Obscure Jewels with Scion MS Workstation V8.2.1 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
- .IQD Dash Queries
- .IRL Dash RuleList
- .IRM Dash Report Template
- .IRO Dash Method Objects
- .MSF AMDIS Data File
- .CDF Content Definition File
- .MSP Spectrum List
- .TXT Text 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 as to 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. System Control should be closed before powering off the GC, to maintain interconnection between instrument and MS Workstation. 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.
- GC Remote Control allows view of status of gas chromatograph from a remote computer, typically through Team Viewer or similar app. (C:\Program Files\Scion GC Tools\GC Remote Control). Access is through Taskbar icon:



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5. **Change time/value** for any timeprogrammable parameter while running, if the step has yet to be executed

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



 Instrument Log – lists activities for the instrument, including faults with time/date stamp. Historical logs are available at C:\ScionWS\MSLOG.

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 Ready
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 Method.
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-Temp Zone

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Valve 0 Valve 0 Valve 0



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. Access any method – even if it does not match current Setup.

MSWS 8 : System Control - Garden Grove - Ready File Inject Automation Instrument Windows Help

45X-GC 44

Ready

Start

Reset

Method ...

ide Keypad View Setup... | GC Ctrl... | Resume Plot |

GLP...

Run Time : 0.00

Status:

tunTime: 0.00 min

ndTime: 20.00 min

alves: +1 -2 -3 -4 -5 -6 9 through 16 Not

Ready

No Fault

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

Instrument

Ready

MS Setup

Method Editor

Status:

Task Pane



10. **Resume Plot** - permits visible display of active baseline drift and noise without starting a run.

Method:

Data File:

Min.

Col Oven

Front FID:

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OZone 4:

Resume Plot

Automation F

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11. **FID/NPD/PDD Detector Full Scale** - the electrometer for these three 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.

12. Entry and display of temperature zones in 0.1 °C increments.

tatus: Ready	Status: Ready Run Time : 0 00 Min.	Method: Automation File:	C:\BrukerWS\me	thods\ECD 2020\ECD Master.mth
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Method Editor	No Fault GLP Valves: 1 -2 -3 -4 -5 -6 -7 -8	DZone 4:	N/A N/A	Contact Potential: -399 mV Detector Signal: 356.049 mV Frequency : 5 Hz

for

temperature

minutes

0.006 °C.



14. Data Rates for GC Detectors – All detectors, including Electron Capture Detector (ECD), have full range of data rates, from1 Hz to 600 Hz, in 12 steps.



Hethod Builder - [randy.mth] X Eile Edit View Window Help -8245<u>88888×</u>688 Help Data Acquisition 🖺 randy.mth Method Notes 43X-GC - Address 44 Detector Frequency: 600 - Hz 43X-GC Control Noise Monitor Length: 64 + points (0.107 sec) Configuration Autosampler The following settings will be ignored for all detectors other than the FID and NPD. B Injector E Flow/Pressure FID/NPD Detector Full Scale Column Oven Detector 10 V Front -Cutput Data Acquisition 10 V -Middle: Rear: 10 V -Auxiliary Heaters Channel Front=Front 🗄 💹 Data Handling Integration Pa Column Oven End Time: 20.00 min lav Help Top

13. Stability of temperature zones -

variation

Detector. Average is 250.015 ±

Electron

over

10

Capture

15. Ready "Green"/Not Ready "Red" status lights.

Common Hints for Both MS and GC Detector Operations

- 16. **Concurrent instrument control and data collection** for MS and GC with single Method.
- 17. **Concurrent data collection** for MS and GC with single SampleList.





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



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

ector Root Mean MS Data Review. MSWS and use line for noise	MS Data Review - Plot Chromatograms and Sp File Chromatogram Spectrum Spectrum List Plot Chromatograms and Spectra Plot Chromatograms and Spectra 2020/88/04165631 - 2020/88/04165631 - 2020/88/04172832 - 2020/88/04178438 - 2020/88/04184001 - 2020/88/0418400 - 2020/88/0400 - 2020/88/0400 - 2020/88/0400 - 2020/88/0400 -	etra Search Integrate Prefere Integrate Prefere PI Chromatogram Markers Features Chr Noise	ences View Wi Nots View Chroma Nots View Spectra Plot Prefe TL Ann romatogram Colors	ndow Help togram Pane Pane rences otations n Plot Plot Labels	AMDIS A Titles DH Axes	× Annotations H Annotations Font
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21. Up to 50 calibration levels.



22. Calibration plots of response factor versus log[concentration] - from Lotus Consulting. Conventional plots of detector response versus concentration does not provide good visibility of linearity over wide concentration ranges. Results displayed as a semilog



plots allows easy validation of linearity over wide concentration ranges. Routine available from Lotus Consulting.

- 23. **Response factors computed as** $\frac{\text{Area}}{\text{Concentration}}$, as specified in most EPA methods.¹
- 24. **Recalc List** This screen allows selected data files to be recalculated with a modified or different method. The list can be generated automatically by entries in SampleList.



¹ US EPA, Compendium Method TO-15 Determination of Volatile Organic Compounds (VOCs) In Air Collected In Specially-Prepared Canisters and Analyzed by Gas Chromatography/Mass Spectrometry (GC/MS), 1999, https://www3.epa.gov/ttnamti1/files/ambient/airtox/to-15r.pdf, p. 15-23.

26. Calculation 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.



30. 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.

Method Notes.

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31. Notes - Free-form user commentary on various activities:

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 - Sample List Notes.

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• Injection Notes.



• Sequence List Notes.

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32. **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 drag-drop into window.



33. 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

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34. Name of Operator can be entered when a SampleList of Sequence is initiated and cannot be changed postrun.

35. 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.

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36. **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.

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6		-		eck	o.		Samples co	ellected 90n 07	28-2020		-
7		-		1.000						-	1
8		1									-
9		-		Bro	wse			0K	Cancel		-
10		-				-	r				-

37. Echo - This AutoLink application inserts a string in the Message Log. Use the following syntax in the AutoLink field in a SampleList or RecalcList:

command-line: echo

other-parameters: <descriptive text to be "echoed" in the Message Log>

38. 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
- 39. Live display of all valve activities on System Control screen.

Instrument	45X-GC.44
Status: Ready	Status: Ready
	Run Time : 0.00 min.
Task Pane	456-GC.44 - Ready
	GC Operation
MS Setup	RunTime: 0.00 min Start
	EndTime: 13.00 min Reset
Valves:	-1+2+3-4-5-6-7-8
Met	9 through 16 Not Installed



40. **Stream Selector Valve Controller** – from Lotus Consulting. Control of sampling position for loading gas samples is set through SampleList. Access is with Task Bar icon:



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

Instrument	-43	8K-GC.44	Nethod	C:Grd	kerinSh	methods/ECT	test[Det 250.4	CH4R	10 mu 10 EC	D Test Sam	sie.	Re-Arthon
attus: Ready	Sta	tus: Ready	new Ma	lana a							<u> </u>	the resolution
-	8.4	Time: 0.00	Automation File Min.	- Copra	kerias)	cate curve	Anian-change	reab 16	\$15.549			stiple name:
		0.00	Data File:	1.							fr	ijection #: 0
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AND DAMAGE	or obse	ikn	emp.comes	38.4	cona	FION DEED	CIDE EFEC STRUE		10 u	600	002	A
Po anap	Runtime	0.00 min Start	Col Gven	30.0	80.0	Type 14			1	200×	T -9	60
	EndTime	12.00 min Recet	First S/SL:	2210	220.0	Citabled: Ye	is fleady. Tes	raut N	° /0	0/200	515X9	000
	😣 Ready	Method	OZera 2	1175	M/A	Ch 1 Binks	el Set Of As	0.00		1001		000
Method Editor	🗧 No Fax	a GLP	@Zore 4	N/A	N/A	Ch 2 Relea	ence Set 11.3.	Actual	11.3 100	5	1	20
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									10	- 1	n -	57
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		NUMBER OF STREET, STREE								10		
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Acquisition	Hide Keype	d View Setup GC D	t. BenmePar	Ven Fic	cnt Crily	• Facez	Delector EFC S	kalus	•			
Acquisition	Hick Keype	d Vew Selua GC D ፦ (히디) (조슈)(태	N. Beam-Par	Ven Fic	ant Ordy	• Front	Delector EFC S	kalus	•			/
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Data Process	Hick Keyper	d View Setus GC D ⊷ 🗗 🖾 🛧 III SampleList (40X-GC): Ar	nt BeranoPic 	Ven Fic	ant Orily	Fice	Delector EFC S	latus	•			
Data Process Report	Hick Coppe	d Vew Setus GC D ••• 🐨 🖾 🖾 🔺 111 SampleList (4XX-GC): Ar Sample Name	AL. <u>BenamePic</u>	Ven Fic SMP Cal. Ievel	ent Orij	Fictor	Delector EFC S AutoLink	tatus Vial	* Injection Volume	Injector: Used		
Data Process Report	Hick Keyps	c View Setus SC D SempleList (4XX-SCI: An Sample Name	AL. Benerie Pix	Vex Fic SMP Cal. Ievel	ont Only	Fictor Injection Notes	AutoLink Det 100 AcCH	Vial	* Injection Volume	Injectors		
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Acquisition Data Process Report System Log	Hick Kepsel 1 1 8400 1 2 3 4 5 5 7 8	d Vew Setup GC D ee C C C A A III Sample List (ACC GC AC Sample Name - Test Sample 100 - Test Sample 100 Test Sample 200 Test Sample 200	Kt. Beramb Pix CH4 Det Temp Texts Sample Type Actuate Method Ansjvis Actuate Method Ansjvis Actuate Method Ansjvis Actuate Method Ansjvis	Vex Fic	Inj. 3 3 3	rore rore	AutoLink Det 100 AcCh 100 ACCH	Vial 0 0	 Injection Volume 10 10 10 10 	Injectors Used Pos 1 • Pos 1 • Pos 1 •		Add Inset Delete Fil Down Add Lines Details
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Method Editor	EndTime: 12.00 min Ready NoFault	Reset Method GLP	Front ECD: Zone 3: Zone 4:		250.0 250.1 N/A N/4 N/A N/4	Ch 1 (Mai Ch 2 (Rei	ce up) Se erence) S	et 0.0, Actual Set 11.3, Act	L 0.0 Nual))	0000
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Acquisition Data Process Report	Valves 1-2-3-4 Hide Keypad Views U S Control Views U S Control Views I Sample Name Text Sample	5 6 7 8 Not installed ietup. GC Ctr Ctr Sample Ts Analysis	t. Flexure PPC Cal. level	Flor	View Front Da Injection Notes none	Ny 💌 From AutoLink none	Vial 0	for EFC Statu Injection Volume 1.0	Injectors Used	Amount Std (IS, NZ only)	Unid Peak Factor 0	Multip
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42. Direct access to Inject Single Sample by clicking on vial position in 8400 display.

43. Run Counter - available from Lotus Consulting. It is designed to complement MS Workstation, adding the ability to track the maintenance lifetime of one or more co Run Counters increments a cycle co designated components each sam providing a message log entry and on-se when the configured lifetime has

> Feb 03 Feb 03

been reached. Additionally. counter details can be reviewed including percentage of useful lifetime and predicted end-of-life

mponents.	Si Acknowledge 3 c	ounters in alert status
ounter for	Injector	Counter reads 20, threshold 10, 200.0 % of usefule life Maintenance cycle began 1/8/19 12:49 AM Last incremented 1/8/19 12:50 AM Reached end of life 1/8/19 12:50 AM
creen alert	Cold Trap	Counter reads 20, threshold 15, 133.3 % of usefule life Maintenance cycle began 1/8/1912:49 AM Last incremented 1/8/1912:50 AM Reached end of life 1/8/1912:50 AM
	Valve One	Counter reads 20, threshold 20, 100.0 % of usefule life
):02:49 Scion MS Workstation J:17:20 Data File 2019-02-03 1 J:17:23 Ran AutoLink Commar	DDE Interface termi 0-02-19 467833 soa nd: "c:\program files!	inated DDE conversation sk inj 1 - hip46 12-23-2018.run created for '467833 Soak', Inje ylotus consulting incjkittyhawk hip cycle gas analysis(mswsdde.
10:17:25 No counter to 10:17:25 Septum run c	kens recovered, ounter reached	, incrementing 1 counter end of useful life 1-31-19 02:11 AM, counter reads 3
0:17:25 Recalc list and Datafil	e information succes	ssfully processed
0:17:25 Scion MS Workstation	DDE Interface termi	inated DDE conversation
0:32:51 DDE conversation est	ablished with HIP Cy	ycle Gas Analysis
J:32:51 Activating Method C:\E	IrukerWS\methods\h	iip40 12-23-2018.mth
C32:53 Automation Besumed		



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





46. Edit out obviously invalid data points in calibration plot by right clicking on specific points. Excluded points are indicated in red.

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

🔳 X <> Y	×
Enter Amoun	it or Peak Size
Amount (X)	Peak Size (Y)
2.00000	22454.3
Calculate	Cancel

				1	1.
Print	Print <u>A</u> ll	Export	<u>O</u> verlay	Point Info	<u>C</u> oefficients
External Curve T	pdfid mast Standard / ype: Linear Force	er lod.mth: 45X- malysis	GC.44.Midd	le: Column Me Resp. Fact. F Coeff. Det.(r ²)	ethane RSD: 8.565%): 0.993187
Poin	t Info				>
-Select F	Point				
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Evel	ida Salactar	Point from Calcu	lation		OK
		KI KOO I IT OOM	~ ~ ~ ~ ~ ~ ~ ~ ~ ~		
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-File: c: Amoi	\ 2.0% qc1 unt: 0.1017	pdfid03 inj5 201 Peak Siz	6-11-16 14-4; e: 1387	2-45 - Deviation: 2	21.44%
-File: c: Amoi	\ 2.0% qc1 unt: 0.1017	pdfid03 inj5 201 Peak Siz	6-11-16 14-4) e: 1387	2-45 - Deviation: 2	21.44%
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-File: c: Amou I z 100 e	V 2.0% qc1 unt: 0.1017	pdfid03 inj5 201 Peak Siz	6-11-16 14-4; e: 1387	2-45 - Deviation: 2	21.44%
File: c: Amou I z 100 e	000-	pdfid03 inj5 201 Peak Siz	6-11-16 14-4; e: 1387	2-45 - Deviation: 2	21.44%
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File: c: Amou I Z 100 e	 2.0% qc1 unt: 0.1017 000- 	pdfid03 inj5 201 Peak Siz	6-11-16 14-4: e: 1387	2-45 - Deviation: 2	21.44% 4 ¹ 5 <u>Exact View</u>
Peak Nam	 2.0% qc1 unt: 0.1017 000- a <l< td=""><td>pdfid03 inj5 201 Peak Siz</td><td>6-11-16 14-4; e: 1387 </td><td>2-45 - Deviation: 2</td><td>21.44% 4 ¹5 <u>Exact View</u> <u>S</u>ave</td></l<>	pdfid03 inj5 201 Peak Siz	6-11-16 14-4; e: 1387 	2-45 - Deviation: 2	21.44% 4 ¹ 5 <u>Exact View</u> <u>S</u> ave
Pile: c: Amou z 100 e Peak Nam Origin	2.0% qc1 unt: 0.1017 000- 01 e: 1. Colu ude	pdfid03 inj5 201 Peak Siz	6-11-16 14-4: e: 1387	2-45 - Deviation: 2	21.44% 4 ¹ 5 <u>Exact View</u> <u>Save</u> Revent

49. 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.

MSWS II : System Control - Canby - S File Inject Automation Instrument

50. Approaches to opening method:

•

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





View/Edit Method Edit Compound Sets Print Method Share with Skype Move to OneDrive 7-Zip CRC SHA 😯 Scan with Windows Defender... A Share Open with... Restore previous versions > Send to Cut Сору Create shortcut Delete Rename Properties

- Method Builder icon on Task Bar. Method Builder • File View Help Ctrl+N XD @? New Ctrl+O Open od File Prompt for Action at Startup Look in: SIM M • • • • Print Setup... Date modified 7/28/2019 1:38 PM 7/28/2019 1:37 PM Recent File 17 Exit ation Method Libratien 19 11:15 AM 07-23-2019 1/27/2019 7:18 AM MS Workstat /27/2019 11:59 AM MS Workstat ff 07-23-2 7/2019 12:48 PM ACS Active Compounds Set Editor 1000 Log Viewer < 100 ed Applications Help 🥳 Method Builder + Qpien Cancel He name Files of by • bods C att P Autolink Help Automation File Editor
- 51. **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.



Untitled	l.smp - Generic Samp	leList	_		ſ	
	Sample Name	Sample Type	Ĩ	AutoLink	Ca 🔺	Add
1		Activate Method	-	PDFID Master.mth		<u> </u>
2		-	-			Insert
3			•			Delete
4		-	•			Fill Down
5			•			1 11 0 01111
6			-			Add Lines
7			-			Defaults
•			•			
8						LOOD OT

52. Activate method through SampleList.

53. Activate "Last Edited" method.





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

55. Sep Codes - indicated in reports.

C	hann	el Middle	= FID - Result	s							-		×	
<u>F</u> ile	<u>S</u> earc	:h Fo <u>n</u> t	Options <u>M</u>	<u>/</u> indows	<u>H</u> elp									
1	⊛ ∘	8 🛯		A 202	0-12-25	00) 🖺	2020-12-25	06)	Chan	nel: Mide	dle = FID]
Title														
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Metho	d Fi	le : c:	\scionws\20	20-12-2	5 06-	50-47 m	utgr inj	1 -	gel5 m	naster	12-12-	2020 -	87c	
Sample	e ID	: MT	GR						-					
Injec	tion	Date: 3	2020-12-25	06:50	Cal	culatio	n Date:	2021	-01-02	09:50	0			
Operat	tor				Det	ector T	wher 4XX	-90	(1000	Volts				
Works	tati	on: Win	dows		Bus	Addres	s : 44							
Instr	amen	t : GC1	5		San	ple Rat	e : 20.	00 H	z					
Chann	el 👘	: Mid	dle = FID		Run	Time	: 86.	003	min					
** Sc:	ion 1	4S Work	station - (V8.2.1D	ash 0	3/14/19) Versio	n 8.	2.1 **	02333	L-7701-	bb0-40	4d *	
Run M	oae 		: Analysis . Deck Dece											
Coloni	loti	arement	. Peak Alea											
Carcu.	Lacr	on rype	. reicent											
				Re	τ.	Time				Width				
Peak		Peak	Result	Ti	me	Offset	Are	a	Sep.	1/2	Statu	IS		
No.		Name	(ppbC)	(11	uin)	(min)	(coun	its)	Code	(sec)	Codes			
												-		
1	190	Ethene		3 18	.697	0.002	64	204	BV	9.7				
2	200	Ethane		6 18	.912	0.018	141	.643	VB	7.9				
3	300	C3		11 21	.676	0.001	269	834	BB	5.5				
4	425	c2C4=		3 27	.442	0.008	81	.389	BV	3.5				
	445	1204==		2 27	. /56	0.004	45	019	100	3.3				
	412	22rlU3		3 28	.142	-0.002	86	039	VB	3.5				Y
<													>	
														_

SepCodes	Peak Onset	Peak End
BB	Baseline	Baseline
BV	Baseline	Valley
VV	Valley	Valley
VB	Valley	Baseline
TF	Tangen	t Fused
TS	Tangei	nt Skim
PB	Perpendicular Drop	Baseline
BP	Baseline	Perpendicular Drop
PB	Perpendicular Drop	Baseline
VP	Valley	Perpendicular Drop
PV	Perpendicular Drop	Valley
GR	Grouped Pe	aks by Time
HF	Horizontal Bas	seline Forward
HB	Horizontal Base	eline Backwards

56. **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".





53 6 Antocampler Type: Autocampler Type: Data file Patic: 5 Data file Name: 6	B Ceneric C'ScienWS data Wes create and update a new	ж		57. Export SampleList to Excel
7 RecalcList Generation: 8 RecalcList Name:	RecalcList c scionws unitled.rcl			
10 Overwrite the RecalcLast each time the Sam	sleList Begi No	AutoLink Command 2 Other Other	Methor	
12	storaget - Const.	Parameters 1 Parame	eters 2	
13 1 14 2	Calibration 425362			
ta € Ge (1	1			
Select Excel File to Im	port List\Test.xlsx		×	
Select Excel File to Im	port eList\Test.xlsx ne SampleList. eList\Test.smp	Browse	×	58. Import SampleList from Excel.
Select Excel File to Im C:\ScionWS\Sample Select path to save ti C:\ScionWS\Sample	port eList\Test.xlsx he SampleList. eList\Test.smp	Browse Browse		58. Import SampleList from Excel.

60. Copy/paste lines in SampleList with "Shift - c" and then "Shift - v".

<u>S</u>ave

Analysis

Cancel

61. Copy/paste lines in RecalcList with "Shift - c" and then "Shift - v".

none

1

none

0

-Export

none

Import

Automation File Editor - [Untitled.smp] _ X File Edit Help 26866 🔝 Untitled.smp - Generic SampleList Dilution Sample Weight Cal. level Inj. Injectior * Notes Sample Name Sample Type Factor Add 1 425362 nalysis 2 Dilution Sample 3 4 5 Factor Weight Fill D<u>o</u>wn 6 Add <u>L</u>ines. 1 1

62. Move columns in SampleList

by right-clicking in header.



63. **Relabel column header** in SampleList.

64. **Security** – Passwords, Application Lock and File Revision Settings. Details displayed with "Help".

-	Reporting import export o
1	Security
1	Standard MS Report

Scion MS Workstation - (V8.2.1Dash 03/14/19) Security	Scion
Passwords Application Locking File Revision Settings	Pass
Password for this application	
You may set, change or remove the password required to enter this application.	
Change Password	
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	
Remove Method Passwords	
You may remove passwords required to save changes to Methods. Click on the button below to select the Method.	
Select Method	
Done Help	



	Look in	methods	-	← 🗈 🚰 💷▼	
	4	Name		Date modified	Туре
	Quick access	Method Archive		2020-07-27 09:42	File folder
	QUICK DUCCSS	2020-07-28 09-20-35 46c0056 vent in	ij 1 - hip	2020-07-28 09:43	MS Worksta
		2020-08-04 17-28-29 test inj 1 - calib	ration 0	2020-08-04 17:48	MS Workstat
	Desktop	2020-08-05 08-11-04 test inj 1 - calib	ration 0	2020-08-05 08:53	MS Workstat
		th		2020-08-06 14:14	MS Workstat
cholonivo methodo Calibr	ation 07-27-2020.mth I-05-08-11-04 text ini 1 - cal	bration 07, 77, 3020, middle mith		2020-07-29 13:30	MS Worksta
c) sciences methods (2020-0	5-04 17-28-29 test ini 1 - cal	bration 07-77-2020-middle.mth		2020-07-20 12:21	MS Worksta
C:\ScionWS\methods\HIP46	D 07-27-2020.mth			2020-07-29 10:01	IVID WORKSLO
C:\ScionWSImethods\HiP46	C 07-27-2020mth				
c1scionws\methods\2020-0	7-28 09-20-35 46c0056 vent	inj 1 - hip46c 07-27-2020middle.mth			
Cr\ScionWSImethods\Calibr	ationumth				
Cr\ScionWS\methods\HiP46	07-12-2020.mth				
C:\ScionWS\methods\Randy	col 60 Flow 4. temp prog.m	th.	Dee	ant Cilas	
C:\ScionWS\methods\HiP46	C 12-05-2019.mth		nec	ent riles y	
CillScionWSlmethods\Randy	r col 60 flow 4.mth		A		
	col 60 flow 4 fil 220.mth				· ·
CliscionWStamethods\Randy				-	Onen
:\ScionWS\anethods\Randy :\ScionWS\methods\Edwar	d.mth				
:\ScionWSumethods\Randy :\ScionWSumethods\Edwar :\ScionWSumethods\Randy	dimth i mth				open

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

66. Enable Automated Printing – must be checked for proper printing after each run.

File Inject Au	tomation	Instrument Windows Help						
-Instrument	Automa	ition File Editor	1					
Status: N	Begin S	ampleList						
	Begin S	equence						
	Begin A	t Selected SampleList Line						
Task Pane	Begin A	t Selected Sequence Line						
	Suspend Automation							
MS :	Resume Automation							
	Stop Automation							
	Reset Modules							
Metho	Enable /	Automated MS Data Processing						
	Enable /	Automated Printing						

67. Specify/Create data file folder from SampleList.

					D	ata File Generation		×
Generic S	ampleList: Lotus (09-22-2020.SMP				Specify the names for Data Files ge Numbers will be appended to file na extension in the Data File name.	neratec mes if t	I by detector modules using this Sample∟ist. he file already exists. Do not include the file
	-		1 1		2 2	Directory for Data Files		Data File names
	Sample Name	Sample Type	Cal. level	Inj. 📥 📊		🗁 c:\	~	%d %t %s Inj %i - %h
1 *		Autolink 👻				🕞 🗁 brukerws		· · ·
2 *		Autolink 👻		Insent		🕞 🤂 data		Example:
3 ×		Activate Method 👻		Delete		2020		
4 *	Test	Analysis 👻		1 Fill Down		🕞 12 december		ZUZI-UI-UZ US-SS-41 Sample 1 Inj 1 - TestMethod
5	-	Autolink •	- 12 I	AddLines		2021		1 CSUMCUIOU
7	199951 Prohest	Activate Metriou		1		👝 01 january		
8	105551116164	Autolink •		Defaults			· .	
9		Activate Method 👻	1	Import				Use the following symbols to enter the
10	4011395 Vent	Analysis 🗸		1 Export				corresponding variable data to the file
11		Autolink 🚽	1					name.
12		Activate Method 🛛 👻					v 1	%s = Sample ID
13	468522 Vent	Analysis 🔹		1		1		%i = Injection number
14		Autolink	<u>.</u>			New Felder		%d = Date
15	Disabled	Activate Method	: N	ata Files i		New Folder		%m = Detector Module name %t = Injection Time
10	Disabled	Autolink		<u>ucu (NCO.</u>				%h = Method Name
18		Activate Method				Drives		%o = Operator Name
19	4680852 Soak	Analysis 🗸		1				%n = Instrument Name
20				•			-	
1			•	•			_	
Begin	Suspend Bes	ume	Dat	a Files Becalcl ist		OK		Cancel
209n.	1103	<u>1997.0</u>						

68. Status/Error Codes

```
Compounds
       S - Internal Standard Peak
       R - Reference Peak
       T - Relative Retention Peak
       NA - Not Active
   Data Files
       IMF - Number of Identified, Missing, and Failed compounds
       TUD - Number of Tentatively Identified, Unknown, and Duplicate
             unknown peaks
   Result Codes
    R : Reference Peak.
    # : Factors not updated.
    * : Negative result. Check calibration curve.
    + : More than one result in range. Check calibration curve.
    V : Peak fails Verification.
    M : Missing Peak.
    C : Result out of Tolerance or Calibration Range.
    S : Internal Standard Peak.
    U : User-defined EndPoints.
    0 : Saturated Peak Amplitude.
    T : Relative Retention Time Peak.
    D : Can't quantitate. Reporting Peak Size.
    I : Can't create chromatogram. Check scan functions, time range.
    L : Missing Library or Search failed.
    N : No internal stds found to quantitate Unknowns.
    Q : Result < Compound Report Threshold.
    H : Cali levels too low. Reporting Peak Size.
    W : Spectrum Match < Threshold. Check Identification params.
    Y : Peak not detected or not in Search Window. Check RT, Int parms
    Z : Ion Ratio failed. Check Qualifier parameters.
    F : Missing some scan functions. Quantitating available scan funcs.
    a : S/N less than threshold.
    b : RRT out of tolerance.
    e : Peak size < curve minimum. Check calibration curve.
    f : Peak size > curve maximum. Check calibration curve.
    g : No Calibration Data. Reporting Peak Size.
    h : No Reference Peaks. Reporting Peak Size.
    j : Internal Std Missing or Not Active. Reporting Peak Size.
    1 : Too many similar spectra. Search may be incomplete.
    m : Too few points to quantitate. Check time range.
    p : Peak < Size Threshold. Check Integration params.</p>
    q : Manual integration of qualifiers.
_____
Separation Codes
    BV : Baseline to Valley
    BB : Baseline to baseline
    MB : Mended end to baseline
    VB : Valley to baseline
    VV : Valley to valley
    MM : Mended end to mended end
    MV : Mended end to valley
    TS : Separated tangent peaks
    TF : Fused tangent peaks
    GR : Group peak, post run calculation function
    BM : Baseline to mended end
    VM : Valley to mended end
    HF : Horizontal forward
    HB : Horizontal backward
    HM : Horizontal minimum
```

69. SampleList AutoLink commands:

• **WAIT** - This AutoLink application pauses for a specified time before terminating; it can be used to perform injections on a specific timetable, for example, start up the GC early in the morning and run the daily check sample automatically.

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.

	· fuers	ed berg - Generic Sperg	léLeit						a a a
		Sample Name	Sample Type	Col. Inj Injection Aread Inj Nature		Injection Noter	AutoLink	Amour (IS, N2	400
	1	2	tara et 🔹				30: FIPW		ined
	2	Detact Scale	Sumith T		-	1016	GED 1	-	Canto
	4] .	-		1			Fillipe
	5		ż			_	-		Addi_mes.
AutoLink Parameters									
Command		0	ther parar	mel	ers				
WAIT :00		[
Browse		.,				0	K	Car	ncel
L									

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:



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

X B B X

🖺 Eile Edit View Window Help

866 / 68

Auxiliary Heaters
 Channel Front=Fron
 Data Handling
 Minegration P

-Peak Table

Deviation Tolerance (%) 10 +

Out-of-Tolerance Action C No Action C Increment Error Cour

Command: GOTO <line-number>

Other-parameters: Inject or Recalc or Print

- WAIT and GOTO can be used to create an infinite loop to perform an injection every preset time interval to monitor a process stream.
- 70. **"Verification" run type** reported results compared to values in a calibration level.

rint Date: 14 Feb 2009 1	19:41:25		Target Compound Report 1	for #11 from45 pm toxics 6 min	nutes.sms - Page 11	1						💽 Untitle	d.smp - Generic Samp	leList			- • •
imple ID: strument ID: easurement Type: xquisition Date: alculation Date: imple Type: . Sample Notes:	0.1 ppbv r Varian lor Area 2008-05-0 2009-02-1 Venficatio None	td Trap 7 20.02 4 19:31 n	Operator: Last Calibration: Calibration Type: Data File: Method:	RSB 2009-02-14 19:31 Internal Standard toxics 6 minutes.sms urve_cal_10_2_08 mt	h	Peak No.	Peak Name	Expected Result ()	Calculated Result ()	Dev.	Ret. Time (min)	1 2 3 4	Sample Name Calbration	Sample Type	Cal. Inj. 1	Injecti * Note	Add Igsett Dokte
npound Information Peak Name: Result Index: ntification	Trichlo 11	roflucromethane Compound Number: 9	CAS Number	None Ide	ntified	1 H 2 O 3 N	ydrogen xygen	125.8000 25.1500 49.9400	126.0991 27.3469 49.9810	0.2 8.7 0.1	5.980 6.457 7.230	5 6 7 8					Add Lines
Parameter Search Type Retention Time Match Result		Specification Spectrum 20.044 +/- 0.100 N-R >= 800	<u>Actual</u> 20.051 min. 874	<u>Sta</u> Pas	ss ss	4 H	ethane	24.8600	24.8167	0.2	8.182	9		-	1	•	Export
egration and Quantita Parameter Quan Ions IS Peak Name	ation	Specification 101.0 Bromochloromethane	Actual	Sta	itus	T	otals:		228.2437	S					_	Data Files	RecalcList
Calibration Equation Area Height Amount Verification Deviation	n	Linear, Force, 1/nX2 >=100 >= 0.005 ppbv +/- 30.00%	y = +5.0748x 172238 32375 0.099 ppbv 8.51%	Pas Pas	85 85 85	Verifi	unt ication De	eviation		>= +/	- 30.009	opov 6			8	099 p 51%	vaqo

71. Access data file actions from Windows Explorer, with a right-click on .RUN/.XMS files.

File Home Share	View View Cost Paste sourcet Sheek C Inv +	Detter filmans Detter filmans Detter filmans Detter filmans Detter filmans Detter filmans Detter filmans Hore Ho	A Open	en - Historian Stear and Stear and Stear States D - Composition	0	
4	Nars	Cate medited		Noe Size Date created	~	
* Quick access	A 2020-12-17 12-18-56 nov	st Cht View/idt Otromatourum		M5 Warkstation D., 107 K8 2029-12-17 12/13		
Desktop #	A 2020-12-17 12-04-31 r					-
🕹 Dizwnicazk 🕜	A 2008-12-17 11-53-47 (📥 2020-12-17 12-18-58 noise che		View/Edit Chromatogram		
Documents #	A 2000 12 17 11 45 07 /	A 2020-12-17 12-04-31 poirs che		view/Eure enronatogram		
and Packards of the	A 2020-12-13 15-45-10 r	Lozo Iz-II Iz-04-31 hoise che		AIA Import/Export		
Exclana Indian	A 2020-12-13 15-34-18 -	A 2020-12-17 11-53-47 noise che		Convert Raw Data and Results to AIA Fo	ormat	
- receip taking	A 2020 12 18 15 21 19 s	A 2020-12-17 11-43-07 noise che				
Seconded.ett	A 2025-12-13 14-47-22 F	A 2020 12 17 11 22 22 pairs she		Convert Raw Data and Results to ASCII		
	A 2005-12-12 16-40-56 e	2020-12-17 11-52-25 Holse che		Print Standard Report		
- Obelinve	A 2020 12 12 16 12 04 v	A 2020-12-13 15-46-18 noise bot		Den deren Gestern Gesterbilite Den ert		
This PC	A 2020-12-12 12-39-55 P	A 2020-12-13 15-34-18 short sign		Produce system suitability Report		
35 Objects	A 2020-12-12 12-27-44 e	A 2020 12 12 12 11 10 1 11		View Chromatogram in MS Data Review	N	
Desktop	A 2020-12-11 15-12-04	2020-12-15 13-21-19 short igni		View Results Only		
Documents	A 2020-12-11 13-45-56 r	📥 2020-12-13 14-47-22 mtgr inj 1		new needed only		
- Denadicana	A 2020-12-11 12-17-51 r	A 2020-12-13 14-39-00 mtor ini 1		View Standard Report		
Distance	A 2020-12-10 17-31-50 a		B	Share with Skype		
I Videor	A 2020-12-10 16-03-48 r	2020-12-12 10-40-56 noise che	-			
L Windows (C3	A 2020-12-10 12-48-48 r	A 2020-12-12 16-12-04 noise test		Scan with Microsoft Defender		
	A 2020-12-09 13-06-54 #	A 2020-12-12 12-35-55 poirs che	B	Share		
- Harvert	A 2020-12-09 10-58-05 r			Once with		
and the second second	A 2020-12-09 10 43-21 F	2020-12-12 12-27-44 noise che		openmin		
H Litems (litem selecter	3 5V0 N8	📥 2020-12-11 16-11-56 mtgr inj 1		Restore previous versions		
		A 2020-12-11 15-13-04 mtor ini 2	-	2 112		
		Loco le l'indirigini e		Send to		
		A 2020-12-11 13-45-36 mtgr inj 1		c .		
		📥 2020-12-11 12-17-51 mtgrinj 1		Cut		
		A 2020-12-10 17-21-50 mtor ini 1		Сору		
		- 2020-12-10 17-51-50 migring 1				
		A 2020-12-10 16-03-48 mtgr inj 1		Create shortcut		
		📥 2020-12-10 14-41-02 mtgr inj 1		Delete		
		A 2020-12-10 12-49-49 mtor ini 1				
		- 2020-12-10 13-40-40 mitgring I		Kename		
		A 2020-12-09 13-06-54 mtgr inj 1		Properties.		





74. **Cannot overwrite data files.** - If new data name matches an existing file in the same folder, then three digits are

automatically appended to the end the name and incremented thereafter



Suggestions for Operations with .XMS data files

- 75. **Peak processing for chromatograms for .XMS files** is discussed in Peak Detection with Varian MS Workstation: http//lotusinstruments.com/wp/wp-content/uploads/ Peak-Detection-with-Varian-MS-Workstation.pdf
- 76. Suspend and Resume buttons in Active SampleList During automated operations, the SampleList can be suspended that will stop activities the end of the current sample. This allows additional entries to the list, or adjustments to the active method. Then Resume will continue with the next sample line.



77. Single method for full simultaneous control of both MS and up to three GC detectors.





78. Active Compounds

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

79. Hot Keys in MS Data Review

```
Data Files Pane
   Mouse Click
                - Replace data file
   <Ctrl> + Click - Add data file
   F5 - Update All Drives and Directories
 _____
                _____
Plot Descriptors Pane
   Mouse Click - Replace descriptor
<Ctrl> + Click - Add descriptor
   <Shift> + Click - Add range of descriptors
   <Alt> + Click - Add descriptor to active chromatogram
                          _____
Chromatogram Plot Control
   Single-Click Actions
       s - Display Spectrum
       <ctrl> + s - Display Spectrum in Empty Plot Area if Available
      1 - Library Search Selected Spectrum
       j - Target List Search Selected Spectrum
       e - Export Selected Spectrum to Active Spectrum List
   Single-Click Point/Spectrum Selection Override
       a - Nearest Apex
       t - Nearest Point
   Click-And-Drag Actions
       z - Zoom Chromatogram
       w - Average Selected Spectra
      n - Calculate Noise
       r - Calculate Time Range
      m - Move Chromatogram
      i - Integrate Area
       b - Export to Clipboard
   Double-Click Override
       u - Only Auto Scale Vertical Scales
   Keyboard Actions
      left arrow - Previous Spectrum
down arrow - Previous Spectrum
      right arrow - Next Spectrum
                 - Next Spectrum
      up arrow
                      _____
Spectra Plot Control
   Single-Click-Actions
      1 - Library Search Selected Spectrum
       j - Target List Search Selected Spectrum
       e - Export Selected Spectrum to Active Spectrum List
       p - Create New Chromatogram Plot using Mass
       r - Enable Mass Ruler
   Click-And-Drag Actions
       z - Zoom Spectrum
       p - Create New Chromatogram Plot using Mass Range
       b - Export to Clipboard
       r - Enable Mass Ruler
   Mass Ruler Mass Selection Override
      a - Highest m/z
      t - Nearest m/z
                  Window Arrangement
    c - Cascade
    h - Tile Horizontally
    v - Tile Vertically
                   Miscellaneous
   Fl - Help
```

80. **QML Commands** (Quadrupole Macro Language) – reserved for Scion Service operations. This is not intended for user operations.





d Reports

>

83. Format in View Results - report format can be altered with options available through menu from MS Data Review > View > View Results > Preferences > Results List Columns. See following list for choices.

All



Columns to Display

Description

Acquisition Data	
Acquisition Date	The time and date when data tile was created.
Amount	The calculated result. Amounts are calculated from the calibration curve for all miles, including Calibration and verification tiles. Areas of neights are reported if the error conditions that prevent calculation of the result calculated result is not available. N/A is reported for some error conditions that prevent calculation of
, inount	the result
Amount Reject	Compounds with calculated results less than this are reported as Missing. Applies only to Analytes in Analysis files.
Amount Units	Verification files. Areas or heights are reported if the calculated result is not available. N/A is reported for some error conditions that prevent calculation of the
Amount/RE	The calculated result. Target Compounds report the RF or RRF for Calibration files. Areas or heights are reported if the calculated result is not available. N/A
Amountaria	is reported for some error conditions that prevent calculation of the result.
Amount/RF Units	Units for the Amount/RF results. They are specified in the method for compounds. Unknown peaks that are quantitated with an Internal Standard report the units of
Area	the internal standard, when integrated areas or neights are reported to rule results, the units are reported as Counts.
Alca	The integrated and of the peak. Needs yielder unan 393393 are reported in solenitin invation.
Baseline Code	definitions)
Calculation Date	The time and date when the data file was last quantitated
Cali Curve Calculations	The Curve Fit Type Origin Point and Repression Weighting used to calculate a calibration curve
Calibration Amount	The compound calibration I way among the section mediating accurate the data and the calibration can be
Calibration Date	The time and date when a Calibration data file was last processed
Calibration Equation	The equation of the calibration curve.
CAS Number	A unique 3-part identification number assigned to a compound by the Chemical Abstracts Service.
Channele	The physical channels on which the scan functions to create the chromatogram were generated. Merged is reported if all available channels are combined.
Channels	Merged is always used to quantitate Unknown Peaks.
Coeff. Det.(r2)	A measure of how well the calibration points fit the calculated curve.
Conc./IS Ratio	The Target Compound Amount divided by the Internal Standard Amount that is specified in the method.
Data File	The name of the data file.
Delta RT (min)	The difference between the expected compound retention time specified in the method and the actual retention time of the result.
Dev%-Amount	The % Deviation of the Target Compound Amount in a Calibration file, relative to the Calibration Level Amount in the method.
Dev%-Curve	The % Deviation of the Target Compound Amount in a Calibration file, relative to the calibration curve.
Divisor	A divisor factor specified in the recalc list that is used to calculate Analysis and Verification results. The Divisor can be edited in the Automation Editor.
Error	Single-character result codes that report problems which occurred when the peak was processed. (Select the Results Codes Help menu item for definitions.)
Expected RT (min)	The expected compound retention time that is specified in the method.
F. Match	A measure of how well a sample spectrum is contained in a library or reference spectrum.
Group Name	All compounds assigned to a method-specified group are reported as a single summed result in addition to the individual compound results.
Height	The baseline-corrected height of an integrated peak. Heights greater than 999999 are reported in scientific notation.
In Lib Prob.	The probability that the reported match is in the searched library. This applies only to Normal - Forward searches of Unknown Peaks.
Ion Ratios	The ion ratio specifications and results for the qualifier ions that have been specified for a compound.
IS % Dev	The % Deviation of the Internal Standard peak size from the average of the Internal Standard sizes in all of the files.
IS Amount	The nominal amount of the Internal Standard used to quantitate an Analyte as specified in the method.
IS Area	The integrated area of the internal Standard peak used to quantitate an Analyte.
IS Factor	A factor used to adjust the Internal Standard Calibration Amount on a per-sample basis. Applies only to Analysis files. The IS Factor can be edited in the
IC Llaight	Automation Editor.
IS Reight	The baseline-corrected neight of the internal standard peak used to quantitate an Analyte.
IS Peak Name	The name of the Internal Standard used to quantitate an Analyte.
br #	The literation time of the internal standard peak used to quantitate an Analyte.
Library	The local of the library that contains the match reported from the library earch of an Unknown Feak.
Match Prob	The name of the money intercontants are matchine ported into the interact sector of an intervent reak.
	The Froward or Reverse Match result used in any search or an Unix own reak is concern, assuming una use one check match is in the database.
Match Result	searching.
Match Type	Specifies whether matches from a search are ranked by Forward or Reverse Match results.
Multiplier	A multiplier factor specified in the recalc list that is used to calculate Analysis and Verification results. The Multiplier can be edited in the Automation Editor
Peak Name	The name of a Target Compound that is specified in the method, or the name of the match that was reported from the library search of an Unknown Peak.
Peak Reject	Peaks whose area or height are less than the Peak Reject method specification will be rejected. The Peak integration events will be displayed in the chromatogram, but leave Peak integration are the second and Teach Compared on With a desired on Mission events will be displayed in the chromatogram,
	but Unknown Peak tesulis will not be reported, and i rarget compounds will be designated as Missing. The bask types of ther than Analyte that may be specified in the method for a Tarret Compound: SP: Internal Standard REE: Reference, RRT: Relative
Peak Type	Retention Time.
Peak Width Spec.	The 1/2 height peak width that is specified in the method.
Peak/IS %	The Target Compound peak size divided by the Internal Standard peak size, expressed as %.
Peak/IS Ratio	The Target Compound peak size divided by the Internal Standard peak size.
Peak Width	The width in seconds at 1/2 height of the integrated peak.
Quan lons	The ions that are specified in the method to create the chromatogram used for quantitation. RIC is specified when all available ions should be used. The ions are
D. Matal	extracted from the ions that are available in the scan functions that are specified for the chromatogram.
R. Match	A measure of how well a library or reference spectrum is contained in a sample spectrum.
Robuit #	nie me nanwer or me reported result. Compound Result Yunes are Identified Missing or Failed (Failed one or more Ion Ratio specifications). Hoknown Pask Result Tunes are TIC (Tantatively
Result Type	Identified Compound pupicate (maps to a reported Compound result), or Unknown.
Ret Time	The retention time of the integrated peak.
RF Used	The Response Factor specified in the method to quantitate Unknown Peaks: Nearest IS, Nearest Pure IS, or Absolute.
RF/RRF	The Response Factor (External Standard) or Relative Response Factor (Internal Standard) calculated for a Target Compound in a Calibration file.
RRT	The retention time of a compound in a data file relative to that of another compound in the data file that has been designated as the RRT Reference in the method.
RRT% Deviation	The Deviation of the RRT result from the RRT of the corresponding method Retention Times. The RRT Tolerance Range, Result, and Status are displayed
RT. Window	The time window in minutes around the expected compound retention time that will be searched for the Target Compound peak.
S/n Ratio	The Signal/Noise ratio of the integrated peak. The RMS or Peak-to-Peak Noise Type specified in the method is used.
S/N Reject	The Signal/Noise ratio of the integrated peak, relative to a specified threshold. The S/N Threshold, Result, and Status are displayed.
Sample Name	The name of the sample that was specified when the data file was created.
Sample Notes	The sample notes that were entered in the Sample List for the data file.
Sample Type	The type of the data file: Calibration, Analysis, or Verification. Baseline data files are not supported by MS quantitation, and are quantitated as Analysis files.
Scan Descriptor	A description of the scan functions from which to create the chromatogram. It is independent of the physical channels that the scan functions are on in a given data file scanard Margarian and the scanard functions are on in a given data file scanard that the scanard file scanar
Scan Number	me segment, mengeu is reported il ani available scan functions are compined, merged is always used to quantitate Unknown Peaks.
	The scan humber or are appex point or the integrated peak. The search type specified in the method to identify the internated peak. Tarriet Compounds: Spectrum Nearest Highest First or Last Unknown Deaks.
Search Type	Library Search, or None.
Slone Sensitivity	A Peak Start is detected when the chromatogram slope exceeds this threshold. The number of points used to calculate the slope is determined by the data
clope constituty	rate and the specified Peak Width.
Status	
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86. Excel Report Templates.

85. Edit/Lock Calibration Coefficients – Some protocols required multiple standards to set up calibration factors. To accomplish this, one standard is initially run to set up its factors. Then those factors are locked, and the next standard is run so that the initial coefficients are maintained. In addition, if response factors are computed off-line, they can be entered manually as appropriate.



84. Calibration Reports.

- 87. Dash Reporting report authoring system that provides tools for designing and generating reports of analytical data from Scion MS Workstation, as well as other relational database sources. The system works by querying the MS Workstation database and applying a report method to the data to produce a report, or finished report, in a wide variety of output layouts. Scion Dash is both an interactive reporting system (using the Designer) as well as a non-interactive report generation system integrated within MS Workstation. Using the Designer, report methods can be designed and previewed interactively, and then stored and used by multiple users in non-interactive mode. Included in package are instruction videos/
- 88. Tune Reports are accessed through an icon on System Control for the Scion SQ Mass Spectrometer. Common tune molecule is Perfluorotributylamine (FC-43, Scion P/N 392035300). Many EPA GCMS protocols mandate performing specific tune routines to ensure that NIST library matches are confirmed, including EPA Method TO15, EPA Method 624.1) and EPA Method 625.1). Common target compounds are 4-Fluorobromobenzene (BFB, CAS # 460-00-4, 1 ppmV/V Scion P/N ULSTS110N) and Decafluorotriphenylphosphine (DFTPP, CAS # 5074-71-5, 2,500 µg/m in methylene chloride, Restek P/N 31001). Although the requirement is specifically listed in many standard procedures, NIST has adjusted their search algorithm to minimize the need to perfectly match the EPA criteria and still achieve appropriate matches.



89. **System Suitability** - is a custom report template used to compute and report system suitability indicators from Scion MS Workstation data files. The following types of reports may be generated:

1. Resolution between selected target compound peak pairs.

2. Degradation estimates for selected target compounds, where the degradation products are also quantitated as target compounds.

3. Tailing Peak and Gaussian Peak Factors for selected target compounds (TPF-GPF Report).

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4. Tune reports for BFB (bromofluorobenzene) or DFTPP (decafluorotriphenylphosphine) based on EPA method 524, 624, CLPVOL, 8240, or 8260 criteria for BFB or method 525,625, CLPSEM, 8250, or 8270 for DFTPP.



91. EnviroPro Reporting -• 23 Tune Criteria for 8270 Current Method provides detailed Tune Criteria Tune Criteria: 624 Relative Abundance Limits Comparison Tune File information on reporting m/z Acceptance Criteria Low1 High1 Low2 m/z1 m/z Method Title: 198 EPA Method 624 Matrix: WATER 30-60% of m/z 198 30 60 results for common 1.999 68 <2% of m/z 69 OT 69 Initial Calibration: 69 Present 0.001 100 USEPA methods - 524. 70 <2% of m/z 69 1.999 01 69 EPA Method 127 40-60% of m/z 198 Tune Criteria 40 60 198 Volatiles SemiVolatiles 525, 624.625, 8240, 0.999 197 <1% of m/z 198 0 0 198 C 524 C 525 Use CCC As Tune File 198 Base peak 199 5-9% of m/z 198 100 100 C 625 01 0 8250, 8260, 8270, 8270, 0 198 5 9 Tune Report Setup C 8240 € 8250 275 10-30% of m/z 198 10 30 0] 198 CLPVOL and CLPSV. C 8270 Matrix WATER 365 >1% of m/z 198 1.001 100 0 198 C 8260 C CLPVOL C CLPSV Tune Reports can be Help Save Set Initial Calibration generated. Help Close

NIST 08 MS and AMDIS 2.6 ^

A very quick guide to AMDIS

Connect NIST MS software

AMDIS Help

AMDIS_32

MS Interpreter

92 NIST Automated Mass Spectral **Deconvolution and Identification System** - AMDIS - allows an automation of a complex process of extracting data

from a GC/MS data file. AMDIS works by finding all of the ions that rise and fall at the concurrently and then associating them to a single component. Once has found this it component, it compares it





93. NIST 20 (Scion P/N 4121057) and NIST 20 Upgrade (Scion P/N 4121058) - 350,704 electron ionization (EI) spectra for 306,643 compounds, 43,774 replicate spectra (39,729 more compounds than NIST 17) and retention indexes for 139,963 compounds.



(E)

- 94. Wiley FFNSC Library Mass Spectra of Flavors and Fragrances of Natural and Synthetic Compounds, 3rd Edition, 2015 (Scion P/N 394105201) - 3,462 mass spectra, linear retention index (Kovats index) data, calculated Kovats RI, and searchable chemical structures of compounds of interest for the flavors and fragrances industry.
- 95. Pfleger, Maurer, Weber Mass Spectral Library of Drugs, Poisons, Pesticides, Pollutants, and their Metabolites, 2016 edition (Scion P/N 392052195) 10,430 spectra of potentially harmful substances, including 7,800 from metabolites. This reference is made up of an electronic database accompanied by two hardbound volumes.
- 96. **Rosner Mass Spectra Library of Designer Drug** 2019 (Scion P/N 392052102 is the largest collection of chemical signatures of new psychoactive substances (NPS) and drugs of abuse in the world. This impressive mass spectral library was developed to support forensics and toxicology labs to combat this global health epidemic.
- 97. Wiley 12th Edition Mass Spectral Library 2020 Wiley Registry Mass Spectral Library is the most comprehensive mass spectral library available, making it an essential tool for general unknown compound identification. Included in the combination package are over 1 million El mass spectra, over 1 million searchable chemical structures, and over 840,000 unique compounds.
- 98. **Multicompound Software** (Scion P/N 393036191) 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.
- 99. mzXMS Conversion Utility legacy operation; not applicable with .XMS files

100. ToxProPlus MS Reporting Software

(Scion P/N 393036291) - software includes three separate custom software packages: multi-compound software, ion ratio summary report software, and screening software to aid reporting.

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alpha -Benzylsuccinic acid	7.119	4735414	2.3	150	RFit	724	Duplicate
2,6-P iperazinedione, 4- (phenylmethyl)-	7.227	1958913	1.7	510	RFit	731	Duplicate
Amphetamine PFP	7.815	2256121	1.6	456	RFit	822	Duplicate
4(axial)-n-Butyl-2(equat methyl-trans-d)- 8.335	1564992	1.6	607	RFit	704	Duplicate
Methamphetamine ptp	8.407	6453251	1.8	150	RFit	865	Duplicate
Methamphetamine ptp	8.542	9648030	2.0	121	RFit	680	Duplicate
Methamphetamine pfp	9.208	12416020	1.9	117	RFit	714	Duplicate
No Match	10.463	248344	0.0	5208	RFit	N/A	Unknown
Sultoxide	10.977	9710617	2.0	145	RFit	721	TIC
3',4'-Dichloro-3- (nicotinoylhydrazono)bu	12.173	7793164	2.0	163	RFit	664	TIC

- 101. Summary Report is only functional with .XMS data files.
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102. Ref Spectrum - is used to identify the peak can be set either from a standard spectrum, or from user adjustments of ions and their intensities.

103. Selected Ions Monitoring (SIM) - Data from multiple ions can be collected to provide positive matching to a reference spectrum with use of multiple characteristic ions for compounds.



104. **Compound Graph** - illustrates scan times and effects of peak window overlap with Selected Ions Scanning (SIS) mode.





105. Expanded view of portion of Compound Graph - allows visual indications of overlapping scan windows. Display area is selected through mouse actions on edges of graph or click/drag inside the presentation. Regions of overlap degrades the quality of the data, especially related to noise levels. In the regions where these windows coincide, scan times are divided up and data points are not collected for the full time for the target compound ions.





106. **Multiple Quan lons** – To boost peak response, specially for low responders such as propene and chloromethane, muliple ions can be defined as scan functions to enhance peak detection, especially for SIM mode 107. SIM (Selected Ions Monitoring) Peak Confirmation - To confirm identification of a compound when only selected ions are set in SIM mode, qualifier ions can be set up with ion ratios to the base peak. A match is labeled as "ID" in the final report. Obviously NIST library searches do not apply.





108. **Convert** .**XMS** files to Content Definition File - .CDF - is a file format from ANSI (American National Standards Institute) allows a .XMS file to be opened in other chromatography systems. The files created in this format are saved with the .CDF file suffix in an XML-based data format.

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109. Convert files to AIA (Analytical Instruments Association)² -ASTM E1947 98(2014) _ Standard Specification for Analyt Data Interchange Protocol Chromatographic Data. This generates .CDF files that can exported/imported into other brands chromatography software compat with AIA format.

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² D.C. Nelson, Chemometrics and Intelligent Laboratory Systems, 26 (1994), p. 43. www.sciencedirect.com/science/ article/abs/pii/0169743994900175

110. **Export to NetCDF** (Network Common Data Form) is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data. It is also a community standard for sharing scientific data. The Unidata Program Center supports and maintains netCDF programming interfaces for C, C++, Java, and Fortran. Programming interfaces are also available for Python, IDL, MATLAB, R, Ruby, and Perl.

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To NetCDF		
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111. XMS data files for MS possess:

- Raw data points
- Last computed results
- Copy of last method used
- Link to original method
- Complete calibration data
 - Response Factors
 - Calibration Point Information
 - Calibration Amounts
 - Calibration Peak Sizes
 - Deviations from Curve
 - > Replicates
 - Link to Calibration .XMS data file
 - Calibration Levels (up to 50)
 - Coefficients
 - Curve Fit Factors

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Hints with Operations with GC Detector .RUN Data Files

112. **Peak processing for chromatograms for GC detector run files -** are discussed in Peak Detection with Varian Star Workstation. http://lotusinstruments.com/wp/wp-content/uploads/Peak-Detection-with-Varian-Star-Workstation.pdf

113. **Display of peak details in Interactive Graphics**. Highlight desired peak and carefully drop straight down to expose other peak information.





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





118. Change background colors of displayed live chromatograms.

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00	w M & R Horz w M & R Vert w F,M,R Horz w F,M,R Vert
0.0	w M & R Horz w M & R Vert w F.M.R Horz w FM R Vert
-0.3 -0.2 -0.2	w M & R Horz w M & R Vert w F,M,R Horz w F M R Vert

119. **Display of live chromatograms in System Control** - single, double or triple, and horizontal or vertical.

120. Change Run Time in Active Chromatogram

- Keyboard on Scion 436/456 is active during a run, and the column oven hold time in the final step can be adjusted longer or shorter time to impact both the GC run time and GC detector(s) data collection end time. This change does not alter the Scion SQ run time.



121. **Hide Keypad** – to set chromatogram display for full screen.





125. **Detector frequency** - This parameter impacts data collection with number of data points used to define the peak combined with monitored noise level.

🖺 Method Builder - [Method1*]	_	
Eile Edit View Window Help		- 8 ×
1	8	
Method1*	Data Acquisition	^
Method Notes	Data Acquisition	_
🗄 🔁 45X-GC - Address 44		
E 45X-GC Control	Detector Frequency: 25 - Hz	
	Noise Monitor Length: 64 📫 points (2.560 sec)	
🛅 Sample Delivery	The following settings will be ignored for all detectors	
🔁 Injector	other than the FID and NPD.	
🖺 Flow/Pressure	- FID /NPD Detector Full Scale	
🔁 Detector	Front: 1000 V	
Bi Output		
	Middle: 1000 V 💌	
🔁 Auxiliary EFCs		
	Rear: 10V	
🗄 🗄 Channel Front=FID		
🛱 🚟 Data Handling		
Integration Parameters		¥
Ready		NUM

126. Single method possesses:

- Full set of parameters for control of GC
- Full set of parameters for computation of results
- Complete calibration data
 - Raw data points
 - Last computed results
 - Copy of last method used
 - Link to original method
 - Complete calibration data
 - Response Factors
 - Calibration Point Information
 - Calibration Amounts
 - Calibration Peak Sizes
 - Deviations from Curve
 - > Replicates
 - Link to Calibration .XMS data file
 - Calibration Levels (up to 50)
 - Coefficients
 - Curve Fit Factors
- Formatting for chromatograms and reports
- Baseline subtract data points

127. RUN data file for GC detectors possesses:

- Raw data points
- Instrument run log
- Last computed results
- Copy of data handling sections from last method used
- Link to original method
- Baseline subtract data points
- Complete calibration data
 - Raw data points
 - Last computed results
 - Copy of last method used
 - Link to original method
 - Complete calibration data
 - Response Factors
 - Calibration Point Information
 - Calibration Amounts
 - Calibration Peak Sizes
 - Deviations from Curve
 - > Replicates
 - > Link to Calibration .XMS data file
 - Calibration Levels (up to 50)
 - Coefficients
 - Curve Fit Factors
- 128. **Display of data points** provides visualization of proper definition of peak shape. Data interval is set by detector frequency and expected peak width. Optimum settings should yeild 10 data points across top of peak.



129. **Open Original Method** - .RUN files possess a link to the original method used to collect the data.

s	ielect me	hod to o se	pen with th rukerws\me	e loaded data file Method Fil ethods\calibration	:(s): e n 07-27-2020.	.mth	Run File 2020-08-10 07-20-07 test inj 1 - test C
0	Onen en Orig	Recalc nal Met	Method	70			
	Open	Origina	l Method		Cut+W		
	New M	1ethod Methor	4		Ctrl+M		
	New C Add/F	hroma emove	togram Chromat	:ogram	Ctrl+N Ctrl+O	•	



131. **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.





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

133. Adjustment of retention time by Reference Peaks (peak windows in blue). Update only occurs when "calibration" is performed.





- 134. **Add peak table entry-** by rightclicking in window below the chromatogram.
- 135. **Add timed events** by rightclicking in window below the chromatogram.



136. Graphically relocate time events with mouse.

137. Reporting and Printing of Results:

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





• Chose printing parameters in method. Printouts on injection can be suppressed to prevent operations to be locked up if printer jams.

Method Builder - [ecdtest det 250 cp	-580 r10 mu 10.mth] — 🗆	×
Eile Edit View Window Help	- 6	×
ecttest det 250 cp - 580 r10 mu 10.mth Method Notes H 43X-6C - Address 44 H 43X-6C Control H 43X-6C Control H - Configuration	Calibration Type Calibration Cali	^
	Replicate Treatment	
-En Detector -En Output -En Data Acquisition -En Auxiliary EFCs	C Average Calibration Replicates Averaging Weight	
Auximity Heaters Auximity Heaters Di Channel Front Di Channel Front Data Handling Auximity Heaters Auximity Heaters Data Handling Auximity Heaters Auximity Heaters Data Handling Auximity Heaters Pack Table	Apply this weight to new replicates (%): 50 +	
Calibration Setup Verification Setup Time Events Table		~
Ready	NUM	

- 138. **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".
- Method Builder - [ecdtest det 250 cp -580 r10 mu 10.mth] X Eile Edit Yiew Window Help 🗎 ecdtest det 250 cp - 580 r10 mu 10.mth Calibration Type Replicate Tr Method Notes C 3 (No Calibration) 43X-GC - Address 44 Internal Standard Average Calibration Replicate 43X-GC Control External Standard . Configuration C Normalized % t to %) 50 ÷ Replicate Tolerance Replicate Tolerance Always add new replicates Never add new replicates Always add new replicates Add reglicates within this tolerance (%): Never add new replicates Out of Tolerance Action Calibration Range Tolerance C Add replicates within Peaks outside the range + tolerance generate calibration range errors. this tolerance (%): 0.5 Bange Tolerance (%): 10.0 ÷ Out of Tolerance Action ... Out of Tolerance Action. Edit/Lock Calibration Data... NUM

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ethod Builder - [Det Limit GC14.mth*] X	Det Limit 6C14.mth*] - X 2. Window Help - 0 X R120 R2 R2 4 1 10 Mr	Method Builder - [Det Limit GC14.mth*] - - × ≥ Eife Edit View Windtow Edito - - - - - - > ≥ Eife Edit View Windtow Edito -
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e Edit View Window Help - 6 > 2 Dies N. Salash Rai Vieslei Vi		
	Creak Detection	
Method Notes	Normal Taylor Bo	Method Notes Vesseement Type Solution Blank Baseline Measurement Type Solution

139. Replicate Tolerance in Method Builder -

replicates".

Peak Tak

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

40. Baseline Subtraction - The baseline run is a reduced set of 257 to 512 data points across the chromatogram run time by a bunching process, is stored within the method used for its collection and is subsequently subtracted from sample runs prior to peak detection. Baseline Subtraction is activated by enabling it in Method Builder > Integration Parameters > Subtract Blank Baseline, and by indicating the first run in a series in SampleList as Sample Type – "Baseline".

141. **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. Sep Code in report is labeled as "GR".

	🛅 Method Builder -	[2020-04-30	13-30-38 a 03	4 - 012 b inj 2 - m	aster sqa	qmd 25.3	3 ml loop (01-24-20-middle.mth]	- 0	×	
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At Scion MS Wor	estation = (V8)	2 IDach (3/14/191	Version 8	2 1 **	* 00101	-2311-	AB1-4118 **			
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Peak Measuremen	t: Peak Area										
Calculation Typ	e: External Star	ndard									
		Ret	Time			Width					
Peak Peak	Result	Time	Offset	Area	Sep.	1/2	Statu	5			
No. Name	(ppmC)	(min)	(min)	(counts)	Code	(sec)	Codes				
								-			
1 Methane		5.360					м				
2 Carbon Mo	nox 1.69	6.352	0.487	2920	BB	26.7					
5 MINLOC	0.52	17.205	0.026	10652	GR.	0.0		-			
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142. Grouping by peak label -

After computations are perfomed for peak concentrations, selected peaks can be grouped by peak name. Examples include summing up peaks separate in of measurement polychlorinated biphenyls, toxaphenes, and aromatic hydrocarbons.

143. **Natural gas calculations** - reports values for mol%, BTU, specific gravity, gallons per thousand, and compressibility.³ Available from Lotus Consulting.





144. Pattern Matching for Polychlorinated Biphenyls (PCBs) available from Lotus Consulting. User selects standards and application compares them to unknowns and reports back matches, and compositions of mixtures.

³ Gas Processor Association, 6525 East 60th Street, Tulsa, Oklahoma 74145, http://ihsmarkit.com/products/gpa-standards.html



145. Master/Slave Gas Chromatographs Some applications require more hardware capabilities than are available in one instrument. By combining two gas chromatographs Master/Slave configuration, in а 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 chromatographs. The configuration allows a single method to fully control two separate temperatureprogrammable column ovens, six GC detectors and a mass spectrometer, 12 electronic flow controllers, 6 detector flow controllers, two 8400 AutoSamplers (up to 200 liquid sample vials), and up to 32 external events. Typical examples are full speciation of hydrocarbons in exhaust (http://lotusinstruments.com/wp/wpvehicle content/uploads/Quantitation-of-Hydrocarbons-in-

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