## Can Your Mass Spec Data System Do This?

## - Powerful Capabilities of Varian MS Workstation 6.91

by:

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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**

 Colorful AutoSampler<sup>™</sup> 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.

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





 Readily convert between Full Scan, Single Ion(s) Monitoring, MS-MS, MS<sup>n</sup> and Chemical Ionization in one chromatographic run.



4. Compute areas on live chromatogram.



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



- Green light Red light status of GC thermal zones.
- 9. Quick access to details of thermal zone by clicking on zone label.

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#### 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.

	Print Custom MS Report
	Print Standard MS Report
	View Custom MS Report
	View Standard MS Report
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Show and Hide Applications on Toolbar			
Applications shown on Toolbar Select applications you wish to remove from the Toolbar and click on the Remove button. Batch Reporting Custom MS Reports Edit Automation Files Review / Process MS Data Standard Chrom Reports Standard MS Reports System Control / Automation View / Edit Chromatograms View / Edit Chromatograms	>> <u>B</u> emove>>	Applications not shown on the Toolbar Select applications you wish to add to the Toolbar and click on the Add button. Quick Start! Security Administration	
ΟΚ	bdd<<	Cancel	

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







**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.

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4	16.672		1,2-Dichlorotetrafluo	85.0, C:M 📑
5	16.885		Chloromethane	49.8, C:M
6	17.336		Vinyl chloride	61.7, C:M
7	17.491		1,3-Butadiene	54.0, C:M
8	18.673		Bromomethane	94.0+96.0, C:M
9	19.109		Chloroethane	49.0, C:M
10	20.054		Trichlorofluorometha	101.0, C:M
11	21.329		Ethanol	44.9, C:M
12	22.041		1,1-Dichloroethene	60.9, C:M
13	22.054		1,1,2-Trichlorotrifluor	100.9, C:M
14	22.634		Acetone	58.U, C:M
15	22.66		Carbon disulfide	75.8, U:M
10	23.204		2-Propanoi Mathulana Chlavida	44.9, C:IVI
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							Actions

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

18. Functionlabeling for valve operations by right-clicking on header for clearer operations.

- Address 40

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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	e Name	Sample Ty	ре	Ca lev	al. /el	lnj.	AutoLink	Rack
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	6	Aroclor 1248	<b>•</b> • • • •			_	1	1	none	1
			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.







4 Analysis C Grain Force, Weight 1900 D 17.35%, Coeff Det (/2) 0.860530 (adon Deviation: -11.78% (2) 0.1 Origin Include (E) (7), Weight 1990 D 17.35%, Coeff Det (2) 0.967116 D 17.35%, Coeff Det (2) 0.967116

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

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Norm 100%	Λ	Stacked Overlaid ✓ Normalized

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	+7
	Average Selected Spectra	+\
	Calculate Noise	+ľ
	Calculate Time Range	+F
Ý	Integrate Area	+I
	Export to Clipboard	+E



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**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.

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30.00%			10.31%			P



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

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



## **Data Treatment**

#### 30. Calibration with "Average Response Factors".



## **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.









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 Weighting = 1/x2 or 1/nx2.



**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 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.



## 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).

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Untitled.seq - SequenceList									
Actio	n	Method	Sample/RecalcList	-					
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	Actio	n	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



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

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**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.

		Data File Generation	
		Specify the names for Data Files g Numbers will be appended to file n extension in the Data File name.	enerated by detector modules using this SampleList. ames if the file already exists. Do not include the file
		Directory for Data Files	Data File names
45. "Variables" for automatically	Example: 08-05-14 08-54-06 Sample 1 TestMethod ADCB.17	Inj 1 rts new	[%d %t %s Inj %t %h %m           Example:           08:05:14 08:54-06 Sample 1 Inj 1           TestMethod ADCB.17
naming data mes.	Use the following symbols to corresponding variable data name. %s = Sample ID %i = Injection number %d = Date %m = Detector Module n %t = Injection Time %h = Method Name %o = Operator Name %n = Instrument Name	enter the to the file	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 %n = Detector Module name %n = Method Name %o = Operator Name %n = Instrument Name

## **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.

ne alt nd in	Instrument T Parameters         Instrument:         UTTS         Operator:         Beady File:         Max Errors:

Max Errors: 3

Calibration Results	Analysis Results	
Replicates Addition Mode	Calibration Range	
<ul> <li>Append</li> </ul>	<u>I</u> olerance %: 20.0 I	Out Of Tolerance Action
C Average	Out Of Tolerance Action	
Averaging Weight 🧏 100 📑	No Action	No Action 👻
- Replicates Addition Bule	No Action	
	Terminate Sample I	No Action
<ul> <li>Always Add</li> </ul>	Verification Results	Increment Error Count
C <u>N</u> ever Add		Terminate Sample List
C Add if within 50.0	Deviation Tolerance %; 30.0 📑	r eminate sample List
		Halt Automation
Out Of Tolerance Action	Out Of Tolerance Action	
No Action	Increment Error Count	

**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.

🛄 Log Viewer - [	MSGLOG1_08-04-11_12_11_18.MLG]	
<u>File E</u> dit ⊻iew <u>H</u> e	qle	
📕 🚑 🖌		
Apr 12 00:15:26	Compound Table is empty	
Apr 12 01:21:05		
Apr 12 01:21:05	Data File 08-04-12 00-21-02 100 ppt Det Limit Ini 8 toyics 0.5 minutes 4000 56 SMS created for "	100 nn
Apr 12 01:21:06	Compand Table is empty	100 pp
Apr 12 01:42:13	Module 3800 44: Coolant Timed Out	
Apr 12 10:20:58	Automation TO15 100 not see Suspended	
Apr 12 10:21:58	Module 3800 44: 3800 Has Disconnected from System Control	
Anr 12 10:22:22	Module 3800 44: 3800 Has Beconnected to System Control	
Anr 12 10:22:47	Automation TO15 100 not sea Besumed	
Anr 12 10:24:59		
Anr 12 10:24:59	Data File 08-04-12 10-21-06 100 not Det Limit Ini 8 toxics 0.5 minutes 4000.56.SMS created for "	100 nn
Apr 12 10:25:00	Compound Table is empty.	
Apr 12 11:26:04	Upload3800Log	
Apr 12 11:26:04	Data File 08-04-12 10-26-01 100 ppt Det Limit Ini 9 toxics 0.5 minutes 4000.56.SMS created for "	100 pp
Apr 12 11:26:05	Compound Table is empty.	••
Apr 12 11:31:39	Completed 9 Inject Actions for 100 ppt det limit.smp with 0 Errors	
Apr 12 11:31:39	Completed 0 AutoLink Actions for 100 ppt det limit.smp	
Apr 12 11:31:39	Completed 0 New Calibration Block Actions for 100 ppt det limit.smp	
Apr 12 11:31:39	Completed 0 Calibration Block Report Actions for 100 ppt det limit.smp	
Apr 12 11:31:39	Completed 0 Summary Report Actions for 100 ppt det limit.smp	
Apr 12 11:31:39	SampleList 100 ppt det limit.smp Activated	
Apr 12 11:31:39	Method toxics 0.2 minutes.mth Activated	
Apr 12 11:31:39	Results will append to new RecalcList 100 PPT DET LIMIT002.RCL	
Apr 12 12:31:54	Upload3800Log	
Apr 12 12:31:54	Data File 08-04-12 11-31-51 100 ppt Det Limit Inj 1 toxics 0.2 minutes 4000.56.SMS created for "	100 pp
Apr 12 12:31:55	Compound Table is empty.	
Apr 12 13:37:36	Upload3800Log	
Apr 12 13:37:37	Data File 08-04-12 12-37-33 100 ppt Det Limit Inj 2 toxics 0.2 minutes 4000.56.SMS created for "	100 pp
Apr 12 13:37:37	Compound Table is empty.	
Apr 12 14:43:19	Upload3800Log	
Apr 12 14:43:20	Data File 08-04-12 13-43-17 100 ppt Det Limit Inj 3 toxics 0.2 minutes 4000.56.SMS created for "	100 pp
Apr 12 14:43:20	Compound Table is empty.	
Apr 12 15:49:08	Upload3800Log	
Apr 12 15-40-08	<u>Nata File 08-04-12 14-49-05 100 not Det Limit Ini 4 tovice 0.2 minutee 4000 55 SMS created for "</u>	100 pp

**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.



	Retention Time	Peak Name	Lock Coeffs.	X^3	X^2	×	Intercept
1	16.019	Propylene	V	0	0	2.761	0
2	16.152	Dichlorodifluoromethane	V	0	0	5.1352	0
3	16.672	2-Dichlorotetrafluoroetha	V	0	0	6.6456	0
4	16.885	Chloromethane	1	0	0	0.88742	0
5	17.336	Vinyl chloride		0	0	1.5764	0
6	17.491	1,3-Butadiene	1	0	0	1.1335	0
7	18.673	Bromomethane	1	0	0	1.5734	0
8	19.109	Chloroethane	3	0	0	0.23308	0

- Calibration Curve 1,1,2,2-Tetrachloroethane Print All... Export... Qverlay... Point Info... Qoefficients.. cal\_5\_07\_08 a.mth: 4000.56: 1,1,2,2-Tetrachloroethane Print... Internal Standard Analysis Curve Fit: Linear, Origin: Force, Weight: 1/nX2 Resp. Fact. RSD: 11.53%, Coeff. Det.(r2): 0.979880 v = +0.4516x Replicates 11 15ş Į 10 Ę 15 t 10 ) '20 '30 Amount / Amt. Std. (ppb∨) 40 50 Peak Name: 58. 1,1,2,2-Tetrachloroethane - 3  $\underline{E} xact \, View$ Curve Fit Type: Linear -Curve Only Г Plot Type Save Origin Point: Force • XY Cursor Linear <u>R</u>evert 🔿 Log Regression: 1/nX2 - $\underline{X} \longleftrightarrow Y..$ Cancel
- 52. Display log-log calibration curve to handle wide linear range.

53. Manual entry of coefficients available.

Calibration Curve - 1,1,2,2-Tetrachloroethane

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

> Print... Print All... Export... Qverlay... Point Info... Coefficients. cal\_5\_07\_08 a.mth: 4000.56: 1,1,2,2-Tetrachloroethane

**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	MS Workstation Security	×1
Name: Randy B-Cook	Passwords Application Locking File Revision Settings	
Comments: Adding second revision to log.	Require Revision Log entry when changes to Methods are saved.	
Revision History:		
12/27/2000 5:05 PM: Method upd Method built to test out Method Re-	ated by Randy B-Cook. vision Log	
Adding second revision to log.	dated by Handy B-Look.	

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

		Instrument 1 Parameters Instrument: Varian GC/MS #1
Method File : C:\My Docume Sample ID : ELCD Mix	erator: Rand	ady File:
Injection Date: 12/26/2000 1:36 Pr Operator : Randy Workstation: Instrument : PCB Analyzer Channel : A = ELCD A	1 Calculation Date: 1/5, Detector Type: ADCB (1 \ Bus Address : 16 Sample Rate : 10.00 Hz Run Time : 3.198 mir	DK Cancel

MS Worksta	tion Security	X
Passwords	Application Locking File Revision Settings	
Password	for this application	
You may set, change or remove the password required to enter this application.		
	Change Password	

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 MS Workstation Security х

report of results.



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'

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

Revision Log:

Del Results..

n be set to require a	Change Method Passwords You may set or change passwords required to save changes to Methods. Click on the button below to select the Method, and then modify the password. Select Method	Location: C:\Star\pcb.mth Created: Wednesday, December 27, 2000 17:05:16 Modified: Sunday, December 31, 2000 11:39:08 Size: 3751 bytes Method File Attributes Read-only Hidden Atchive Requires Password on Save
ior to saving to horized changes to	Add Password Enter new password Re-enter new password:	Requires Password on Save

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



61. Methods can password pri prohibit unaut methods.

## Can Your Mass Spec Data System Do This?

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

Da	ta Review	Your Data System	Varian MS Workstation
23.	Single screen for data review of multiple data files		
24.	View and compare two curve fits		
25.	Normalize and overlay ion peaks to aid in sorting out identificatio	ns 🗆	
26.	Graphical assignment of baseline		
27.	Verification runs		
28.	Easy graphical access to timed events		
29.	Export chromatogram or spectrum into .WMF Picture File		
Da	ata Treatment		
30.	Calibration with "Average Response Factors"		
31.	Data filtering by Savitsky-Golay or Mean (Boxcar)		

32. Use of multiple ions for Quan ions33. Tangent% parameter for peak skimming

## **Method Construction**

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

## SampleList, RecalcList and Sequence List

38.	Sequence List	
39.	Automatically create or append RecalcList	
40.	Create RecalcList with drag/drop from Windows Explorer	
41.	Separate multiplier/divisor for each GC detector	
Fi	le Structure	

# 42. Single file contains raw data, results, method, calibration data... 43. Data file names up to 255 characters 44. No possibility of overwriting data files 45. "Variables" for automatically naming data files

Er	ror Monitoring	Your Data System	Varian MS Workstation
46.	Errors incrementing "Max Error" counter		
47.	Fatal Errors will halt all operations		
48.	Message Log		

## **Calibration Process**

49.	Edit calibration curve with graphics	5
50.	Easily choose alternate fit	
51.	Readily delete deviant calibration points with mouse click	
52.	Display log-log calibration curve	
53.	Manual entry of coefficients	
54.	Lock selected coefficients	
55.	X↔Y Converter	

## **Data Integrity**

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

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

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