Quirks with Scion MS Workstation V8.2 User Interface

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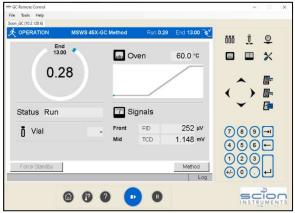
File Extensions

- .MTH Method
- .RUN GC Detector Data
- .XMS MS Data
- .SMP Sample List
- .SEQ Sequence List
- .RCL Recalculate List
- .MLG Message Log
- .MSR Report File
- .IRM Dash Template
- .MSF AMDIS Data File
- .CDF Content Definition File

Routine operations with Scion MS Workstation are quite easy to set up parameters for data collection and report generation. The following is a discussion of hidden quirks that may not be obvious of their usefulness. This discussion assumes that the operator is familiar with basic operations in MS Workstation.

Operations involving control of Scion 436/456 Gas Chromatographs.

- 1. To maintain interconnection between instrument and MS Workstation, System Control should be closed before powering off the GC. Reconnection becomes automatic. If needed, the reconnection can be established by viewing video at http://lotusinstruments.com/reconnecting-a-456436-in-ms-workstation-8/.
- 2. Full access to methods through instrument display, even active one, during data collection.
- 3. GC Remote Control allows view of status of gas chromatograph from a remote computer, typically through Team Viewer or similar app.



on_GC (10.2.128.6)	MSWS 45X-GC N	lethod Run:)	0.00 End: 13.00		
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5. Change run time for gas chromatograph during run, especially useful in method development.

4. Reboot gas chromatographs through GC Remote Control by setting a minor change to System Time through Setup > System.

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File Tools Help		
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6. Instrument Log – lists activities for the instrument, including faults with time/date stamp.

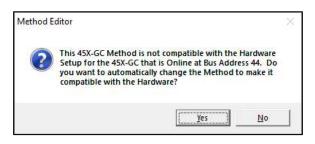
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7. Runlog - documents all actual run conditions on GC in every .RUN file for full recovery at a later time, even changes made during the run.

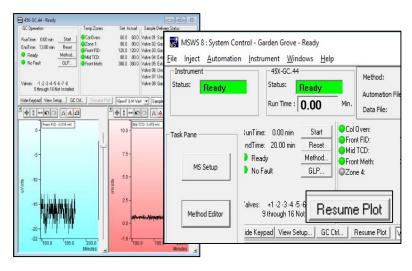
8. Automatic update of method when hardware is added/deleted in Setup. All other hardware and calculations remain intact.

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Ready	1



9. FID/NPD Detector Full Scale - the electrometer for these two detector types has the ability to auto-range over the full range of the detector. To activate this feature, full scale parameter is set to 1000 V.

10. Resume plot – permits visible display of active baseline drift and noise.

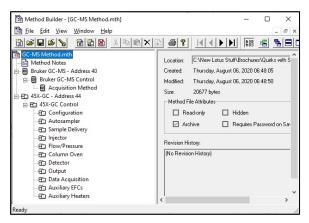


Status: Ready	43X-GC.44 Status: Ready Run Time : 0.00 Min.	Method: Automation File: Data File:		thods\ECD 2020\ECD Master.mth
Task Pane	GC Operation	Temp Zones	Set Actual	Front Detector Status
MS Setup	EndTime: 1999.00 min Reset	Col Oven: Front S/SL : Front ECD: Zone 3:	200.0 200.0 150.0 150.0 350.0 350.0 N/A N/A	Ready: Yes Fault: No Front ECD Electronics: On Range: 10 Time Const: Fast Cell Current: CAP
Method Editor	No Fault <u>GLP</u>	ĴZone 4:	N/A N/A	Contact Potential: -399 mV Detector Signal: 356.049 mV Frequency : 5 Hz

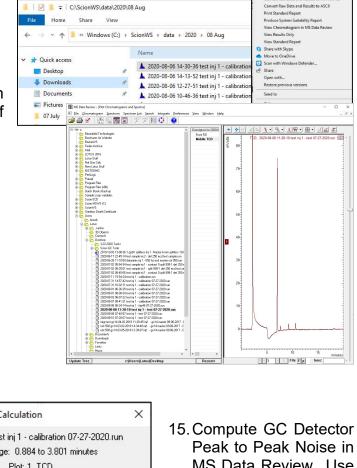
11. Entry and display of temperatures in 0.1 °C increments.

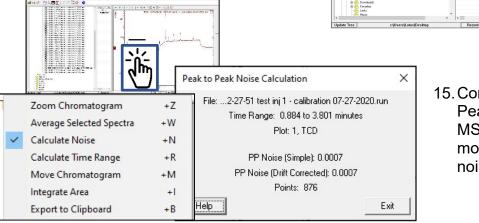
Common hints for both MS and GC detector operations

- 12. Concurrent instrument control and data collection for MS and GC with single Method.
- 13. Concurrent data collection for MS and GC with single SampleList.



14. GC chromatogram can be displayed in MS Data Review, by right-clicking of .RUN file in Windows Explorer.



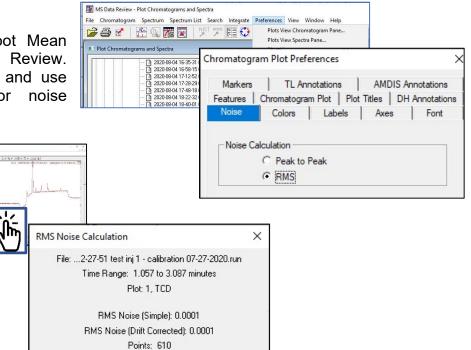


MS Data Review. Use mouse to draw line for noise calculation.

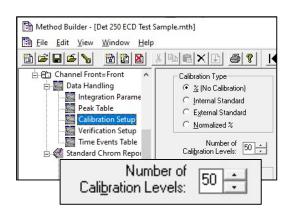
16. Compute GC Detector Root Mean Square Noise in MS Data Review. Open .RUN file in MSWS and use draw line for noise mouse to calculation.

Jh

Help



17. Up to 50 calibration levels.

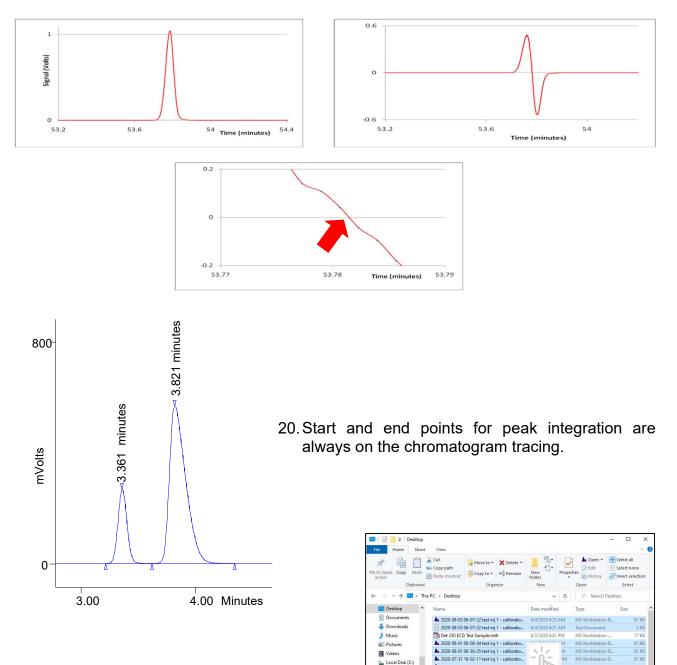


Exit

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11	c:\new lotus stuff\brochures\electron capture primer\reproducibility		Analysis 👻		2		Report
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15	c:\new lotus stuff\brochures\electron capture primer\reproducibility	Test Sample R1	Analysis 👻		6		
16	c:\new lotus stuff\brochures\electron capture primer\reproducibility	Test Sample R1	Analysis 👻		7		
17	c:\new lotus stuff\brochures\electron capture primer\reproducibility	Test Sample R1	Analysis 💌		8		
18	c:\new lotus stuff\brochures\electron capture primer\reproducibility	Test Sample R1	Analysis 🔹		9		
19							

18. Recalc List - This screen allows selected data files to be recalculated with a modified or different method.

19. Determination of Retention Time - MS Workstation establishes retention time of a peak by computing the zero crossover of the first derivative of the peak. It this value does not correspond to a collected data point, precise timing is determined by linear interpolation of points before and after the zero crossing.



Local Dis

2 2 8 2 5 A 8 8 8 8

Data File

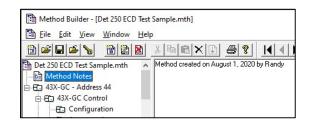
Cal. Inj. Re

21. Drag/drop .RUN files into Recalc list.

22.Create/update SampleList.	files	to	Recalc	lists	from	Append to an existing RecalcList.	lose Dele	
						OK Cancel		

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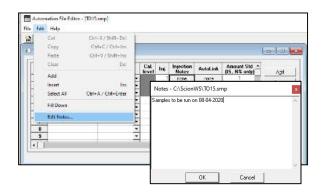
- 23. Sequence List This screen permits multiple actions related to using a series of methods with multiple SampleLists or RecalcLists. The related MessageLog can be printed to provide documentation of actions.
- 24. Notes Free-form user commentary on various activities:
 - Method Notes.



	Sample Name	Samp	la Type	Eal. Invel	lnį.	Injection Notes	AutoLink	Amount Std • (IS, N2 only)	Add
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-			Note	5					X
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• Injection Notes.

• Sample List.



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-	Insert	115		
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-	Fill Down			
-	Edit Nutra.			

Sequence List.

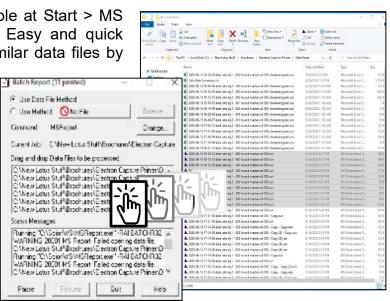
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-	Add		
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1	Edit Notes		7 0
		artic and InnokinshodM02	
8		suits and tomokinested ALC2	
10			
11			

Recalc List.

25. Sample injection time/date and sample name are locked at time of data collection and cannot be changed postrun. Title : Run File : c:\users\lotus\desktop\2020-07-31 14-57-42 test inj 1 - calibration 07-27-2020.run Method File : C:\ScionWS\methods\Calibration 07-27-2020.mth Sample ID : Test Injection Date: 7/31/2020 2:57 PM Calculation Date: 7/31/2020 3:10 PM Operator : Detector Type: 4XX-GC (10 Volts) Workstation: Windows Bus Address : 44 Instrument : Canby Sample Rate : 1.00 Hz Channel : Middle = TCD Run Time : 13 000 min 26. Batch Processing - icon accessible at Start > MS Workstation > Batch Reporting. Easy and quick approach to reprocess lots of similar data files by highlighting desired data files in

Windows Explorer and dragdrop into window.

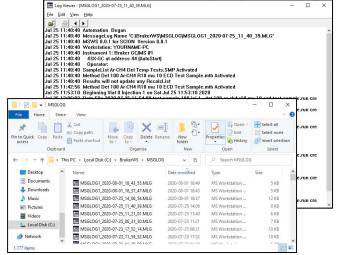




27. Automatic recalculation of data files with sequence list with different method immediately following data collection, with no operator interactions, using Recalc file created with .SMP actions.

alcList Generation	×			-					
You can automatically create or update a RecalcList with files generated during Specify the RecalcList generation options for this SampleList below.	automated injections.		0-08-01.smp]					- [
C Do not automatically create and update a RecalcList.		de Name	Sample	Туре	AutoLink	Cal. level	Inj. ^{II}	njec Nol A	١dd
Create and update a new RecalcList.			Analysis Analysis	-	none		1	nor	psert
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C Append to an existing RecalcList.				Ē			_	_	nes
RecalcList name:	Browse				Recalc		_ist		yks ort
Overwrite the Recalc List each time the SampleList Begins.				-)	ort
OK Cancel							Data Fi	es Rec	calcl

28. MessageLog lists all system control activities, documented with time/date of injection, sample labeling, data file label and location, and errors. These logs are available for recall later.

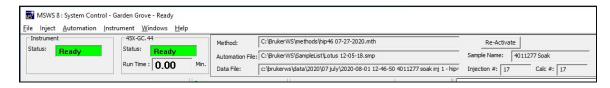


29. Echo - This AutoLink application inserts a string in the Message Log. Use the following syntax in the AutoLink field in a Sample List or Recalc List: command-line: echo other-parameters: <descriptive text

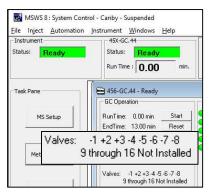
to be "echoed" in the Message Log>

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1 3 x	015.00	ip - Generic SampleL	itt									
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	7			1								1
	8		-						_			
	9				Bro	w/se			DK.	Cancel		-
	10		-					-				1

30. Header block in System Control:



- Listing of active method
- Active automation file
- Last data file collected
- Active sample name
- Injection counter
- Number of calculated files
- Button to reactivate active method

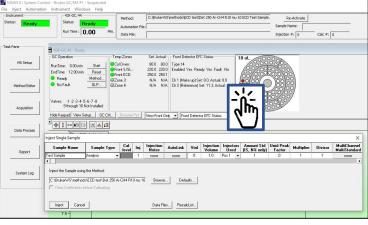


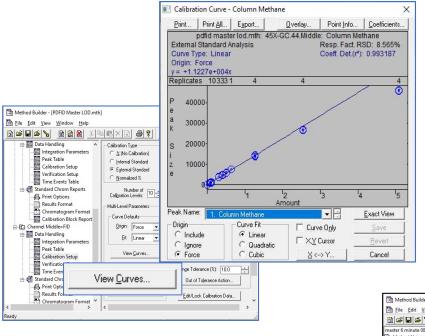
31. Live display of all valve activities on System Control screen.

32. Direct access to SampleList from 8400 display by clicking on center of carousel.

		X-GC.44		Method:	C:\Bru	kerWS methods (E	CD test Det 250	Ar-CH4 R	10 mu 10 EC	D Test Samp	ie.	Re-Activa
tatus: Ready	Stat	us: R	eady	Automation F	le: C:\Bru	kerWS\data\ECD1	2020 Ar-CH4 Det	Temp Te	sts.SMP			mple Name:
	Run	Time : 0	.00	Min. Data File:							In	jection #: 0
ask Pane	4 36-GC.4	U - Readu										
	- GC Operation			Temp Zones	Set A	think - Foort De	Nector EFC Status		10 נ			
MS Setup	RunTime: EndTime:	0.00 min	Start Reset	Col Over: Front S/SL : Front ECD:	80.0 220.0 250.0	80.0 Type 14 220.0 Enabled	Yes Ready: Yes					
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Data Process Report	1	ampleList			Cal	Ini. Injectio		Vial	Injection	Injectors		
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Report	■ 8400 S	ampleList	(4XX-GC): Ar	Sample Type	Cal. level	Ing. Notes	Det 100 Ar CH		Volume	Used Pos 1 -	0:	Add
	1 8400 S	ampleList	(4XX-GC): A nple Name	-CH4 Det Temp Tes Sample Type Activate Method Analysis	Cal. level	Inj. Note:	Det 100 Ar Ci		Volume	Úsed •	0:	Add Insert Delete
Report	₹ * 3 ×	ampleList	(4XX-GC): A nple Name		Cal. level	3 none	Det 100 Ar CH none Det 150 Ar CH	0	Volume 1.0	Used Pos 1 •	0:	Add Inset Delete Fill Down
Report	■ 8400 S	ampleList	(4XX-GC): Au nple Name nple 100 nple 150	CH4 Det Temp Tes Sample Type Activate Method Analysis Activate Method Analysis	Cal. level	3 none	Det 100 Ar CH none Det 150 Ar CH none	0	Volume 1.0	Used Pos 1 - Pos 1 -	0:	Add Insert Delete
Report	1 8400 S	ampleList	(4XX-GC): Ar nple Name nple 100 nple 150 nple 200	CH4 Det Temp Tes Sample Type Activate Method Analysis Activate Method Analysis Activate Method Analysis Activate Method Analysis Activate Method	Cal. level	3 none 3 none 3 none	Det 100 Ar CH none Det 150 Ar CH none Det 200 Ar CH	0	Volume 1.0 1.0 1.0	Used Pos 1 • Pos 1 • Pos 1 • Pos 1 •	0:	Add Inset Delete Fill Down
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Report	1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	ampleList	(400-GC): A (400-GC): A nple Name nple 100 nple 100 nple 200 nple 200	CH4 Det Temp Tes Sample Type Activate Method Analysis Activate Method Analysis Activate Method Analysis Activate Method Analysis Activate Method	Cal. level	Ing. Note: 3 none 3 none 3 none 3 none	Det 100 Ar CH none Det 150 Ar CH none Det 200 Ar CH none Det 200 Ar CH none Det 250 Ar CH none	0	Volume 1.0 1.0 1.0 1.0	Used Pos 1 • Pos 1 • Pos 1 • Pos 1 • Pos 1 •		Add Insett Delete Fill Down Add Lines.
Report	▼	ampleList	(400-GC): A (400-GC): A nple Name nple 100 nple 100 nple 200 nple 200	CH4 Det Temp Tes Sample Type Activate Method Analysis	Cal. level	3 none 3 none 3 none	AutoLink Det 100 Ar CH none Det 150 Ar CH none Det 200 Ar CH none Det 200 Ar CH none Det 250 Ar CH none Det 300 Ar CH none	0	Volume 1.0 1.0 1.0	Used Pos 1 • Pos 1 • Pos 1 • Pos 1 • Pos 1 • Pos 1 •		Add Insett Delete Fill Down Add Lines. Defaults
Report	1 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	ampleList Test San Test San Test San Test San Test San	(400-GC): A (400-GC): A sple Name sple 100 sple 200 sple 250 sple 300	CH4 Det Temp Tes Sample Type Activate Method Analysis Activate Method Analysis	Cal. level v v v v v v v v v v v v v v v v v	Init Note: 3 none 3 none 3 none 3 none 3 none 3 none	PAUGOLINK Det 100 Ar CF none Det 150 Ar CF none Det 200 Ar CF none Det 250 Ar CF none Det 300 Ar CF none	0	Volume 1.0 1.0 1.0 1.0 1.0	Used Pos 1 • Pos 1 • Pos 1 • Pos 1 • Pos 1 • Pos 1 • Pos 1 •		Add Insert Delete Fill Down Add Lines. Defaults. Import
Report	1 () () () () () () () () () (ampleList	(400-GC): A (400-GC): A sple Name sple 100 sple 200 sple 250 sple 300	Activate Method Analysis Activate Method Analysis Activate Method Analysis Activate Method Analysis Activate Method Analysis Activate Method Analysis Activate Method Analysis Activate Method Analysis	Cal. level	Ing. Note: 3 none 3 none 3 none 3 none	AutoLink Det 100 Ar CF none Det 150 Ar CF none Det 200 Ar CF none Det 250 Ar CF none Det 300 Ar CF none	0	Volume 1.0 1.0 1.0 1.0	Used Pos 1 • Pos 1 •		Add Insert Delete Fill Down Add Lines. Defaults. Import
Report	1 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	ampleList Test San Test San Test San Test San Test San	(40X-GC): A uple 100 uple 100 uple 200 uple 250 uple 300 uple 350	Activate Method Analysis Activate Method Analysis Activate Method Analysis Activate Method Analysis Activate Method Analysis Activate Method Analysis Activate Method Analysis	Cal. level v v v v v v v v v v v v v v v v v	Init Note: 3 none 3 none 3 none 3 none 3 none 3 none	PAUGOLINK Det 100 Ar CF none Det 150 Ar CF none Det 200 Ar CF none Det 250 Ar CF none Det 300 Ar CF none	0	Volume 1.0 1.0 1.0 1.0 1.0	Used Pos 1 • Pos 1 • Pos 1 • Pos 1 • Pos 1 • Pos 1 • Pos 1 •		Add Insert Delete Fill Down Add Lines. Defaults. Import

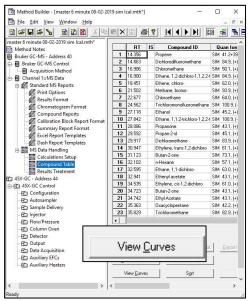
33.Direct access to inject single sample by clicking on vial in 8400 display.





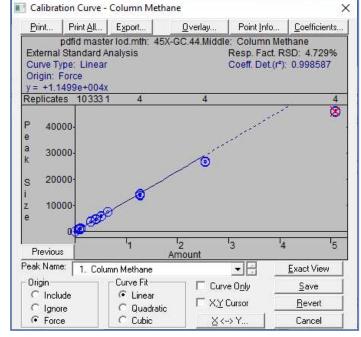
34. Graphic display of calibration plot by Method Editor > Calibration Setup > View Curves for GC detectors.

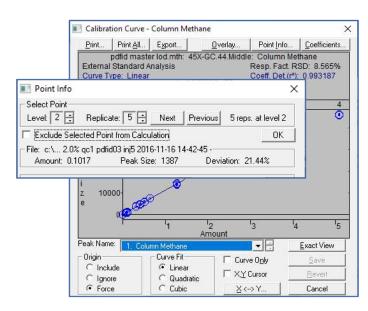
35. Graphic display of calibration plot for MS data through Method Editor > Channel 1=MS Data > MS Data Handling > Compound Table > View Curves.



36. Interconversion of detector response and concentration per calibration curve. This calculator allows anticipation of expected peak size for a given peak size.

Enter Amou	int or Peak Size
Amount (X)	Peak Size (Y)
2.00000	22454.3
Calculate	Cancel



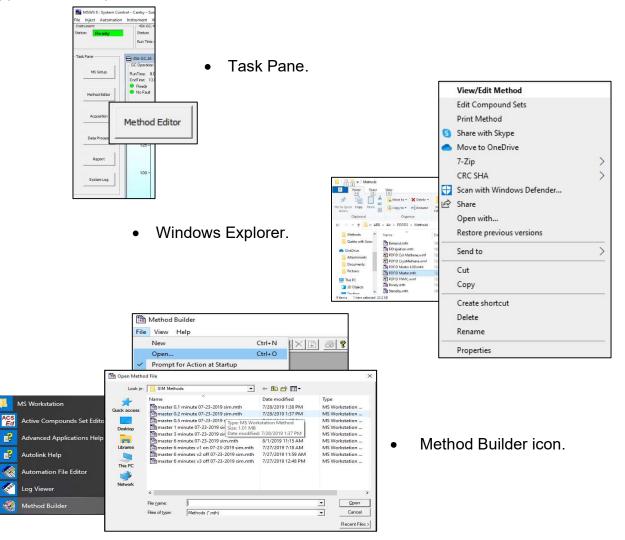


38. Source of calibration data point with Calibration Curve > Point Info.

37. Edit out obviously invalid data points in calibration plot by right clicking on specific points. 39. Edit/Lock Coefficients – When multiple standards with differing analytes are used, coefficients need to be locked after they are calibrated so that the next mixture does not alter them. In addition, coefficients from related analytes can be manually entered. For example, the response values for propane with a flame ionization detector can be applied to other hydrocarbons.

Metho 45X-G(8 45)	AQMD 25.3 3 ml L d Notes - Address 44 -GC Control Configuration pefficients	05-05 A	Calibration T, C 強 (No C C Internal ・ Externa	Calibration) Standard		e Treatment p Replicates Sepa rage Calibration Re ging Weight	
-e-	Retention	Peak Name	Lock Coeffs.	х^з	X^2	×	Intercept
3-	1 2.513	Air/CO	Coens.	0	0	2.8505e+012	0
2-	2 3.440	Carbon Dioxide		ő	-0.0063595	9193.8	0
e e e	3 7.376	Ethane	1	0	-0.34913	9441.7	0

40. Approaches to open method:



41. Indication that Method file has not been saved with an asterisk after the file name in the header. If not manually saved, a prompt will appear for saving.

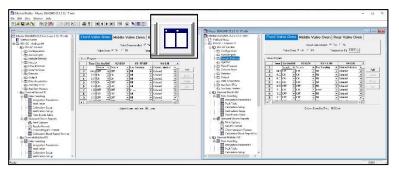


al 🗖	🖆 🎒 🐰 📭					
	l.smp - Generic Samp	des second second				
T	Sample Name	Sample Type		AutoLink	Ca_▲ lev	Add
1		Activate Method	-	PDFID Master.mth		
2			-			Insert
3			-			Delețe
4			-			Fill Down
5			-			
6			-			Add Lines
7			-			Defaults
8			-			
9			-		-	Import
r- d			- 1		` →□	Export

43. Activate "Last Edited" method.

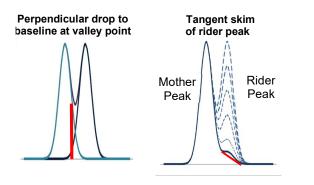
42. Activate method through SampleList.

w\$ [#]	MSWS 8 : System Control - Garden Grove - Runn
File	Inject Automation Instrument Windows
	Activate Method
	Activate Last Edited Method
	Upload Active Method from Modules
	New SampleList
	Open SampleList



44. View multiple methods side-by-side on one screen.

45. Tangent Percent for fused peaks - This compares the height of the rider peak to the height of the mother. If the ratio exceeds the Tangent Percent value, a perpendicular drop is executed, and peak is reported as "Valley/Baseline - VB". If less than this value, a skim is undertaken and marked as "Tangent Skim - TS".



Method Builder - [Master SQAQMD 25.] Eile Edit View Window Help Eile Edit View Window Help Eile Edit N N N N			
	Pesk Detection Subtract Blank Baseline Initial SryL Ratic Initial Peskwidth: Height %: 10	Peak Measurement – Measurement Type © Peak <u>A</u> rea © Peak <u>H</u> eight © Sg. Rt. Height Initial Peak <u>R</u> eject Value: 100	
	angent ight %: 10	•	Peaks Is

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	<u>File Edit H</u> elp							
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		-						
	Untitled.smp - Generic SampleLis	t.						
	Tanana and		10			18.1		
	Sample Name	Sample Type	Cal. Ini	Injection	Autol i	nk 📩		
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F	ile Home Insert Page Layout Formulas Da	a Review View	Help PDFeld	ement Quick	Books	9 12	Insert	
		- Conditional		Ellinsert -				
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Ρ,		: Cell Styles ~		Format ~	Editing Ideas		Fill Down	
c	ipboard % Font % Alignment % N	umber 🕤 Styl	les	Cells	Ideas	~		
KI	3 ▼ : × √ fx					~	Add Lines	
		1.4					Defaults	
2	A Autosampler Type:	B	н	1	J	<u>K</u> =	Deragins	
3							Import	
	Data file Path:	C:\ScionWS\data						
5	Data file Name:	%s					Export	
0		create and update a new						
	RecalcList Generation:	RecalcList						
8	RecalcList Name:	c:\scionws\untitled.rcl						
	Overwrite the RecalcList each time the SampleList Beg	No						
11				AutoLink				
	Sample Number	Sample Name	Command 2	Other Parameters 1	Other Parameters 2	Methoe		
12				Farameters 1	rarameters 2			
13	1	Calibration						
14	2	425362	-					
15	< > 8 Ge (+) 1 (-)	1			L	P P		
			Ħ	100 円		+ 100%		

46. Export SampleList to Excel.

Ē 1 Calibratio 2 425362 1 none 1 none none none Analysis Import Sample List Fill Down \times Add Lines... Defaylts... Select Excel File to Import Import Export C:\ScionWS\SampleList\Test.xlsx Browse... Select path to save the SampleList. C:\ScionWS\SampleList\Test.smp Browse... OK Cancel

Automation File Editor - [Untitled.smp]

12 **2 2 3 4 8 2**

Untitled.smp - Generic SampleList

<u>File E</u>dit <u>H</u>elp

- 0

- -

Add

- • ×

Sample Type Cal. Inj. Injection AutoLink Amc▲ Ievel Inj. Notes AutoLink [IS.] ×

47. Import SampleList from Excel.

48. Default entries simplifies construction of SampleList.

					1	Calibration									
						Calibration		Verifical	tion 👻	1	1	none	none		10000
					2	425362		Analysis	•		1	none	none		Insert
					3				•						Delete
Set Generic SampleList Defaul					4									×	Fill D <u>o</u> wn
set Generic SampleList Delau	ts														Add Lines
Sample Name Sa	mple Type	Cal. level	lnj.	Injection Notes		utoLink	Amount (IS, N% o		Unid Peak Factor	Mu	Itiplie	Divis		iChannel iStandard	
425362 Analys	is 🔻		1	none		none	1		0		1	1		none	Import
•														•	

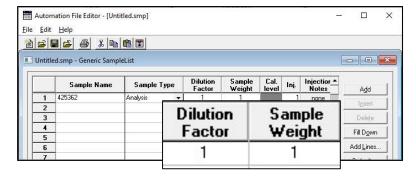
Automation File Editor - [Untitled.smp]

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<u>File Edit H</u>elp

49. Move columns in SampleList by right-clicking in header.

			# 1 Untitled smp - Generic SempleL			
			Sample Name	Sample Type: Col. Int. Intertion AutoLink	Anount Ski Unid Peak Mattylike Divine -	Add
Automa <u>E</u> dit	tion File Editor - [Untit Help	led.smp]		Edit Colur	nn Header	
6	smp - Generic Sample			Move Sele	cted Columns	
Ontitied	Sample Name	Sample Type	Multiplier Divisor		umns to Defaults	101035 2011
1		*			res (rs, wa only) ractor w	
						Ipseit
2						Delete
3						Fil Dowr
3 4		•				
3 4 5		-				
3 4 5 6						Add Lines
3 4 5		•				
3 4 5 6 7		* * * * * * * * * * * * * * * * * * *				Add Lines
3 4 5 6 7 8						Add Lines Defaults.



- 50.Relabel column header in SampleList.
- 51. Copy/paste lines in SampleList with "Shift c" and then "Shift v".
- 52. Copy/paste lines in RecalcList "Shift c" and then "Shift v".
- 53. SampleList AutoLink commands:
 - WAIT This AutoLink application waits for a specified time before terminating; it can be used to perform injections on a specific timetable.

Command: WAIT hours:minutes:seconds

Other Parameters: <none> Hours 0-23 Minutes 0-59 Seconds 0-59

For example, WAIT 15:03:56 will wait for 3:03:56 PM, unless this time is already passed, in which case there will be no wait. Fields can be omitted.

AutoLink Parameters

 Command
 Other parameters

 WAIT :00
 DK

In this case, tailing fields are defaulted to zero, while leading fields are interpreted as the next matching hour or minute. The following examples illustrate most useful cases:

- 13: taken as 13:00:00.
 - 13:10 taken as 13:10:00.

:13 taken as the next occurrence of 13:00 minutes after the hour. At 12:15, this command would wait for 13:13. At 12:10, this command would wait for 12:13.

::13 taken as the next occurrence of 13 seconds after the minute

• GOTO - This application jumps to another line of the sample list or log. Use the following syntax in the AutoLink field in a Sample List or Recalc List:

Command: GOTO <line-number> Other-parameters: Inject or Recalc or Prir

• WAIT and GOTO can be used to create an infinite loop to perform an injection every hour on the hour to monitor a process stream.

	Sample Name	Sumple Type	Cal. Is	i Injection Notez	AutoLink	Amour (IS, NX	Ago
nt 🛛 🔤		Analysis is		1 nore	ncor GD01		Debte
124	20 C				6001	and the second s	FillDown
5	<u>51</u>	-			-		AddLines.
	20 1			1			Defaultz.
Command GOTO 1	1 2 3 4 5	Sample Namer Sa Raza da. 1 Saripli Raza Raza	63 V	Cat Iri I		I toL i AIT :	
						none	.
· · · · · · · · · · · · · · · · · · ·					GI	ото	1

Delete Fil Down Add Lines... Delaults ... Import Export

RecalcList.

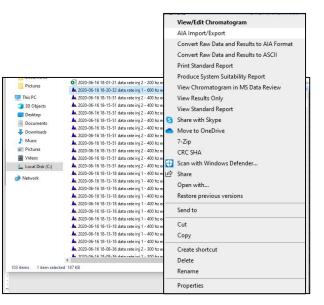
Data Files...

Method Builder - [Det 250 ECD Test Sample.mth*]

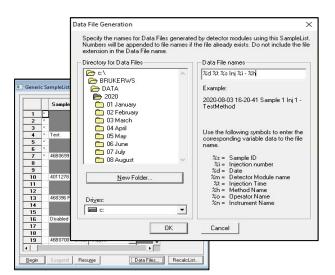
54. "Verification" run type – Reported results compared to values in a calibration level.

om	pared to	values in	a calibr	ation	level.			Eile Edit View Window Help Dig D X Dig
Peak No.	Peak Name	Expected Result ()	Calculated Result ()	Dev.	Ret. Time (min)	Time Offset (min)	(0	C C
1	Hydrogen	125.8000	126.0991	0.2	5.980	-0.010		Imme Events Table Imme Events Table Imme Events Table Imme Events Table Imme Events I
2	Oxygen	25.1500	27.3469	8.7	6.457	-0.009		Automation File Editor - [Untitled smp]
3	Nitrogen	49.9400	49.9810	0.1	7.230	-0.011		File Edit Help
4	Methane	24.8600	24.8167	0.2	8.182	-0.011		
	Totals:		228.2437			-0.041		Ready 4/03/34/0 Foresta Nues Consta Nues Cal. La Injecti *
								Sanplo Name Sample Type Col. Ini. Injecti Add 1 Catization Verication • 1 1 none Igreet

55. Access data file actions from Windows Explorer.

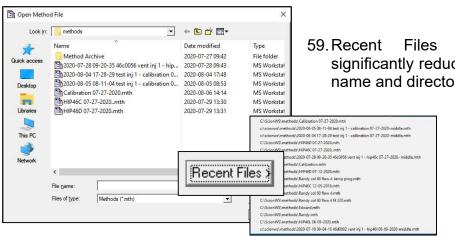


56. Specify/Create data file directory from Sample List.



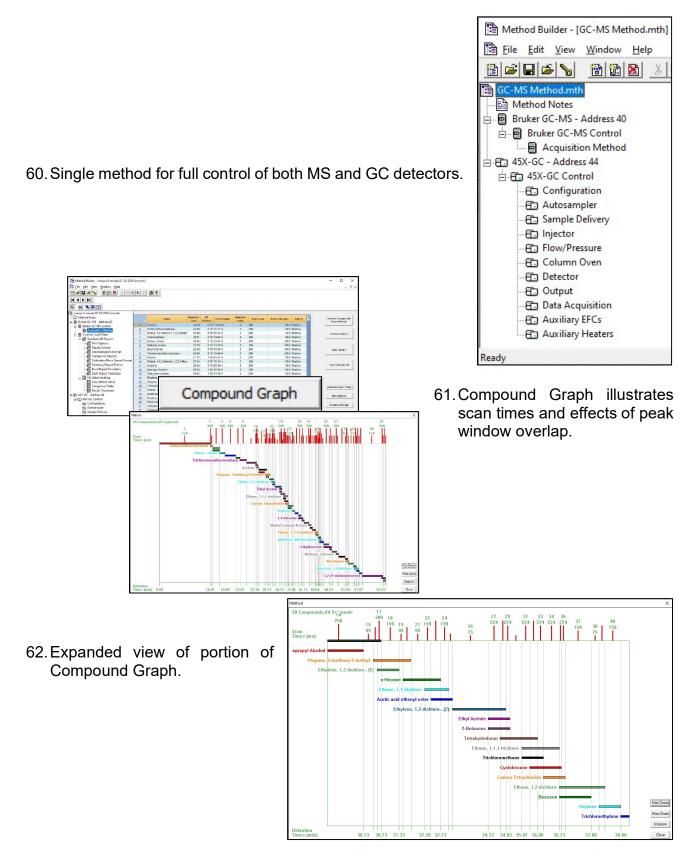
Data File Generation × Specify the names for Data Files generated by detector modules using this SampleList. Numbers will be appended to file names if the file already exists. Do not include the file extension in the Data File name. Directory for Data Files-Data File names 🗁 c:\ %s Brite Scient 🔎 dal Example 57. Automatic data file naming with Sample 1 tokens. Use the following symbols to enter the corresponding variable data to the file Use the following symbols to enter the corresponding variable data to the file name. name. 58. Data file names can have up to 255 %s = Sample ID %s = Sample ID $\begin{array}{l} & \&s = Sample ID \\ & & \&i = Injection number \\ & \&d = Date \\ & & & & Detector Module name \\ & & & & & \\ & & & & \\ & \&t = Injection Time \\ & & \&h = Method Name \\ & & & & \\ & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & & \\ & & & & \\ & & & \\ & & & & \\ & & & \\ & & & & \\ & & & \\ & & & & \\ & & & & \\ & & & & \\ &$ %i = Injection number characters. %d = Date %m = Detector Module name %t = Injection Time %h = Method Name Cancel %o = Operator Name %n = Instrument Name

%f = Data Folder

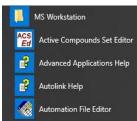


59. Recent Files button. This action significantly reduces errors in entry of file name and directory path.

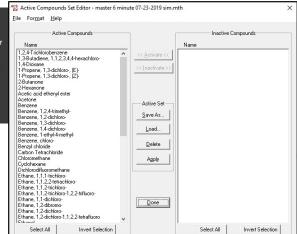




63. Active Compounds Set Editor - ACS is a list of compounds, representing a subset of the Compound Table, which can be saved in a method, and activated during

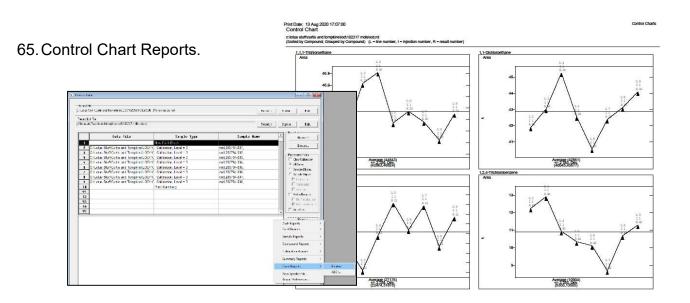


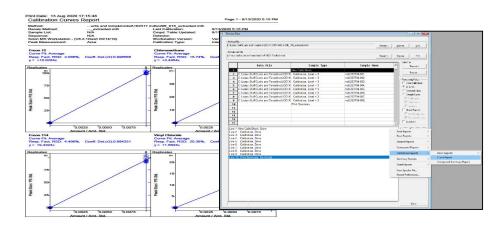
automation. MSWS includes an interactive application (ACTIV2.EXE) to create, edit, delete such sets within a method file. MSWS also includes an automated application (ACTIVATE.EXE) which can be invoked within a sample list to activate one or more sets in the active method.



64. Process Files.

rocess D				
	Shift/Curis an		_ Pecept >	Erxuse Edt
Recelc L c: \lotus s	Proces	s Data	Recent	Bigene. Edt.
		pe	Sanple Hame	Data File Becent >
1		New Calib Block		Browne
	C \Lotus Stuff\Curtis and Tompkins\LOD\10		mdl,283794-001	provise
3	C:\Lotus Stuff\Curtis and Tompkins\LOD\10		mdl,283794-002,	Processing Rules
	C Lotus Stuff/Curtis and Tompkins/LOD/10		mdl,283794-003,	Clear Calibration
	C:Lotus Stuff/Curtis and Tompkins/LOD/10		mdl.283794-004,	@ Al Lines
	C V.otus Stuff/Curtis and Tompkins/LOD/10		mdl.283794-005	C Selected Lines
	C:\Lotus Stuff\Curtis and Tompkins\LOD\10		mdl.283794-006. mdl.283794-007	C Gample Types
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12	1			No Receivable
14	1			F Provent Rapor
15				T AutoLink
				Beparts
				Process





10 ppt - 1.67 ppt Lotus Toxics Area 7/24/2019 9:48 PM 8/23/2020 9:57 AM Analysis

Operator: Last Calibration: Calibration Type Data File: Method:

8/22/2020 7:22 AM External Standard ...e 07-23-2019 sim.xms 7-29-2019/randy.mth

33.6% 25.4%

Identified

<u>Status</u> Pass

Pass Pass

Status

42 649

•

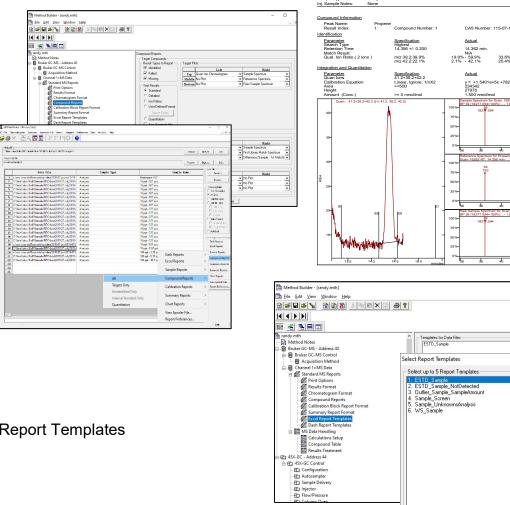
×

Select up to 5

Cancel

66. Calibration Reports.

67. Compound Reports



68. Excel Report Templates

69. Dash Reporting.

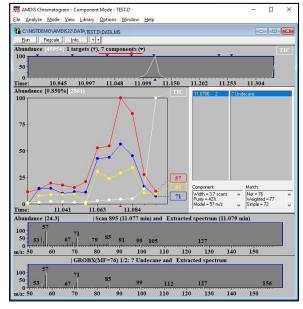
70. EnviroPro Reporting - provides detailed information on reporting results for common USEPA methods - 524, 525, 624.625, 8240, 8250, 8260, 8270, 8270, CLPVOL and CLPSV. Tune Reports can be generated.

		Tune Criter	ia				
		Relative Ab	undance L	imits (Comparis	on lons	
m/z	Acceptance Criteria	Low1	High1	Low2	m/z 1	m/z 2	
a	30-60% of m/z 198	30	60	<u> </u>	198	0	
68	<2% of m/z 69		1.999		69	0	
69	Present	0.001	100		0	0	
70	<2% of m/z 69		1.999		69	0	
127	40-60% of m/z 198	40	60		198	0	
197	<1% of m/z 198	0	0.999	0	198	0	
198	Base peak	100	100	0	0	0	
199	5-9% of m/z 198	5	9	0	198	0	
275	i 10-30% of m/z 198	10	30	0	198	0	
365	i >1% of m/z 198	1.001	100	0	198	0	

Current Method		
Tune Criteria: 624		
Tune File:		
Method Title: EPA	Method 624	Matrix: WATER
nitial Calibration:		
EPA Method		Tune Criteria
Volatiles	SemVolatiles	
C 524	C 525	🖵 Use CCC As Tune File
· 624	C 625	
C 8240	C 8250	Tune Report Setup
C 8260	C 8270	Matrix WATER 🔍
C CLPVOL	C CLPSV	Set Initial Calibration
Help		Close

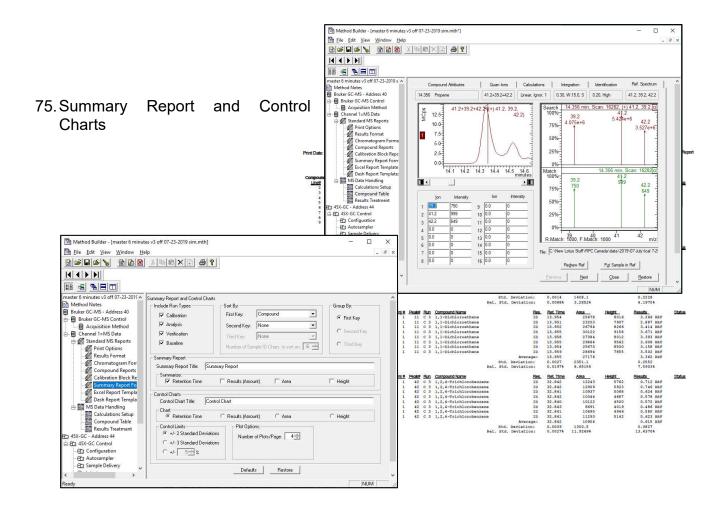
- 71. Multicompound Software 19 templates allow various displays of target compounds, tentatively identified and unknown compounds in 1) graphic and text, 2) graphics only and 3) text only configurations.
- 72. ToxProPlus MS Reporting Software software includes three separate custom software packages: multicompound software, ion ratio summary report software, and screening software to aid reporting.

73. NIST Automated Mass Spectral Deconvolution and Identification System -AMDIS - allows users to automate the complex process of extracting data from GC/MS data file. AMDIS works by finding all of the ions that rise and fall at the same time and associating them to a single component. Once it has found this component it compares it to a library of spectra and retention indices provided.



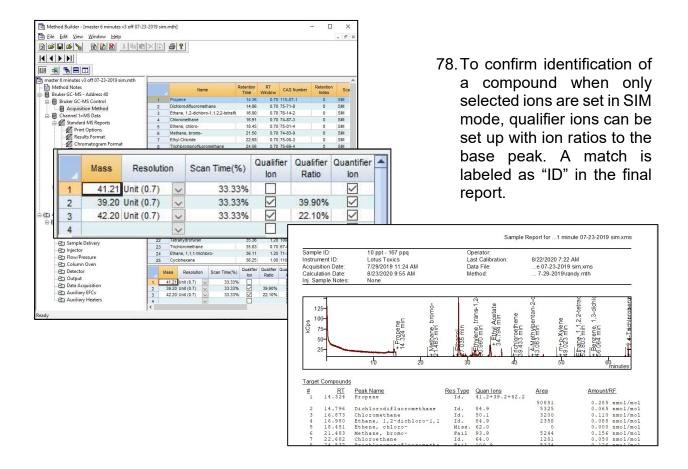
% 🖻 🛱 🏭 🖬 🖬	? → <i>z</i> ← ?	
CHLOROBENZENE	Clear a-z mainlib	•
Chlorobenzen		112
Chlorobenzene Chloro benzene	100-	
Chlorobenzene, mono-		-
Chlorobenzenu		a
Chlorobenzhydrol		
Chlorobenzoic acid		- ~
Chlorobenzol	50-	77 (
Chlorobromodifluoromethane		Γ
Chlorobromoform		
Chlorobromomethane		
Chlorobutadiene	51	~
Chlorobutanol	25 32 38 43 56 61	84 97
Chlorocaps	1 0 min rath a ather a state	the put of the put the
Chlorocarbonate de methyle	20 30 40 50 60 70	80 90 100 110 120 130
Chlorocarbonate D'ethyle	(mainlib) Benzene, chloro-	
Chlorocarbonic acid, ethyl este	Name: Benzene, chloro-	12
Chlorocarbonic acid, methyl es Chlorocarbonylsulfenyl chloride	Formula: CgH5Cl	10
	MW: 112 CAS#: 108-90-7 NIST#: 1680 ID#	1005 DP: mainlin
	Other DBs: Fine, TSCA, RTECS, EPA, HOD	
Chloro (chloromethyl)dimethylsil		JC, NIH, EINECS, INDB
Chloro (chloromethyl)dimethylsil Chloro (chlorosulfanyl)oxometh	10 largest peaks: 112 999 77 453 114 329 51 120	
Chloro (chloromethyl)dimethylsil Chloro (chlorosulfanyl)oxometh Chlorocid	10 largest peaks:	50 961
Chloro (chloromethyl)dimethylsil Chloro (chlorosulfanyl)oxometh Chlorocid Chlorocide	10 largest peaks: 112 999 77 453 114 329 51 120	50 961
Chloro(chloromethyl)dimethylsil Chloro(chlorosulfanyl)oxometh Chlorocide Chlorocide Chlorocidin C Chlorocidin C tetran	10 largest peaks: 112 999 77 453 114 329 51 120 113 691 38 571 75 46 74 43 Swnoryms: 1. Chlorobenzene	50 961
Chloro(chloromethyl)dimethylsil Chloro(chlorosulfanyl)oxometh Chlorocide Chlorocide Chlorocidin C Chlorocidin C tetran	10 largest peaks: 112 999 77 453 114 329 51 120 113 691 38 57 75 46 74 43 Swnonyms: 1.Chlorobenzene 2 Monochlorobenzene	50 961
Chloro (chloromethyl)dimethylsi Chloro (chlorosulfanyl)oxometh. Chlorocid Chlorocidin C Chlorocidin C Chlorocidin C tetran Chlorocid S Chlorocid S	101srgest peaks: 112.999 77.453.1 114.2291 51.120 113.691 38 571 75 461 74 43 Smoortyma: 1Chlorobenzene 2. Monochlorobenzene 3.MCB	50 961
Chloro(chloromethyl)dimethylsil Chloro(chlorosulfanyl)oxometh. Chlorocide Chlorocide Chlorocidin C Chlorocidin C tetran Chlorocid S Chlorocol Chlorocol	10.1arcest peaks: 112.9991 113 691 113 691 123 691 123 75 124 75 125 75 126 74 Synomma: 1.Chlorobenzene 2.Monochlorobenzene 3.MCB 4.Phenyl (Chloride 4.Phenyl (Chloride	50 961
Chloro(chloromethyl/dimethylai Chloro(chloromifanyl)oxometh. Chlorocid Chlorocidin C Chlorocidin C Chlorocidin C Chlorocid S Chlorocol Chlorocol Chlorocosol Chlorocesol Chlorocyan	10.Imment peaks: 112.999 77.4531 114.329 51.120 113 691 38.571 75.461 74.43 Sunonma: 1.Chirobenzene 2.Monochlorobenzene 3.MCB 3.MCB 5.Benzene chloride 5.Benzene chloride 5.Benzene chloride	50 961
Chloro(chloromethyl)dimethylai Chloro(chlorosulfaryl)oxometh- Chlorocid Chlorocidh C Chlorocidh C Chlorocidh C Chlorocol Chlorocol Chlorocol Chlorocyan Chlorocyan Chlorocyande	10.10000000000000000000000000000000000	50 961
Chloro(chloromethyl)dimethylai Chloro(chlorosalfaryl)oxometh Chlorocid Chlorocid Chlorocidn C Chlorocidn C Chlorocidn C tetran Chlorocid S Chlorocol Chlorocresol Chlorocyanide Chlorocyanide (clcn)	10.Imment peaks: 112.999 77.4531 114.329 51.120 113 691 38.571 75.461 74.43 Sunonma: 1.Chirobenzene 2.Monochlorobenzene 3.MCB 3.MCB 5.Benzene chloride 5.Benzene chloride 5.Benzene chloride	i 50 961 i 56 391
Chicor(chicomethoay) methan Chicor(chicomethy) dimethylal Chicor(chicomethylamethylal Chicorcida Ch	10.10000000000000000000000000000000000	50 961

74. NIST 20 and NIST 20 Upgrade - 350,704 electron ionization (EI) spectra -306,643 compounds, 43,774 replicate spectra (39,729 more compounds than NIST 17) and retention indexes for 139,963 compounds.



76..XMS data file for MS possesses:

- Raw data points
- Last computed results
- Copy of last method used
- Link to original method
- Calibration data points
- 77. Selected Ion<u>s</u> Monitoring (SIM) Data from multiple ions can be collected to provide positive matching to reference spectrum with use of multiple characteristic ions for compounds.



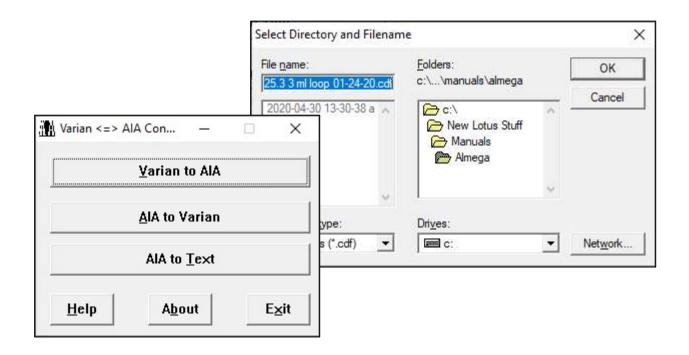
- 79. Wiley Registry of Mass Spectral Data, 11th Edition Comprehensive mass spectral library contains 775,500 mass spectra, over 741,000 searchable structures, and over 599,700 unique compounds.
- 80. Maurer, Pfleger, Weber Library, 2016 Edition includes novel designer drugs and a broad range of AIDS therapeutics, for a total of over 8,800 clinically relevant substances, including more than 3,500 metabolites.
- 81. Rosner Mass Spectral Library of Designer Drugs, 2019 edition provides comprehensive data of novel psychoactive substances with 28,032 mass spectra, 28,032 chemical structures, 21,649 unique compounds, 18,017 measured kovats indices, 353 opiates, 866 fentanyls, 996 cannibiminetics and 112 canniboids.

82. Convert .XMS files to Content Definition File - .CDF used by groups and organizations to share abstract enterprise content management data. The files created in this format are saved with the .cdf file suffix in an XMLbased data format.

otus Stuff\Manuals\RP	C\data\2019\07 Jul	y\2019-07-31 13-	27-19 100 ppb- 5
otus Stuff\Manuals\RP	C\data\2019\07 Jul	y\2019-07-31 13-	27-19 100 ppb- 5
Converting Cullion Lat	in Chuff Manuala DD	Cldsts\2010\07	
	Convertion Cillion Lab	Convertion C (Marci Labor Shi (PM-revolution	Converting C: Wew Lotus Stuff Manuals (IRPC Idata \2019)07

83. ASTM E1947 - 98(2014) Standard Specification for

Analytical Data Interchange Protocol for Chromatographic Data. This app generates .CDF files that can be exported/imported in other brands of chromatography software compatible with AIA format.



Hints with operations with GC detector .RUN data files

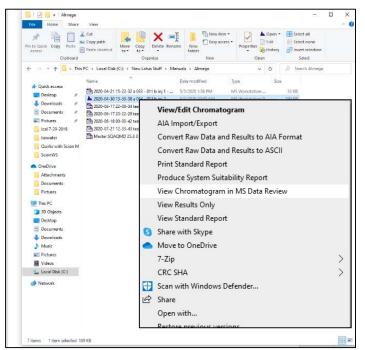
🛦 Interactive Graphics - Method: 2020-08-03 06-07-22 test inj 1 - calibration 07-27-2020-middle.mth for run file 2020-... 🛁 × Eile Edit View Results Edit Method Help 🖆 🗃 🖇 👔 🕼 🖟 🛵 📰 🐼 🐼 🚫 NO File 75 X: 8.4533 Minu Y: -5.24 mVolts Name: Oxygen Result: 21.556 Area: 6048 Counts Width: 3.80 sec 50 mVolts 25 -10.062 6.453 3.177 7 227 0 -84. Display of peak details in 75 X: 6.4483 Minu Y: 5.40 mVolts mVolts 50 -Interactive Graphics. Vame: Oxygen Result: 25.150 Area: 8051 Co Width: 3.60 sec 8.175 10.060 .225 25 -3.448 888 Highlight desired peak and 0 carefully drop straight down to 75-X: 6.4587 Mir Y: 5.65 mVolts 50 mVolts expose other peak Name: Oxygen Result: 27.741 10.068 8.183 6.457 7,232 25 -Area: 8880 Court information. 0 -Nidth: 3.70 sec 75 -X: 6.4667 Min Y: 8.37 mVolts mVolts 50 -0.082 Name: Oxygen Result: 25.150 193 467 242 25 Area: 7791 Cou 0 -Width: 3.70 sec 75-X: 6.4567 Min Y: 5.81 mVolts Name: Oxygen Result: 27.347 Area: 8471 Count: Width: 3.70 sec 50 · mVolts 3.457 .230 82 25

2.5

5.0

0

For Help, press F1

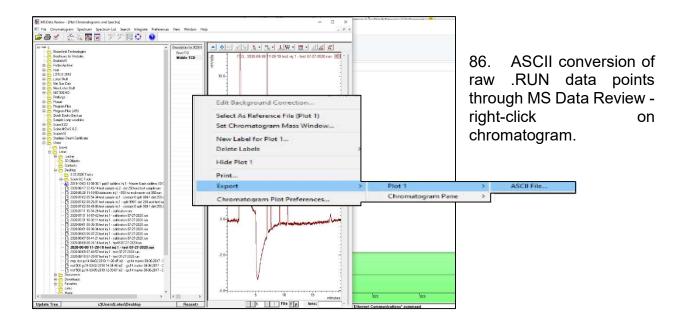


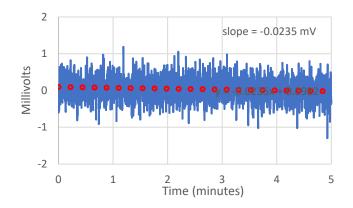
85. Insert .RUN data file into MS Data Review from Windows Explorer by right-clicking on desired data file.

7.5

10.0

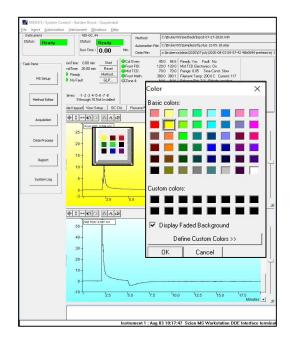
Minutes





87. Detector signal drift computed through Trend Line of ASCII data points via Excel.

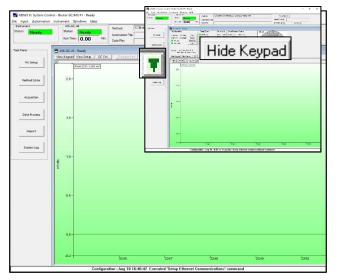
88. Change colors of displayed live chromatograms.

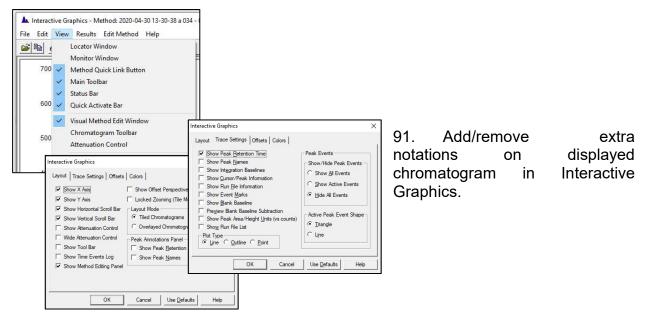


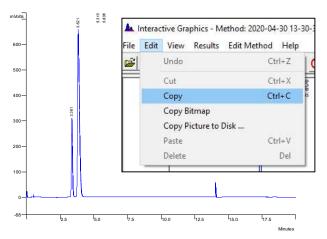
nstrument atus: <mark>Running</mark>	45X-GC.44 Status: Running Run Time : 0.65 min.	Re-Activate Sample Name: Injection #:	Method: C:\Sci Test 9 Calc #:
Vie	ew F & M Ver w Front Only w Middle Onl w F & M Hora	y ly	Set Actual Set 60.0 60.0 Vah 80.0 80.0 Vah 80.0 80.0 Vah 380.0 380.0 Vah Vah Vah Vah
Data Process Report System Log	Font FID: 0.046 mV 150 - 125 - 100 - 25 - 0 - -15 - 25 - 0 - -15 - 25 - 0 - -15 - 25 - 0 -		

90.Set chromatogram display for full screen.

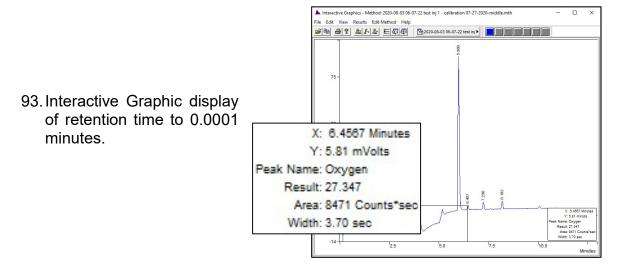
89. Display of live chromatograms in System Control – single, double or triple, and horizontal or vertical.







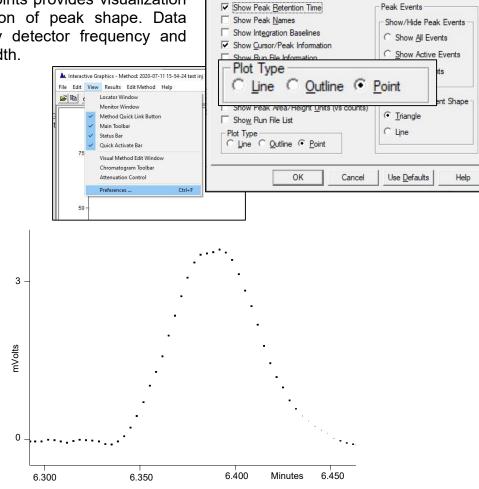
92. To display a chromatogram in external documents, such as Word, "copy" from Interactive Graphics to Clipboard and the "paste into the .docx. This action allows the chromatogram labels to be edited and comments added.



Method Builder - [Method1*]	-
🖺 Eile Edit View Window Hel	p
Method1* ^	Data Acquisition
	Detector <u>F</u> requency: 10 y Hz Noise <u>Monitar Length</u> 64 ÷ points (6.400 sec)
- E Autosampler	

94. Detector frequency. This parameter impacts data collection with number of data points to define the peak and with noise level.

95. Display of data points provides visualization of proper definition of peak shape. Data interval is set by detector frequency and expected peak width.



Interactive Graphics

Layout Trace Settings Offsets Colors

Х

96. Single method possesses:

- Full set of parameters for control of GC
- Full set of parameters for computation of results
- Calibration data points
- Formatting for chromatograms and reports
- Baseline subtract data points

97..RUN data file for GC detectors possesses:

- Raw data points
- Last computed results
- Copy of last method used
- Link to original method
- Baseline subtract data points

- Calibration data points
 - 98. Fill Peak Table is accessible through Interactive Graphics. Clicking on peaks in the displayed chromatogram will add these peaks to Peak Table of active method.

mV ofts	75 - 50 - 25 - 0 -	Set Pass Method Integrat Peak Tal Time Ev Calibrat Verificat	Notes ion Para ble ents ion Setu ion Setu	meters. p			>7.232	> 8.165		10.068 10.325 10.675	
	75 -	Add Me		m		>					
Peak 1	able Retention Time	Peak Name	Ref	Std	BBT	Standard Pea Name	k	Group	Level 1 Amount	^	
	5.990	Hydrogen		11			-	0	125.8		Add
2	6.466	Oxygen	ヨ	盲			-	0	25.15		Insert
3	7.241	Nitrogen	=	11			*	0	49.94	-	Delete
4 5	8.193	Methane	1	10			-	U	24.86		
	e from selection			_	Save	Cancel	<u> </u>				Sort
mVolts	75 - 50 - 25 -					6.467	7.242	8.183		10.082	
	0-14	¹ 2.5		~	5.0)		7.5		40.0	K

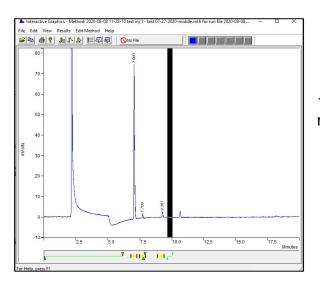
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mvatts	75- 50- 25- 0		s.ar	2022(581 K	
m/olts	75 - 50 - 25 - 0 -		6.651	8272 (50.3	
m/vatts	75- 50- 25- 0		Lasr	0027	200.0	
moats	75 - 50 - 25 - 0 -		186-2		61.8	-
	1		ہ ۳	۲ ه د ا	6 6	Minutes

99. Graphically relocate retention times in Peak Table by right-clicking on yellow window under peak and move to adjust.

100. Add timed events by right-clicking in window below the chromatogram.

101. Deletion of timed events in Interactive Graphics can only be performed in "Tile" mode.

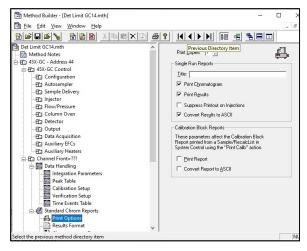
A Interactive Graphics - Method: 2020-08-03 06-07-22 tes	st inj 1 - calibration 07-27-2020-middle	amth for run file 2020 — 🛛	×
File Edit View Results Edit Method Help	Fie E		
75- <u>8</u> 50- 25- 0- 75-	Add Peak Table Entry		
Interactive Graphics			×
Layout Trace Settings Offsets Image: Show X Axis Image: Show Y Axis Image: Show Horizontal Scroll Bar Image: Show Vertical Scroll Bar Image: Show X Axis Image: Show Vertical Scroll Bar Image: Show X Axis Image: Show X Axis		grams	
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C Tiled Chrom		;	
ОК	Cancel Us	e <u>D</u> efaults Help	

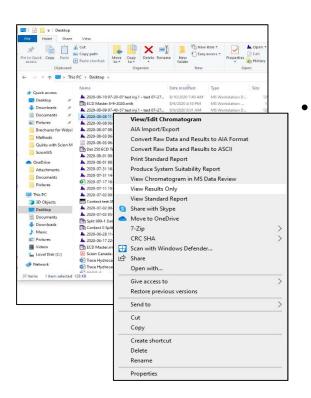


102.Graphically relocate time events with mouse.

103. Reporting of Results:

• Set up for automated printing at run end with Automated Printing enabled.





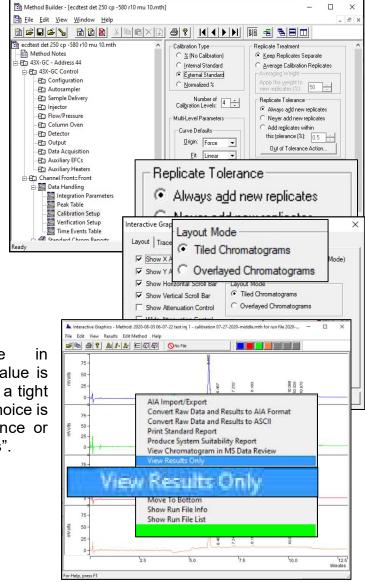
Set up printing parameters in method.

• Access data files from Windows Explorer.

File Edit View Window Help		- 5
ecdtest det 250 cp - 580 r10 mu 10.mth → Method Notes → 13X-GC - Address 44 → 13X-GC Control → 10 43X-GC Control → 10 Autosampler → 10 Sample Delivery	Calibration Type Calibration Type Calibration C Internal Standard C External Standard C External Standard C Averaging Weight C Averaging Weight	es
- ED Injector - ED Flow/Pressure - ED Column Oven - ED Detector - ED Data Acquisition - ED Ata Acquisition - ED Auxiliary FECs - ED Auxiliary Heaters	 Keep Replicates Separate Average Calibration Replicates Averaging Weight 	
	Apply this weight to new replicates (%): 50 + [Nore] Edit/Lock Calibration Data.	

• Interactive Graphics allows up to seven chromatograms to be displayed. If chromatograms are displayed in "tile" mode, as specified in Interactive Graphics > View > Layout, then right-click with mouse in any of them offers its report to be displayed or printed.

104. Replicate Treatment in Method Builder - Preset value is set to Average Calibration Replicates. Often the individual data points are desired to be indicated separately and this parameter can be changed to "Keep Replicates Separate".



105. Replicate Tolerance in Method Builder - Preset value is set to add replicates within a tight tolerance of 0.5%. Better choice is either to widen the tolerance or "Always add new replicates".

19	10 R ×	0	<u>१</u> ।				
	Time Ever	its Program					
Method Notes 45X-GC - Address 44		Time	Event	Value / End Time	Description	-	Add
Channel Middle=Middle	1	2.4404	FP 👻	4.4402	(End time: 0.0-1440.00 min)		Insert
🖻 🎆 Data Handling	2	11.0000	WI 👻	32 sec 💌	(0.5-256 sec)		
Integration Parameters	3	12,9159		14,7040	(End time: 0.0-1440.00 min)		Delete
4	14.51	25 G	R	-	19.89	85.	Sgit

106. Baseline Subtraction - The baseline run is a reduced set of 257 to 512 data points across the

chromatogram run time by a bunching is stored process, within the method used for its collection and is subsequently subtracted from sample runs prior to detection. peak **Baseline Subtraction** is activated by enabling it in Method Builder > Integration Parameters >

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	on MS Worksta					2.1 **	00101	-2311-AB1-	4118 **			
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un Mo eak M Calcul Peak	de : A easurement: P ation Type: E Peak	nalysis - S eak Àrea xternal Sta: Result	ubtract ndard Ret. Time	Blank Bas Time Offset	eline Area	Sep.	Width 1/2	Status	4118 **			
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lun Mo Peak M Calcul Peak No.	de : A easurement: P ation Type: E Peak Name Methane Carbon Monox	nalysis - S eak Area xternal Star (ppmC) 1.69 0.92	ubtract 1 ndard Ret. Time (min) 5.360 6.352	Time Offset (min) 0.487	Area (counts) 2920 18652	Sep. Code BB GR	Width 1/2 (sec) 26.7 0.0	Status Codes	4118 **			
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Run Mo Peak M Dalcul Peak No. 1 2 3 3 3 5 tatus	de : A easurement: P ation Type: E Peak Name Garbon Monox NMNEOC Totals: Codes:	nalysis - S eak Area xternal Sta: (ppmC) 1.69 0.92	ubtract 1 ndard Ret. Time (min) 5.360 6.352	Time Offset (min) 0.487 0.026	Area (counts) 2920 18652	Sep. Code BB GR	Width 1/2 (sec) 26.7 0.0	Status Codes	4118 **			Ŷ

Subtract Blank Baseline, and by indicating the first run in a series in SampleList as Sample Type – "Baseline".

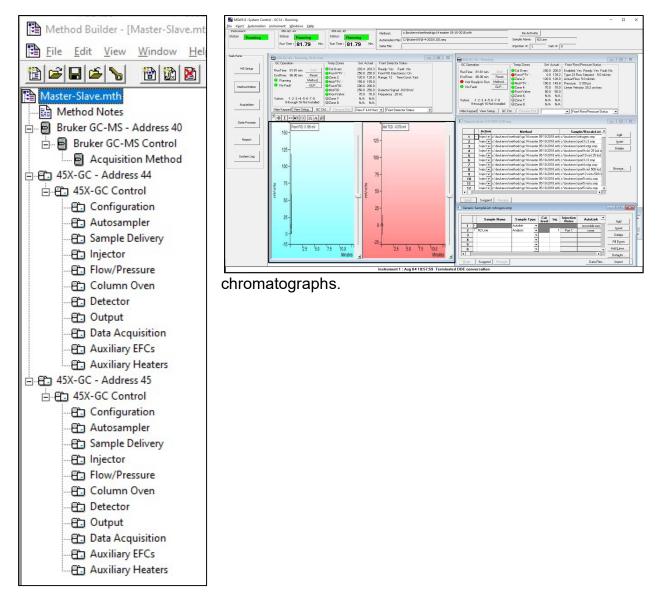
107. Grouping by time interval – detector response can be grouped over a userselectable time interval. This process is often used for grouping non-methane hydrocarbons in EPA Method 25, and for summing up all hydrocarbons in natural gas for Hexane+. Assigned retention time for the group is the midpoint between and starting and ending points.

364	Baseline Analysis Analysis Analysis	•	none	Add			
	Analysis	-	none	Insert			
25364 25365		-					
25365	Analysis		none	Delete			
		-	none	Fill Down			
		-		1-10 D/DAM1			
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Data Acquisition Auxiliary EFCs Auxiliary Heaters		Twee raise:	ro prous		108. Grouping	by	peak label –
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concentrations, selected peaks can be grouped by peak name. Examples include summing up separate peaks in measurement of polychlorinated biphenyls, toxaphenes, and aromatic hydrocarbons.

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109. Master/Slave Gas Chromatographs – Some applications require more hardware capabilities than are available in one instrument. By combining two gas chromatographs in a Master/Slave configuration, accessible resources are doubled. One gas sample is loaded into both instruments, and the master then starts both concurrently. A single method loads parameters for both



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