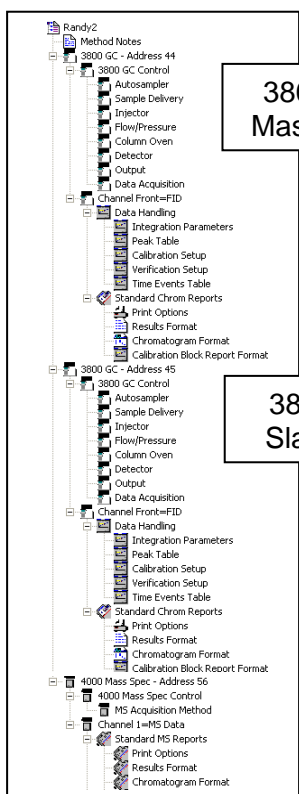
36. *Single method [right] for GC/MS + 3 injectors and 7 detectors [sic], 7 valves, 3 gas sample concentrators, MS data collection, computations, reports, error monitoring and baseline subtraction data.*



3800 with 3 detectors

800 MIB with 4 detectors

4000 MS



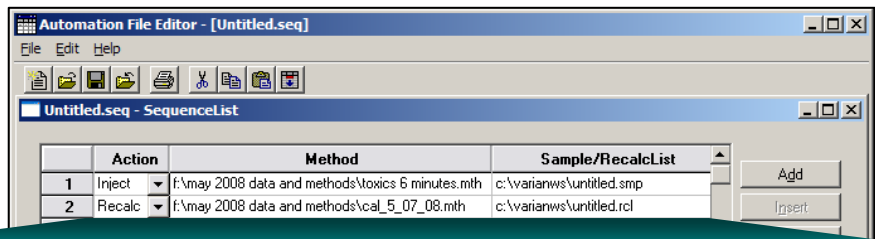
3800 Master

3800 Slave

37. *Single method [left] can control master/slave configuration of two GCs (Addresses 44 and 45) tied together. For example, Hydrogen Fuel Analyzer and Trace Hydrocarbon System, where multiple columns and detectors require two GCs tied together with one sample loading.*

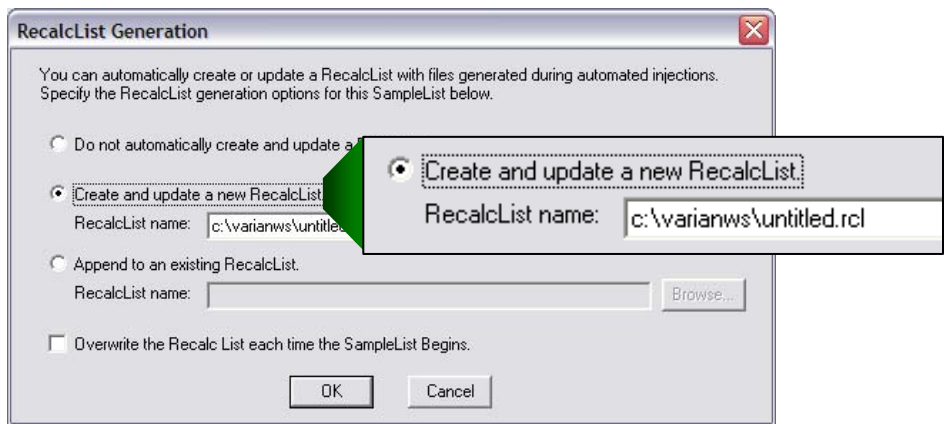
SampleList, RecalcList and Sequence List

38. **Sequence list** allows data collection with one method and then reprocess automatically same (or different) data files with different method(s).

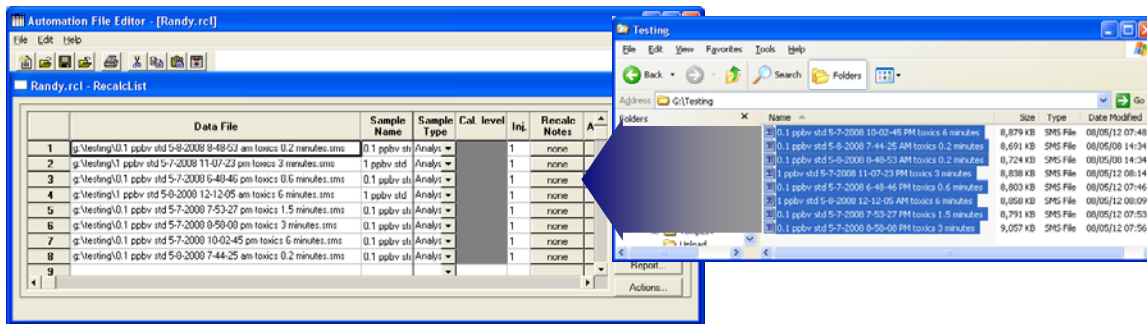


	Action	Method	Sample/RecalcList
1	Inject	f:\may 2008 data and methods\toxics 6 minutes.mth	c:\varianws\untitled.smp
2	Recalc	f:\may 2008 data and methods\cal_5_07_08.mth	c:\varianws\untitled.rcl

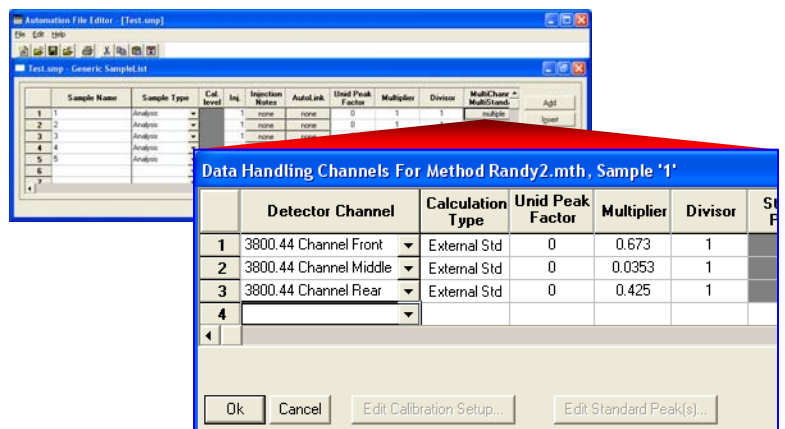
39. **Automatically create or append RecalcList** for later batch reprocessing.



40. **Create RecalcList with drag/drop from Windows Explorer.**

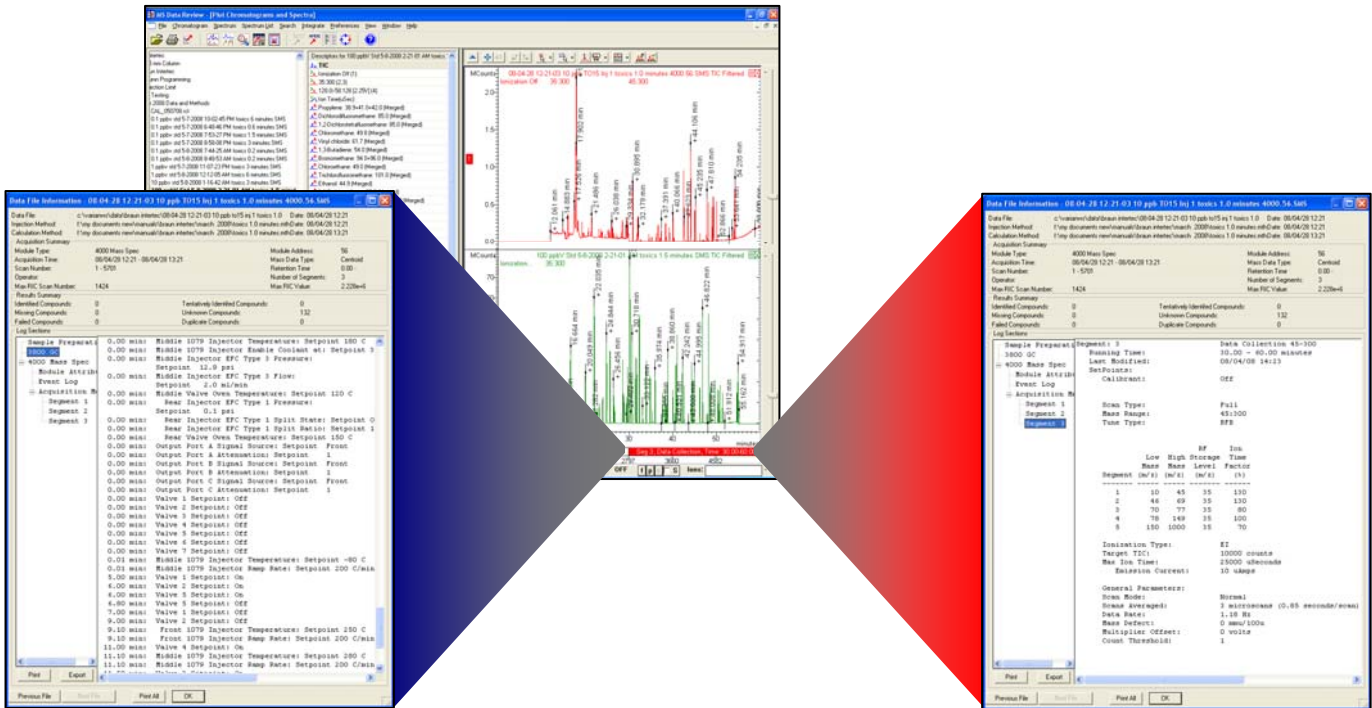


41. **Separate multiplier/divisor for each GC detector** through SampleList.



File Structure

42. Single file contains raw data, results, method, calibration data, errors, instrument logs, sample and recalc notes, module notes, baseline data.



43. Data file names up to 255 characters. No special cryptic coding to 8 characters required.

44. No possibility of overwriting data files. If names match, then XXX (such as 001) are automatically appended to end of file name to make it unique.

45. "Variables" for automatically naming data files.

Data File Generation

Specify the names for Data Files generated by detector modules using this SampleList. Numbers will be appended to file names if the file already exists. Do not include the file extension in the Data File name.

Directory for Data Files:

Data File names:

Example:
08-05-14 08-54-06 Sample 1 Inj 1
TestMethod.ADCB.17

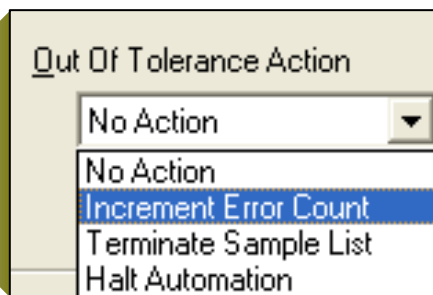
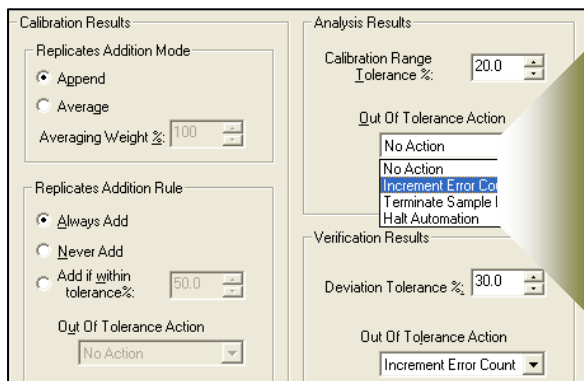
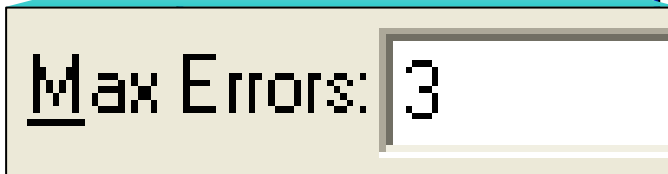
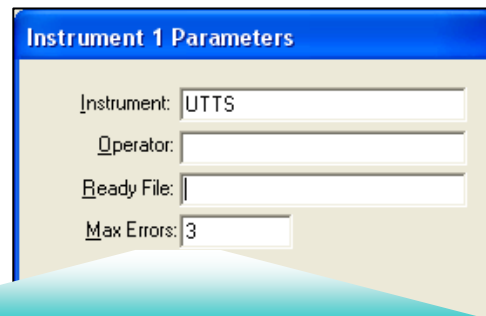
Use the following symbols to enter the corresponding variable data to the file name.

- %s = Sample ID
- %i = Injection number
- %d = Date
- %m = Detector Module name
- %t = Injection Time
- %h = Method Name
- %o = Operator Name
- %n = Instrument Name

Cancel

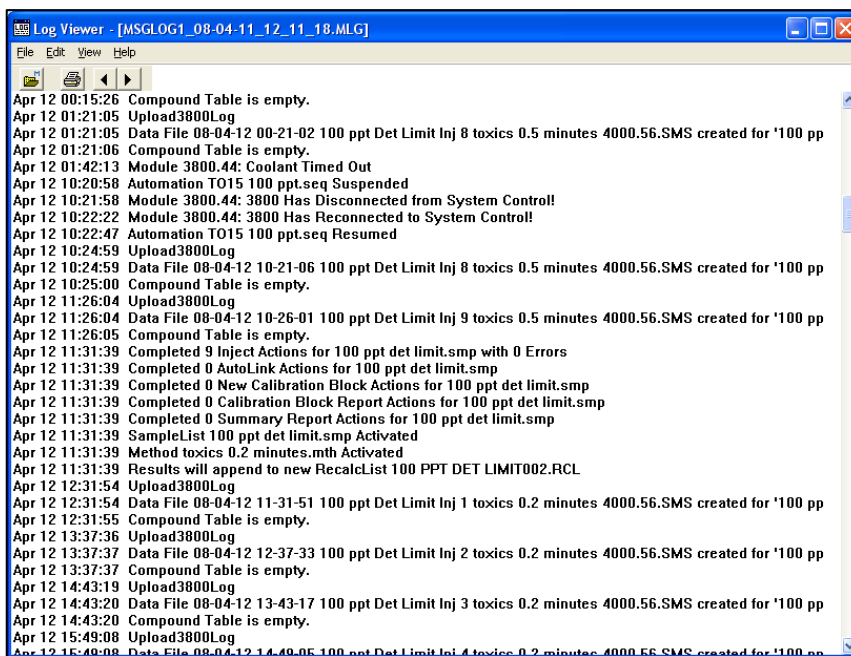
Error Monitoring

46. **Errors incrementing “Max Error” counter.** Some specified errors can be monitored and then trigger a halt to operations, based on operator parameter settings and seriousness of error. “Minor” errors that occur in consecutive runs can be set to take a specific action, including conversion to a fatal error that stops operations. These errors include: outside calibration range, verification failure, replicate standard out of tolerance, missing internal standard, and missing reference peak.



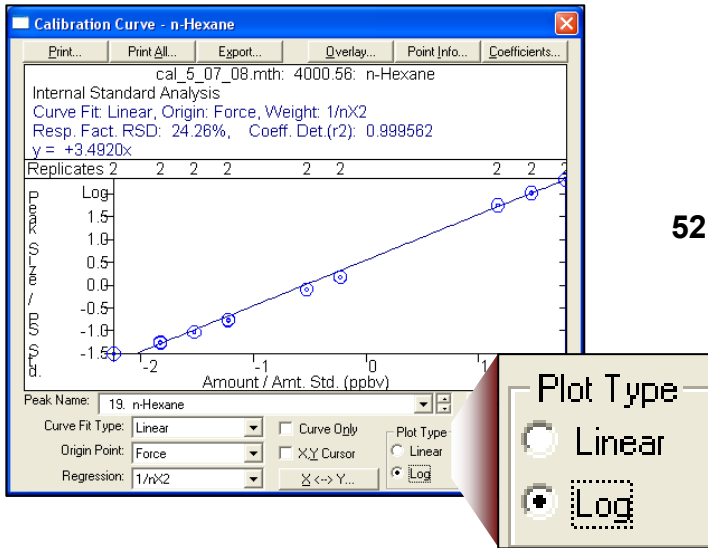
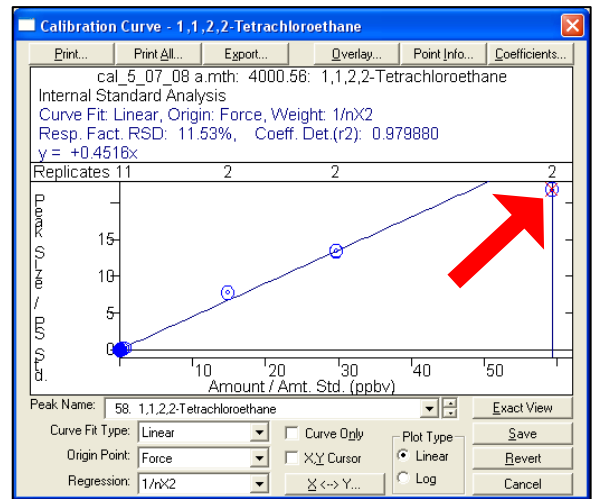
47. **Fatal Errors will halt all operations** until problem is corrected. These types can include: 3800 has disconnected from System Control, End Hardware Check – Module Hardware Problems are Present, Module 3800.44: Coolant Timed Out, among many others.

48. **Message Log becomes documentation** of system operations, including report of errors during runs. Historical logs are saved and recoverable later and cannot be altered.



Calibration Process

- 49. Edit calibration curve with graphics to test other fits, and update method.
- 50. Easily choose alternate fit and save to method.
- 51. Readily delete deviant calibration points with mouse click and new fit is recomputed automatically.



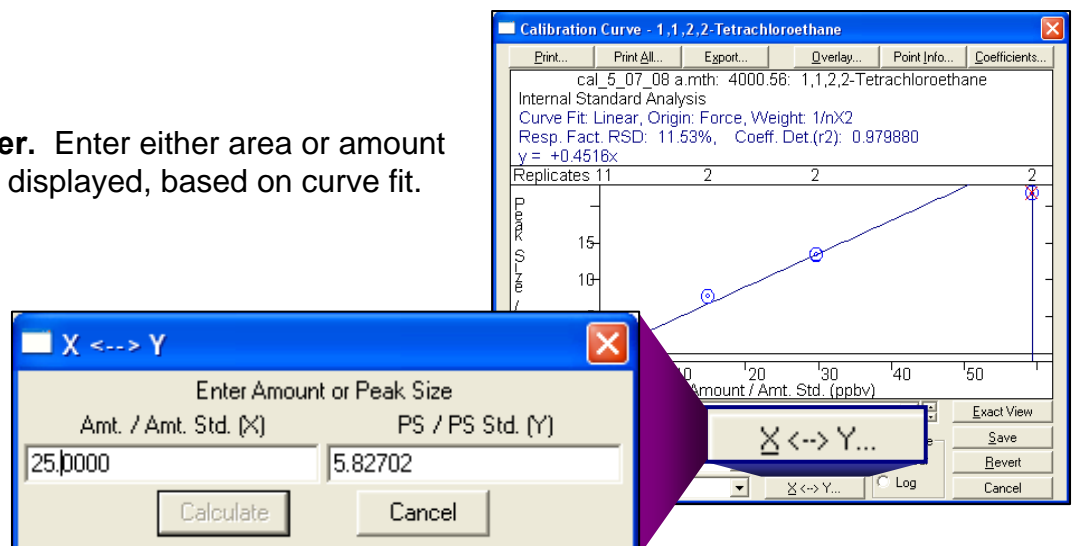
- 52. Display log-log calibration curve to handle wide linear range.

Coefficients							
	Retention Time	Peak Name	Lock Coeffs.	X ³	X ²	X	Intercept
1	16.019	Propylene	<input checked="" type="checkbox"/>	0	0	2.761	0
2	16.152	Dichlorodifluoromethane	<input checked="" type="checkbox"/>	0	0	5.1352	0
3	16.672	1,1-Dichloroethane	<input checked="" type="checkbox"/>	0	0	6.6456	0
4	16.885	Chloromethane	<input checked="" type="checkbox"/>	0	0	0.88742	0
5	17.336	Vinyl chloride	<input type="checkbox"/>	0	0	1.5764	0
6	17.491	1,3-Butadiene	<input type="checkbox"/>	0	0	1.1335	0
7	18.673	Bromomethane	<input type="checkbox"/>	0	0	1.5734	0
8	19.109	Chloroethane	<input type="checkbox"/>	0	0	0.23308	0

- 53. Manual entry of coefficients available.

- 54. Lock selected coefficients, to avoid improper changes to calibration if using multiple standard mixes in multiple standard runs.

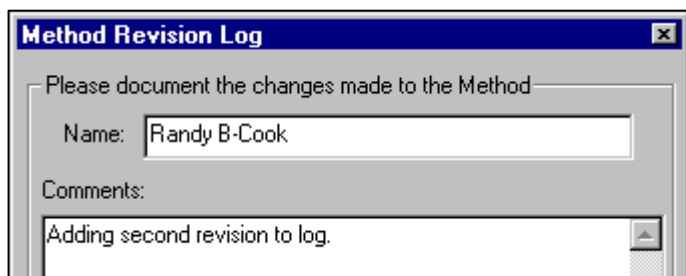
- 55. X↔Y Converter. Enter either area or amount and the other is displayed, based on curve fit.



Data Integrity

56. Cannot change sample name, sample notes, date/time of injection, message logs, nor raw data after data collection. No fudging allowed.

57. To document changes in a method, an optional automatic prompt can be set up to add comments to revision history and these alterations are maintained with the method and with every data file using that method.

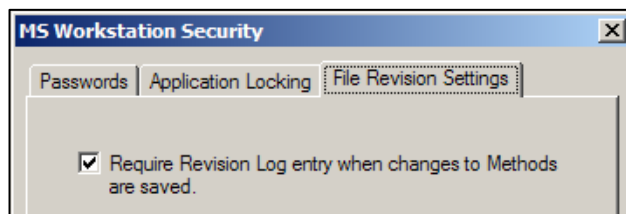


Method Revision Log

Please document the changes made to the Method

Name: Randy B-Cook

Comments:
Adding second revision to log.



MS Workstation Security

File Revision Settings

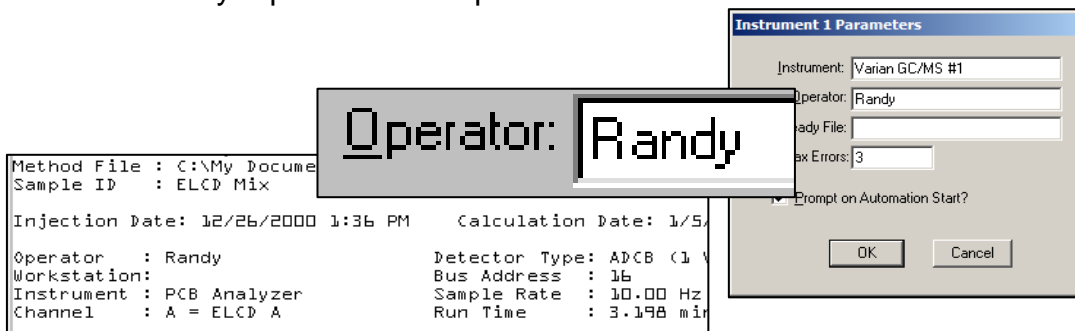
Require Revision Log entry when changes to Methods are saved.

Revision History:

12/27/2000 5:05 PM: Method updated by Randy B-Cook.
Method built to test out Method Revision Log

12/31/2000 12:50 PM: Method updated by Randy B-Cook.
Adding second revision to log.

58. Optional automatic prompt for operator name at start of data collection. Entry for "Operator" is documented on every report in that sequence.



Operator: Randy

Method File : C:\My Document
Sample ID : ELCD Mix

Injection Date: 12/26/2000 1:36 PM Calculation Date: 1/5/2001

Operator : Randy Detector Type: ADCB (1
Workstation: Bus Address : 16
Instrument : PCB Analyzer Sample Rate : 10.00 Hz
Channel : A = ELCD A Run Time : 3.198 min

Instrument 1 Parameters

Instrument: Varian GC/MS #1

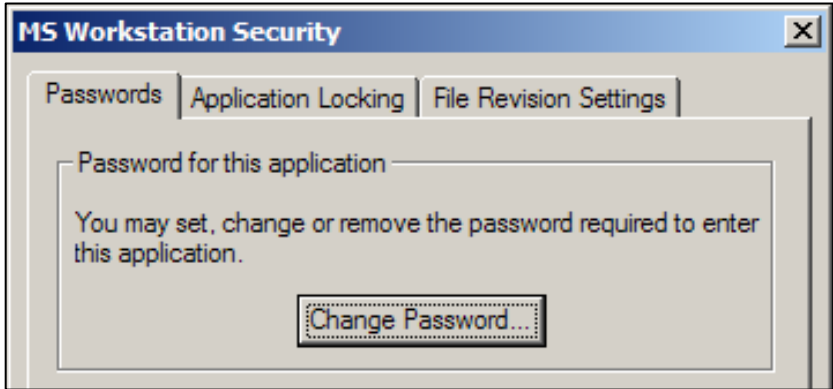
Operator: Randy

Ready File:

Max Errors: 3

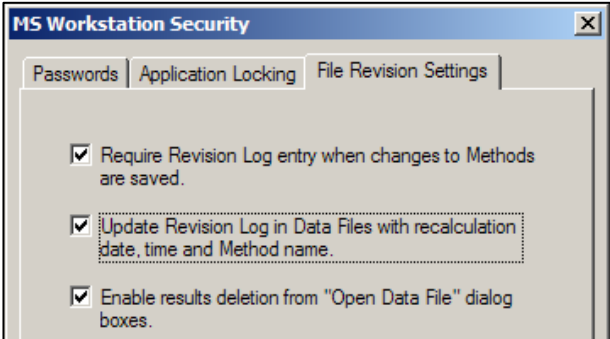
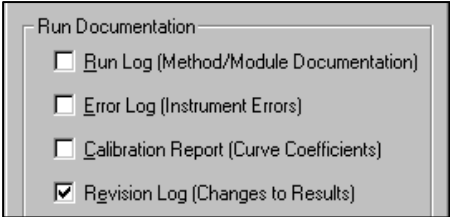
Prompt on Automation Start?

OK Cancel



59. Access to MS Workstation Security application is password controlled, limiting access to changes in security procedures and passwords.

60. Revision log for results. After both checking the box for "Update Revision Log" and enabling the Revision Log in Run Documentation, time and date of operator revisions are independently recorded. This log can be printed as part of every report of results.

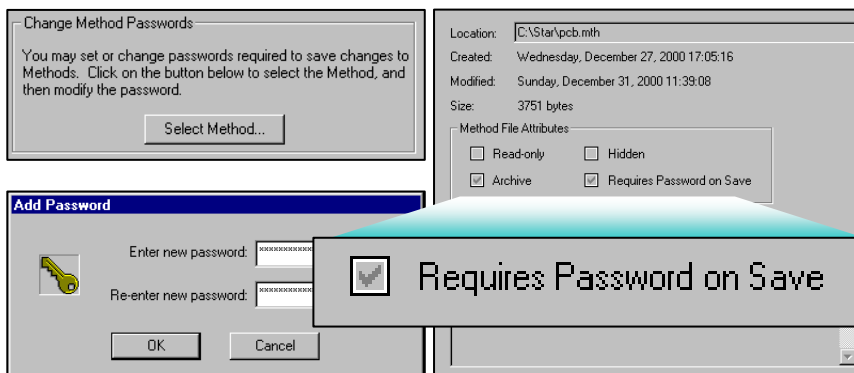


```
Revision Log:
12/27/2000 4:59 PM: Calculated results from channel A using method:
'c:\my documents\brochures\data integrity with star workstation\12-26-00 1:37:00 pm elcd mix-b.mth'
12/27/2000 6:20 PM: Calculated results from channel A using method:
'c:\my documents\brochures\data integrity with star workstation\12-26-00 1:37:00 pm elcd mix-b.mth'
12/31/2000 1:40 PM: Calculated results from channel A using method:
'c:\my documents\brochures\data integrity with star workstation\12-26-00 1:37:00 pm elcd mix-b.mth'
```

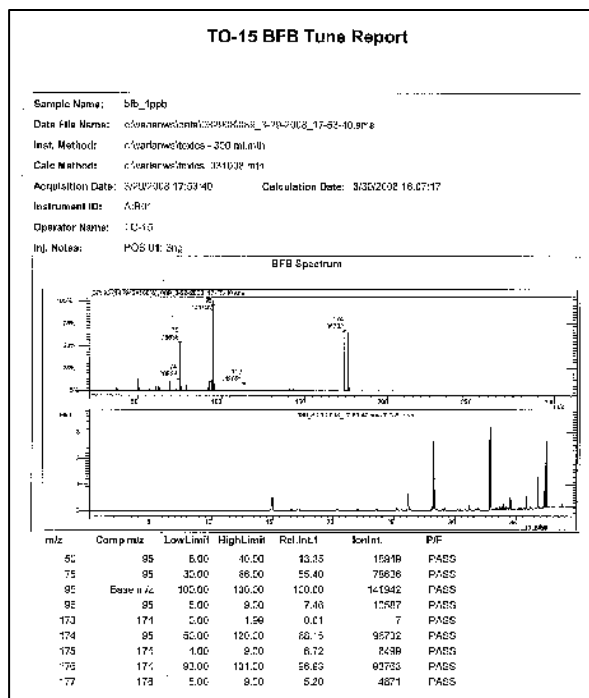
```
Revision Log:
12/31/2000 2:09 PM: Deleted results calculated on 12/26/2000 9:45 PM
from channel B of ADCB at address 16.
```



61. Methods can be set to require a password prior to saving to prohibit unauthorized changes to methods.



62. BFB Tune adjustments allow ion trap spectra to match criteria for EPA library search.



General Parameters | Ionization Control | Internal EI Parameters | Full Scan Parameters

Mass Range: Low Mass: 35 m/z High Mass: 300 m/z

Tune Type: 4000BFB, 5 segments

	Low Mass (m/z)	High Mass (m/z)	RF Storage Level (m/z)	Ion Time Factor (%)
1	10	70	27	200
2	71	78	31	70
3	79	150	31	100
4	151	175	31	110
5	176	1000	31	104
6				

Tune Type: 4000BFB, 5 segments

	Low Mass (m/z)	High Mass (m/z)	RF Storage Level (m/z)	Ion Time Factor (%)
1	10	70	27	200
2	71	78	31	70
3	79	150	31	100
4	151	175	31	110
5	176	1000	31	104
6				

Can Your Mass Spec Data System Do This?

Operator Interface

	Your Data System	Varian MS Workstation
1. Colorful AutoSampler™ Display	<input type="checkbox"/>	<input checked="" type="checkbox"/>
2. Readily convert between Full Scan, Single Ion(s) Monitoring, MS-MS, MS ⁿ and Chemical Ionization	<input type="checkbox"/>	<input checked="" type="checkbox"/>
3. Automatic Method Development for MS-MS	<input type="checkbox"/>	<input checked="" type="checkbox"/>
4. Compute areas on live chromatogram	<input type="checkbox"/>	<input checked="" type="checkbox"/>
5. Library search live chromatogram	<input type="checkbox"/>	<input checked="" type="checkbox"/>
6. Monitor single ions (or ion groups) in live chromatogram	<input type="checkbox"/>	<input checked="" type="checkbox"/>
7. Simultaneously collect MS data, plus runs from up to 7 [sic] GC detectors	<input type="checkbox"/>	<input checked="" type="checkbox"/>
8. Green light – Red light status	<input type="checkbox"/>	<input checked="" type="checkbox"/>
9. Quick access to details of thermal zone	<input type="checkbox"/>	<input checked="" type="checkbox"/>
10. Open data files/ methods/samplelists/sequences/recalc lists directly	<input type="checkbox"/>	<input checked="" type="checkbox"/>
11. Tool Bar	<input type="checkbox"/>	<input checked="" type="checkbox"/>
12. Delete icons in Tool Bar	<input type="checkbox"/>	<input checked="" type="checkbox"/>
13. Recent Files button	<input type="checkbox"/>	<input checked="" type="checkbox"/>
14. Browse button	<input type="checkbox"/>	<input checked="" type="checkbox"/>
15. Get immediate Help	<input type="checkbox"/>	<input checked="" type="checkbox"/>
16. Copy [ctrl C] and Paste [ctrl V] peak table details	<input type="checkbox"/>	<input checked="" type="checkbox"/>
17. Relabeling headers	<input type="checkbox"/>	<input checked="" type="checkbox"/>
18. Function-labeling for valve operations	<input type="checkbox"/>	<input checked="" type="checkbox"/>
19. User-selectable delay in start of MS data collection	<input type="checkbox"/>	<input checked="" type="checkbox"/>
20. Method control of mass flow controller for air sample loading	<input type="checkbox"/>	<input checked="" type="checkbox"/>
21. Correction to results for air sample volume loaded	<input type="checkbox"/>	<input checked="" type="checkbox"/>
22. Auto Start at specific clock time	<input type="checkbox"/>	<input checked="" type="checkbox"/>

Data Review

	Your Data System	Varian MS Workstation
23. Single screen for data review of multiple data files	<input type="checkbox"/>	<input checked="" type="checkbox"/>
24. View and compare two curve fits	<input type="checkbox"/>	<input checked="" type="checkbox"/>
25. Normalize and overlay ion peaks to aid in sorting out identifications	<input type="checkbox"/>	<input checked="" type="checkbox"/>
26. Graphical assignment of baseline	<input type="checkbox"/>	<input checked="" type="checkbox"/>
27. Verification runs	<input type="checkbox"/>	<input checked="" type="checkbox"/>
28. Easy graphical access to timed events	<input type="checkbox"/>	<input checked="" type="checkbox"/>
29. Export chromatogram or spectrum into .WMF Picture File	<input type="checkbox"/>	<input checked="" type="checkbox"/>

Data Treatment

30. Calibration with "Average Response Factors"	<input type="checkbox"/>	<input checked="" type="checkbox"/>
31. Data filtering by Savitsky-Golay or Mean (Boxcar)	<input type="checkbox"/>	<input checked="" type="checkbox"/>
32. Use of multiple ions for Quan ions	<input type="checkbox"/>	<input checked="" type="checkbox"/>
33. Tangent% parameter for peak skimming	<input type="checkbox"/>	<input checked="" type="checkbox"/>

Method Construction

34. Methods can be activated on other similar instruments	<input type="checkbox"/>	<input checked="" type="checkbox"/>
35. Prompt appears for choice to update method	<input type="checkbox"/>	<input checked="" type="checkbox"/>
36. <i>Single</i> method for GC/MS + 3 injectors and 7detectors [sic]...	<input type="checkbox"/>	<input checked="" type="checkbox"/>
37. <i>Single</i> method can control master/slave configuration of two GCs	<input type="checkbox"/>	<input checked="" type="checkbox"/>

SampleList, RecalcList and Sequence List

38. Sequence List	<input type="checkbox"/>	<input checked="" type="checkbox"/>
39. Automatically create or append RecalcList	<input type="checkbox"/>	<input checked="" type="checkbox"/>
40. Create RecalcList with drag/drop from Windows Explorer	<input type="checkbox"/>	<input checked="" type="checkbox"/>
41. Separate multiplier/divisor for each GC detector	<input type="checkbox"/>	<input checked="" type="checkbox"/>

File Structure

42. Single file contains raw data, results, method, calibration data...	<input type="checkbox"/>	<input checked="" type="checkbox"/>
43. Data file names up to 255 characters	<input type="checkbox"/>	<input checked="" type="checkbox"/>
44. No possibility of overwriting data files	<input type="checkbox"/>	<input checked="" type="checkbox"/>
45. "Variables" for automatically naming data files	<input type="checkbox"/>	<input checked="" type="checkbox"/>

	Your Data System	Varian MS Workstation
46. Errors incrementing "Max Error" counter	<input type="checkbox"/>	<input checked="" type="checkbox"/>
47. Fatal Errors will halt all operations	<input type="checkbox"/>	<input checked="" type="checkbox"/>
48. Message Log	<input type="checkbox"/>	<input checked="" type="checkbox"/>

Calibration Process

49. Edit calibration curve with graphics	<input type="checkbox"/>	<input checked="" type="checkbox"/>
50. Easily choose alternate fit	<input type="checkbox"/>	<input checked="" type="checkbox"/>
51. Readily delete deviant calibration points with mouse click	<input type="checkbox"/>	<input checked="" type="checkbox"/>
52. Display log-log calibration curve	<input type="checkbox"/>	<input checked="" type="checkbox"/>
53. Manual entry of coefficients	<input type="checkbox"/>	<input checked="" type="checkbox"/>
54. Lock selected coefficients	<input type="checkbox"/>	<input checked="" type="checkbox"/>
55. X↔Y Converter	<input type="checkbox"/>	<input checked="" type="checkbox"/>

Data Integrity

56. Cannot change sample name, sample notes, date/time of injection...	<input type="checkbox"/>	<input checked="" type="checkbox"/>
57. Optional automatic prompt can be set up to add comments to revision history	<input type="checkbox"/>	<input checked="" type="checkbox"/>
58. Optional automatic prompt for operator name at start of data collection	<input type="checkbox"/>	<input checked="" type="checkbox"/>
59. Access to MS Workstation Security application is password controlled	<input type="checkbox"/>	<input checked="" type="checkbox"/>
60. Revision Log for results	<input type="checkbox"/>	<input checked="" type="checkbox"/>
61. Methods can be set to require a password prior to saving	<input type="checkbox"/>	<input checked="" type="checkbox"/>
62. BFB Tune adjustments	<input type="checkbox"/>	<input checked="" type="checkbox"/>

**This author thanks Carlos Warner and Rand Mahoney of Varian, Inc.,
for assistance in preparing this monograph.**

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