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

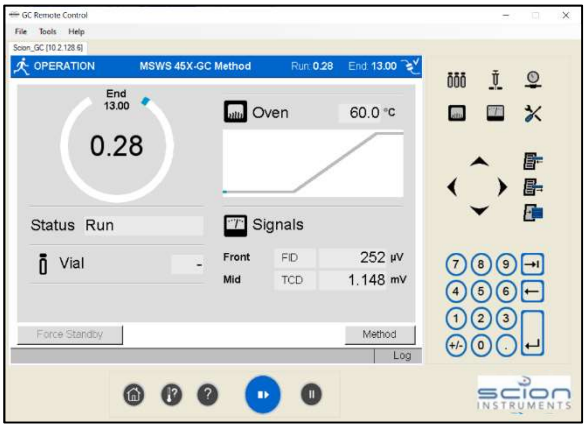
Routine operations with Scion MS Workstation are quite easy to set up parameters for data collection and report generation . The following is a discussion of hidden quirks that may not be obvious of their usefulness. This discussion assumes that the operator is familiar with basic operations in MS Workstation.

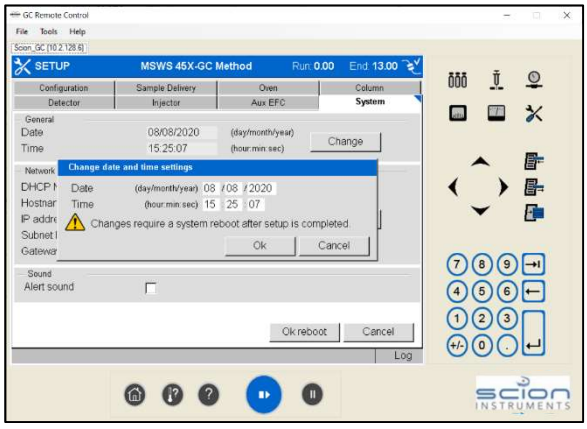
Operations involving control of Scion 436/456 Gas Chromatographs.

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.

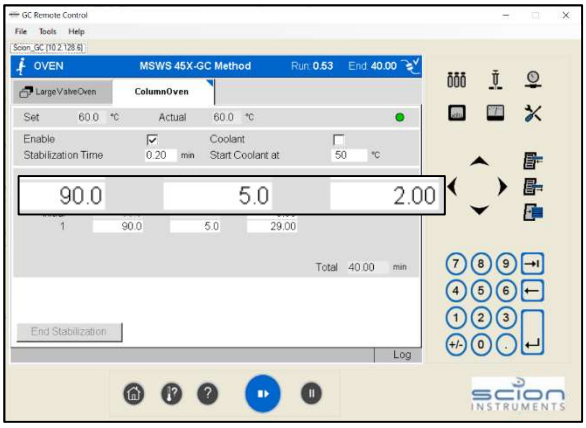
3. GC Remote Control - allows view of status of gas chromatograph from a remote computer, typically through Team Viewer or similar app.



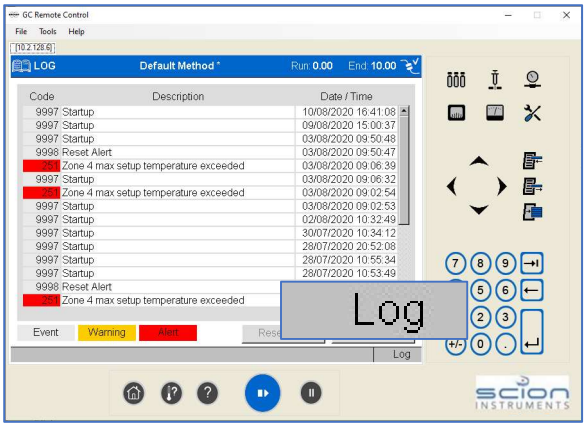


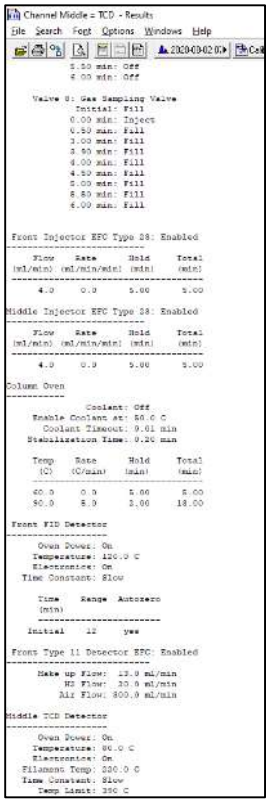
4. Reboot gas chromatographs through GC Remote Control by setting a minor change to System Time through Setup > System.

5. Change run time for gas chromatograph during run, especially useful in method development.



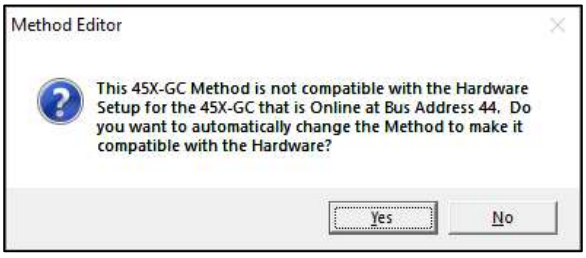
6. Instrument Log – lists activities for the instrument, including faults with time/date stamp.

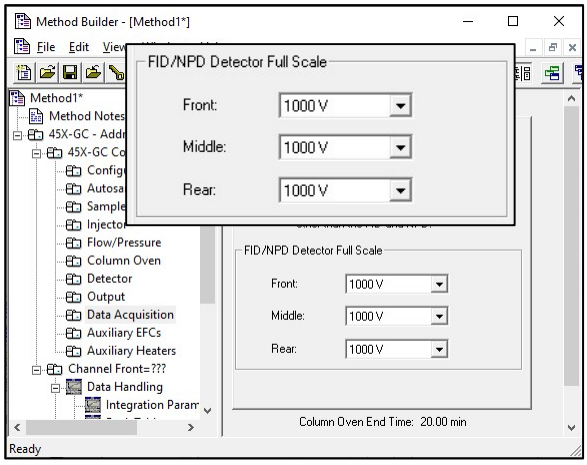




7. Runlog - documents all actual run conditions on GC in every .RUN file for full recovery at a later time, even changes made during the run.

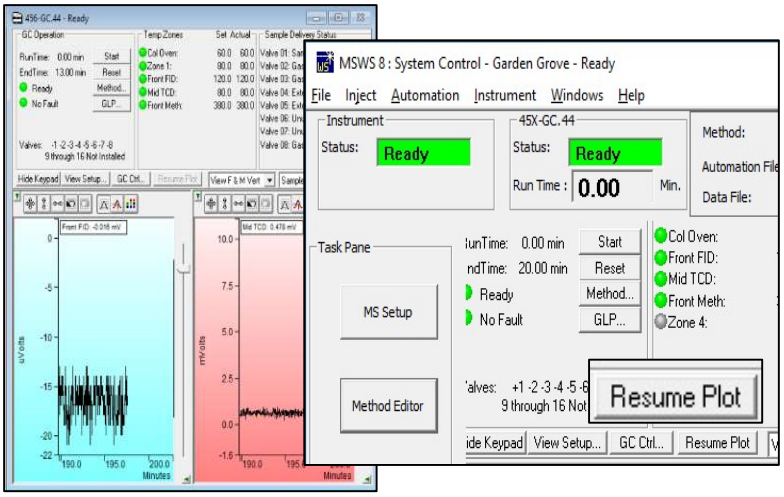
8. Automatic update of method when hardware is added/deleted in Setup. All other hardware and calculations remain intact.



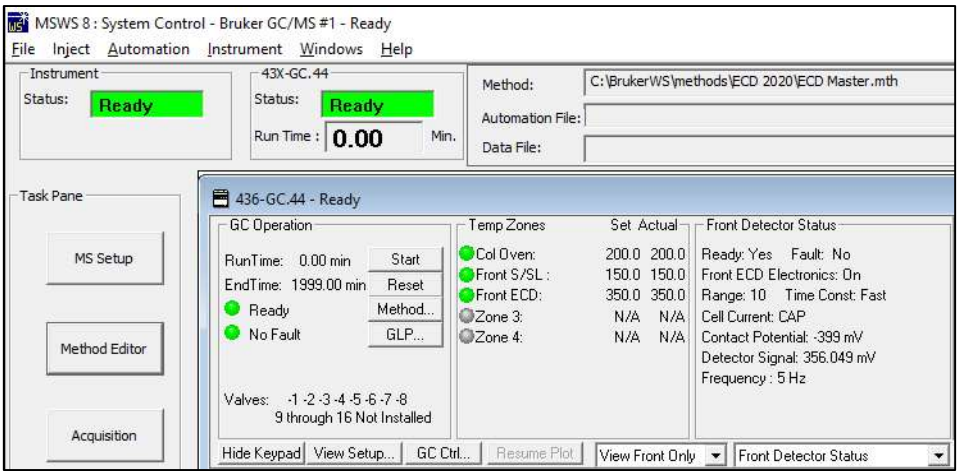


9. FID/NPD Detector Full Scale - the electrometer for these two detector types has the ability to auto-range over the full range of the detector. To activate this feature, full scale parameter is set to 1000 V.

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

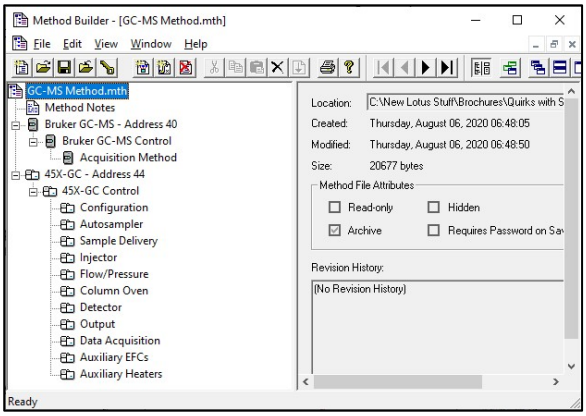


11. Entry and display of temperatures in 0.1 °C increments.



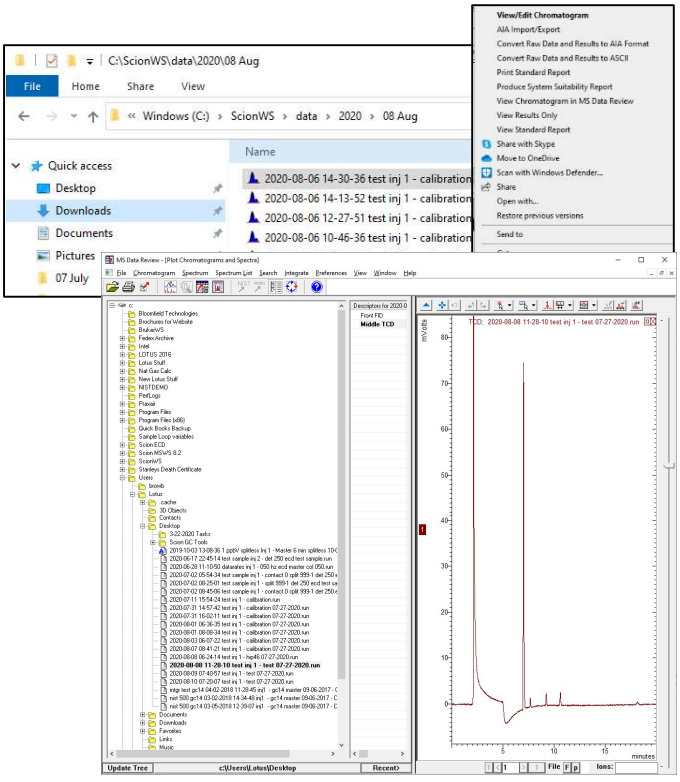
Common hints for both MS and GC detector operations

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

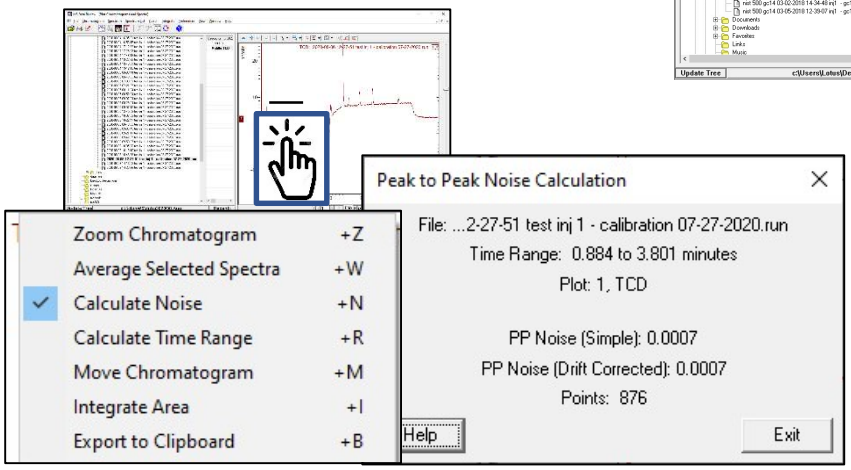


13. Concurrent data collection for MS and GC with single SampleList.

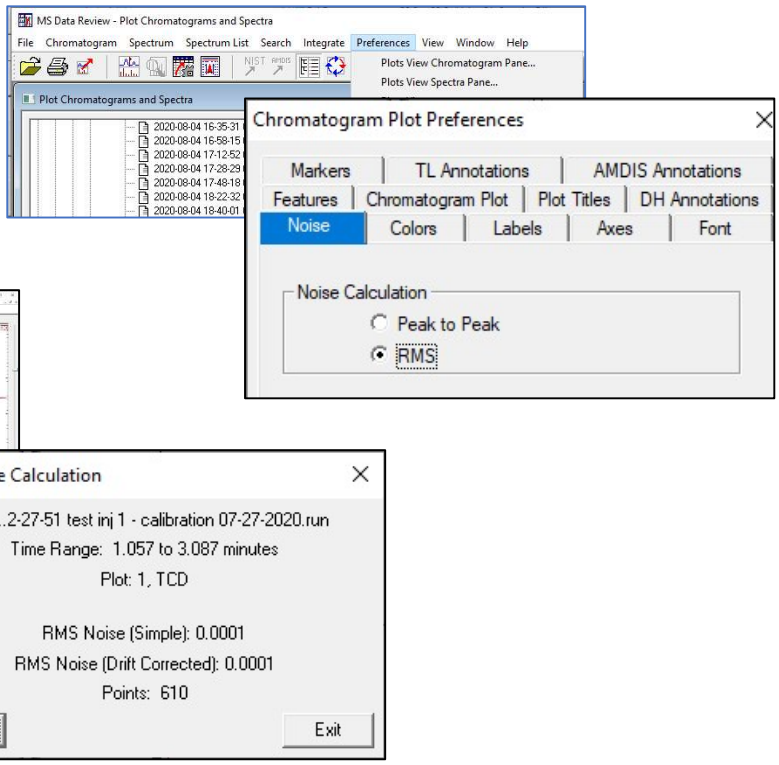
14. GC chromatogram can be displayed in MS Data Review, by right-clicking of .RUN file in Windows Explorer.



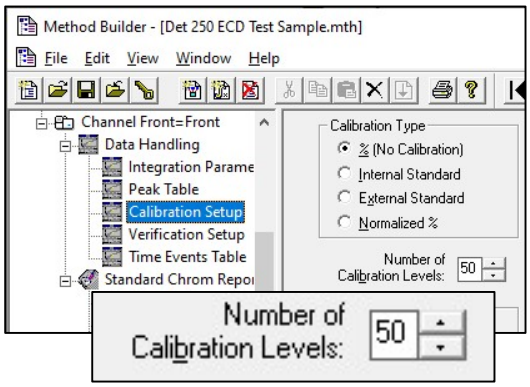
15. Compute GC Detector Peak to Peak Noise in MS Data Review. Use mouse to draw line for noise calculation.

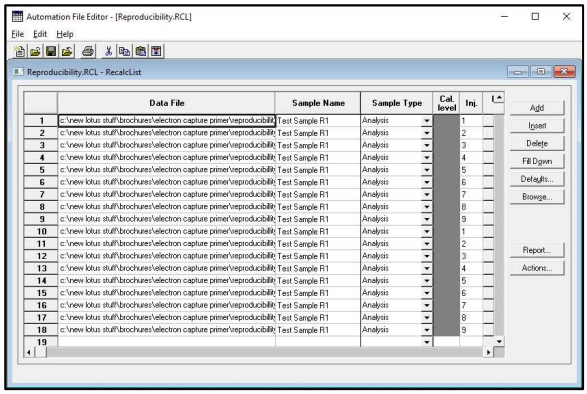


16. Compute GC Detector Root Mean Square Noise in MS Data Review. Open .RUN file in MSWS and use mouse to draw line for noise calculation.



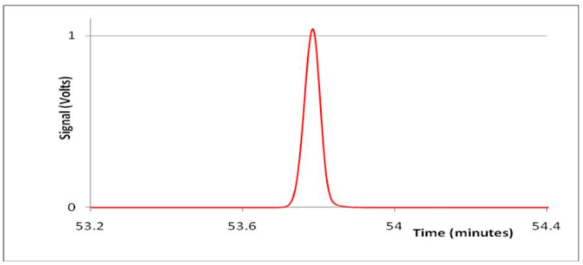
17. Up to 50 calibration levels.

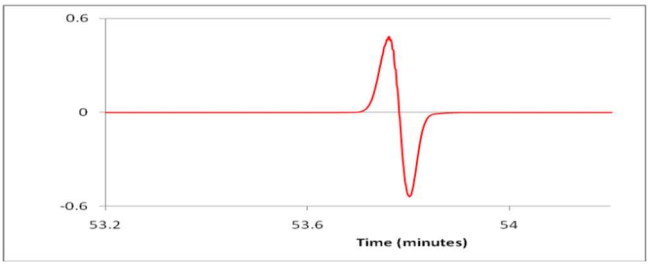


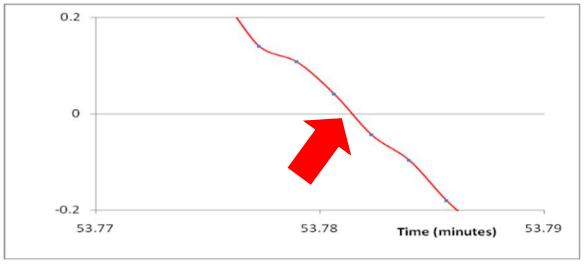


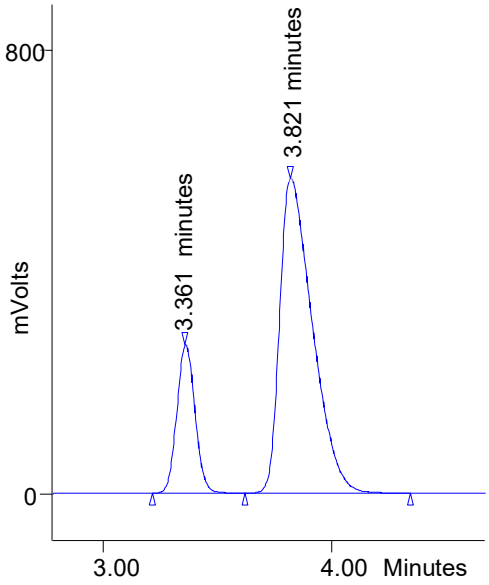
18. Recalc List – This screen allows selected data files to be recalculated with a modified or different method.

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.



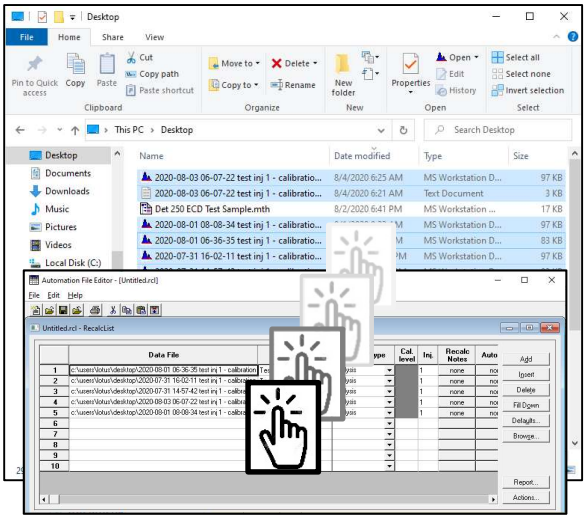




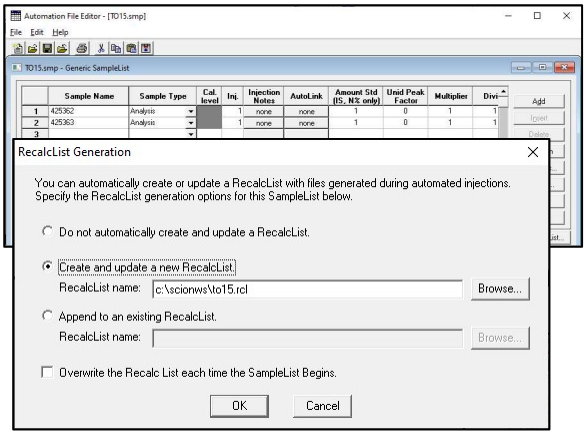


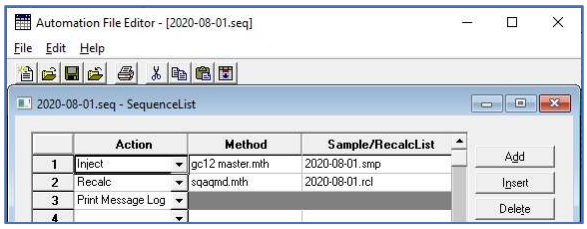
20. Start and end points for peak integration are always on the chromatogram tracing.

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



22. Create/update files to Recalc lists from SampleList.

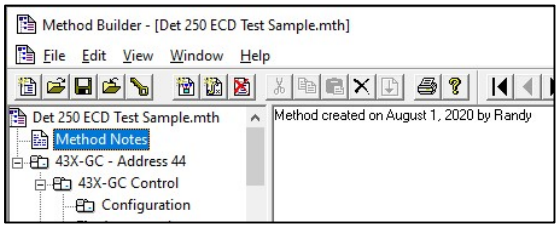


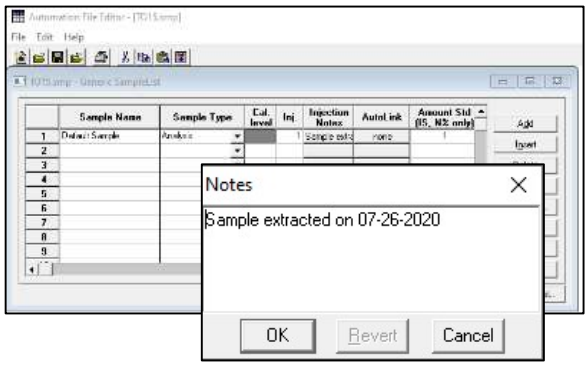


23. Sequence List – This screen permits multiple actions related to using a series of methods with multiple SampleLists or RecalcLists. The related MessageLog can be printed to provide documentation of actions.

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

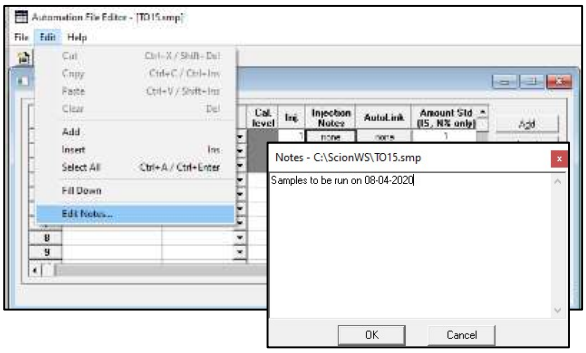
- Method Notes.

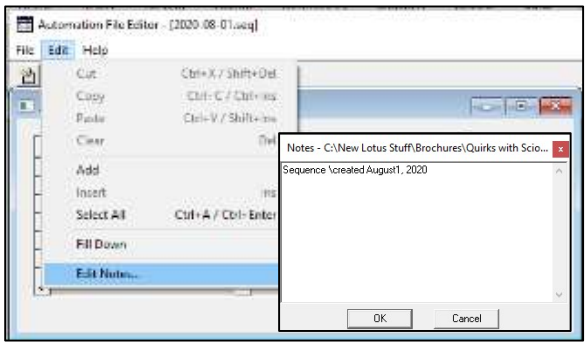




- Injection Notes.

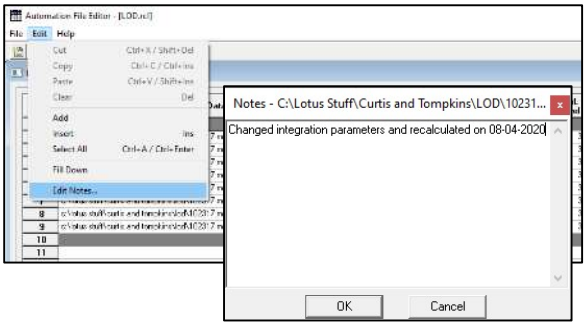
- Sample List.





- Sequence List.

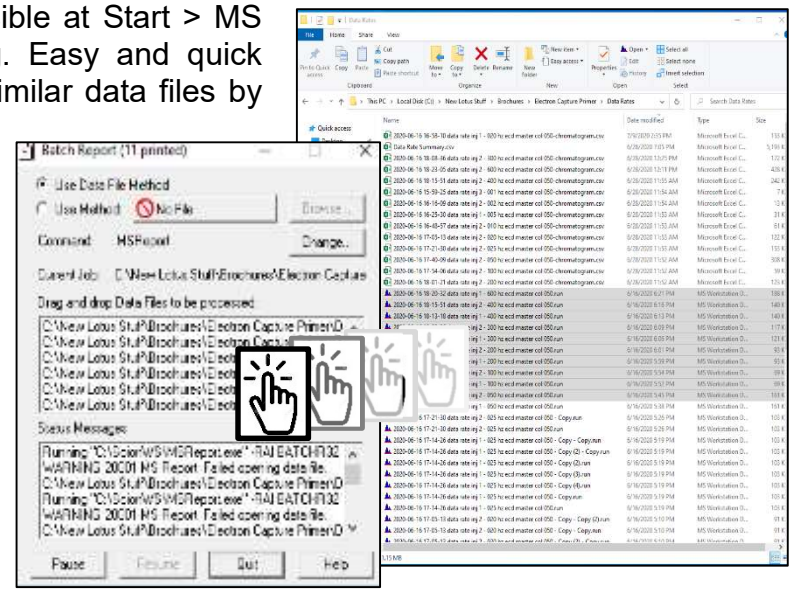
- Recalc List.



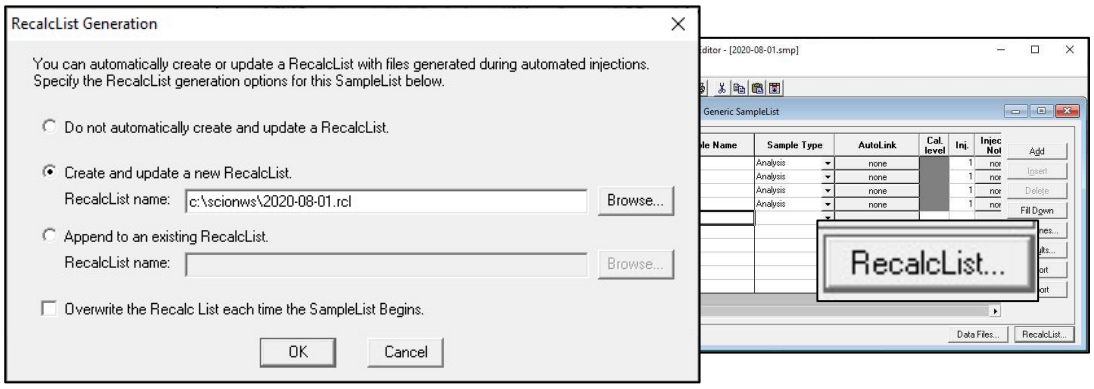
25. Sample injection time/date and sample name are locked at time of data collection and cannot be changed postrun.

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

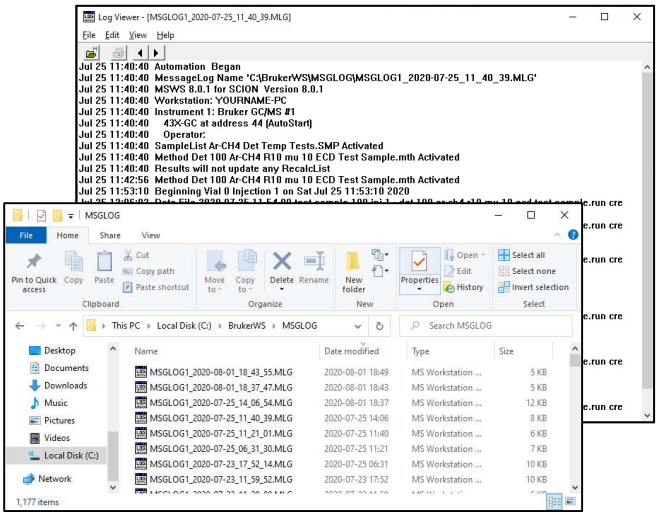
26. Batch Processing - icon accessible at Start > MS Workstation > Batch Reporting. Easy and quick approach to reprocess lots of similar data files by highlighting desired data files in Windows Explorer and drag-drop into window.



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.



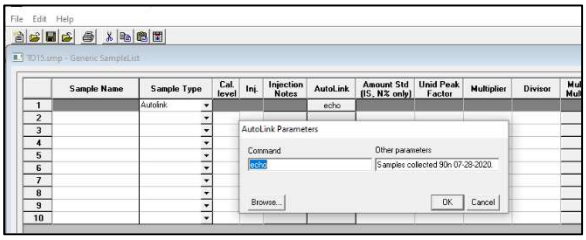
28. MessageLog lists all system control activities, documented with time/date of injection, sample labeling, data file label and location, and errors. These logs are available for recall later.



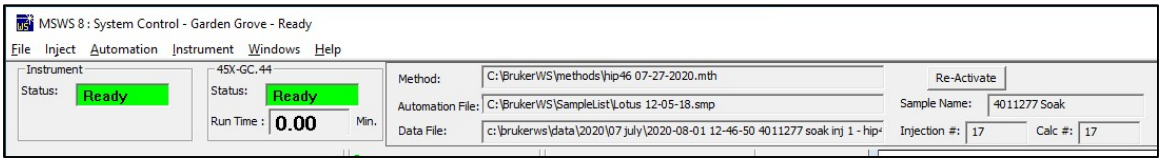
29. Echo - This AutoLink application inserts a string in the Message Log. Use the following syntax in the AutoLink field in a Sample List or Recalc List:

    command-line: echo

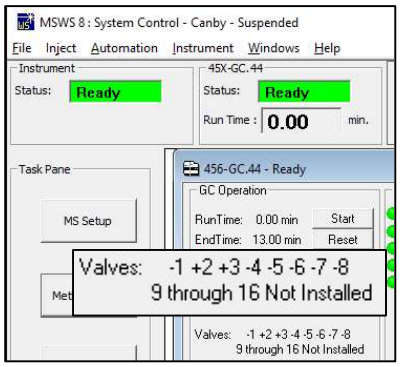
    other-parameters: <descriptive text to be "echoed" in the Message Log>



30. Header block in System Control:

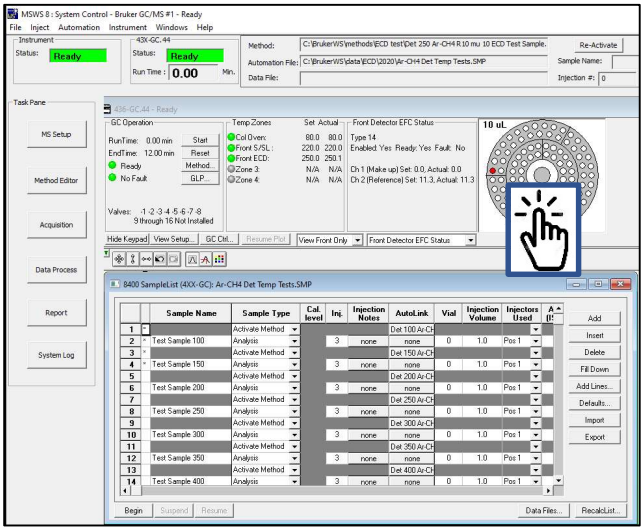


- Listing of active method
- Active automation file
- Last data file collected
- Active sample name
- Injection counter
- Number of calculated files
- Button to reactivate active method

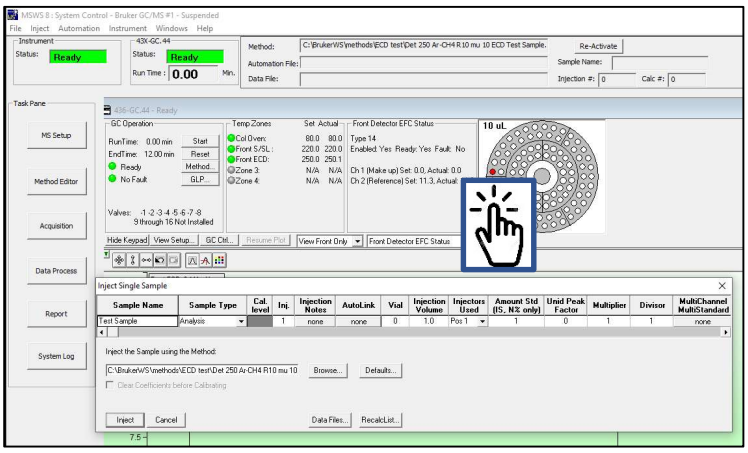


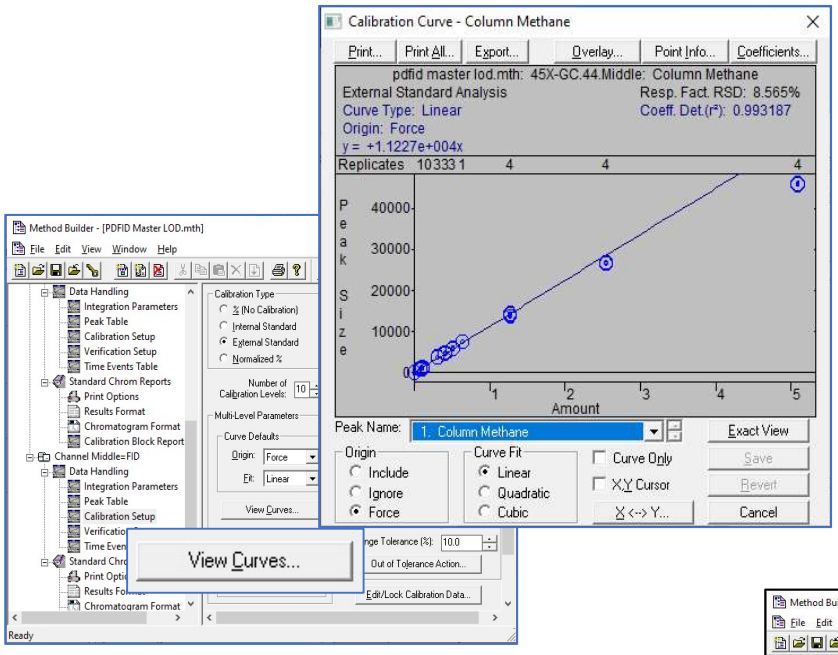
31. Live display of all valve activities on System Control screen.

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



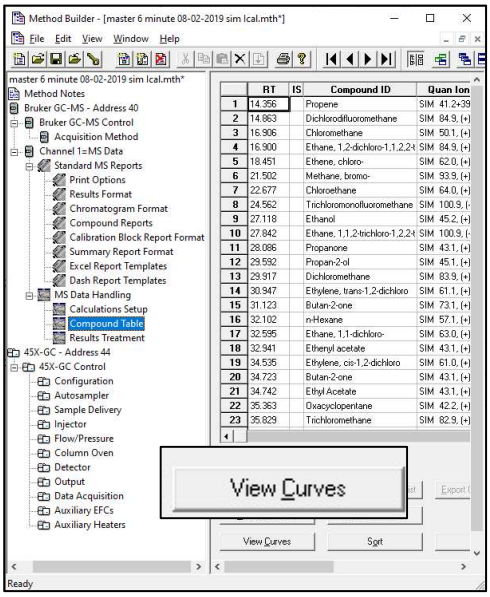
33. Direct access to inject single sample by clicking on vial in 8400 display.



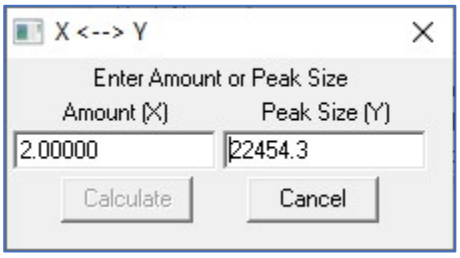


34. Graphic display of calibration plot by Method Editor > Calibration Setup > View Curves for GC detectors.

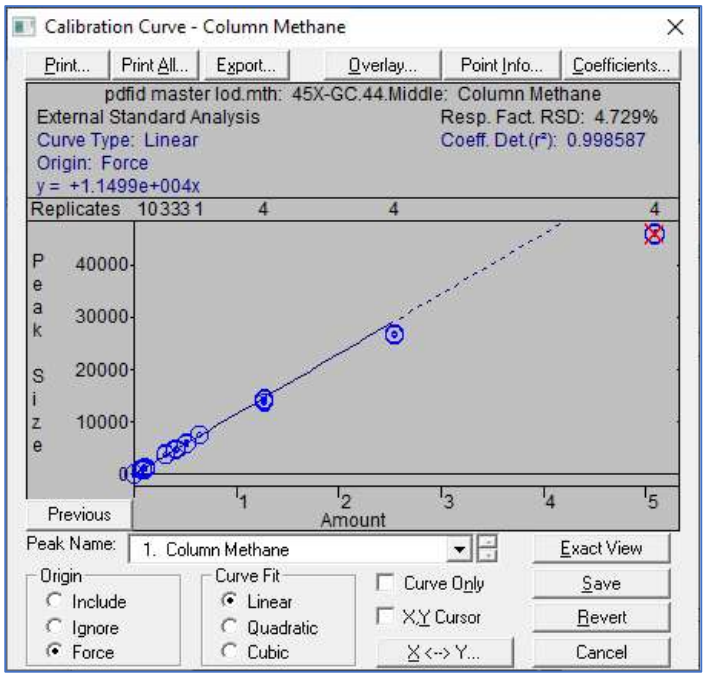
35. Graphic display of calibration plot for MS data through Method Editor > Channel 1=MS Data > MS Data Handling > Compound Table > View Curves.

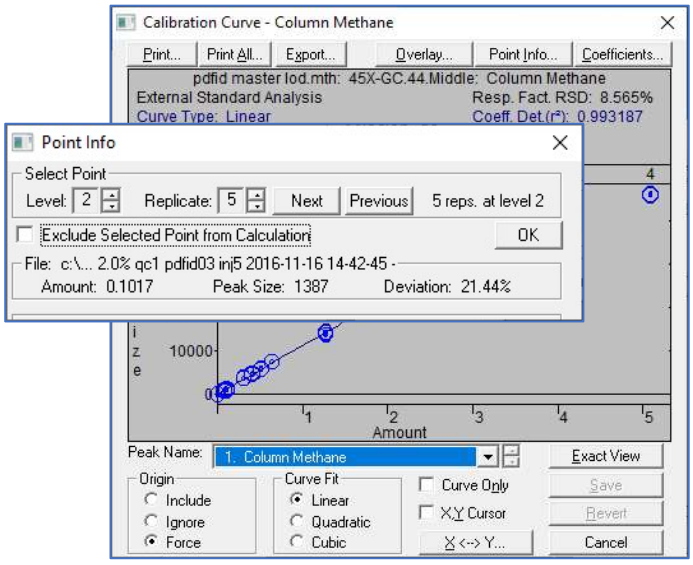


36. Interconversion of detector response and concentration per calibration curve. This calculator allows anticipation of expected peak size for a given peak size.



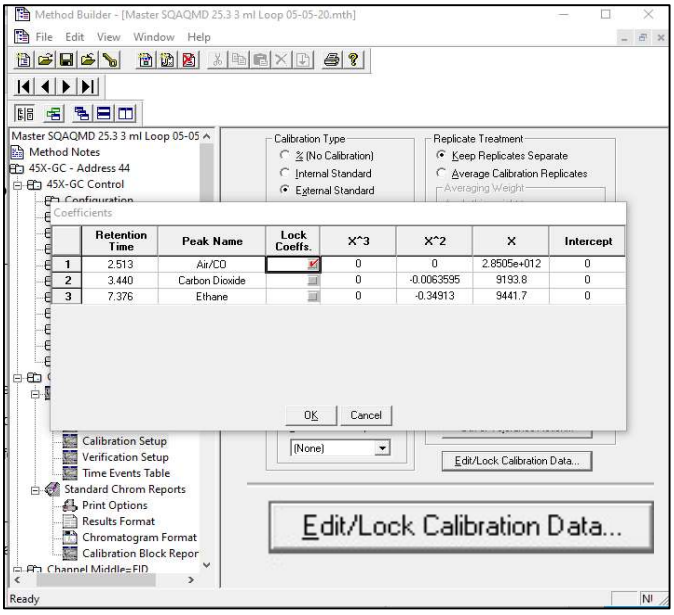
37. Edit out obviously invalid data points in calibration plot by right clicking on specific points.



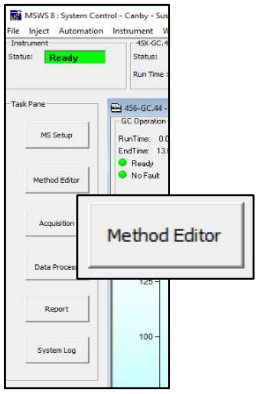


38. Source of calibration data point with Calibration Curve > Point Info.

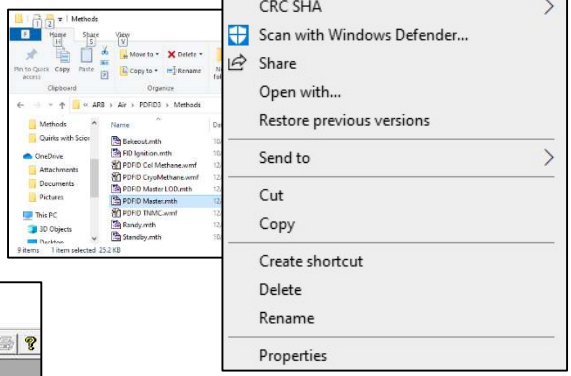
39. Edit/Lock Coefficients – When multiple standards with differing analytes are used, coefficients need to be locked after they are calibrated so that the next mixture does not alter them. In addition, coefficients from related analytes can be manually entered. For example, the response values for propane with a flame ionization detector can be applied to other hydrocarbons.



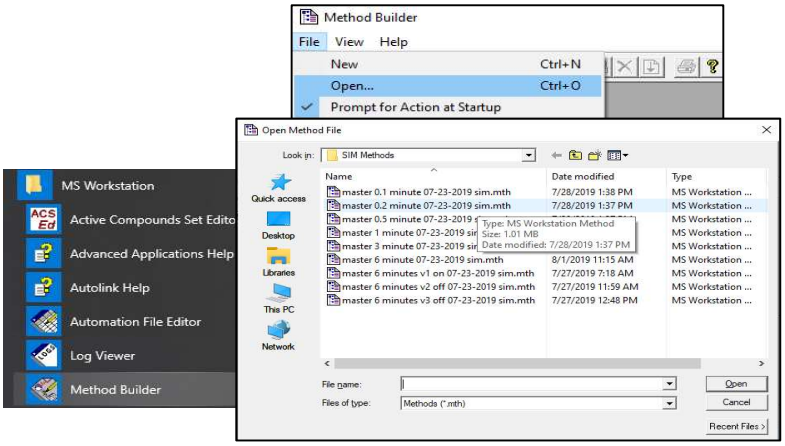
40. Approaches to open method:



- Task Pane.

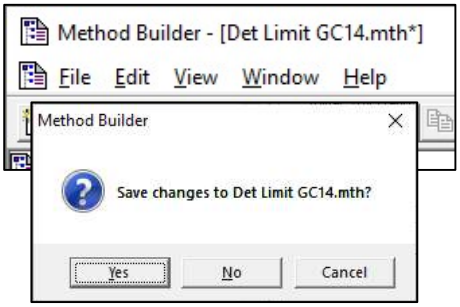


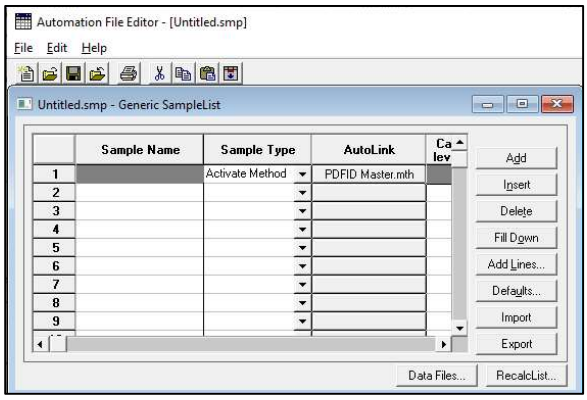
- Windows Explorer.



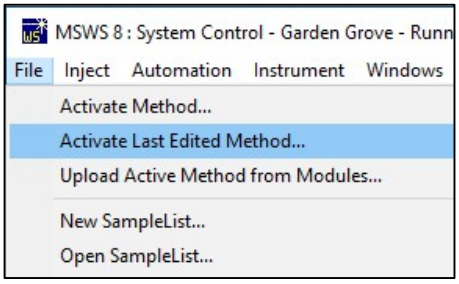
- Method Builder icon.

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.

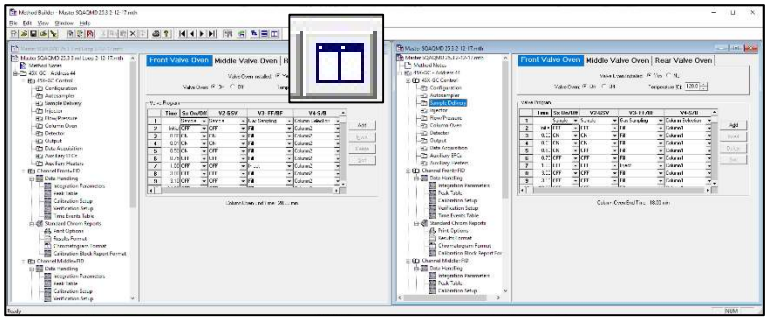




42. Activate method through SampleList.

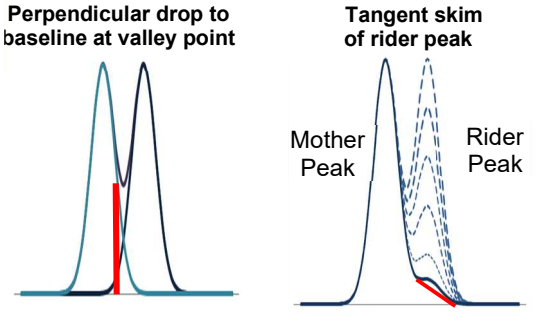


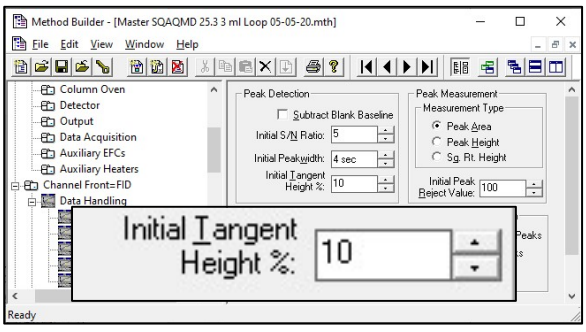
43. Activate “Last Edited” method.



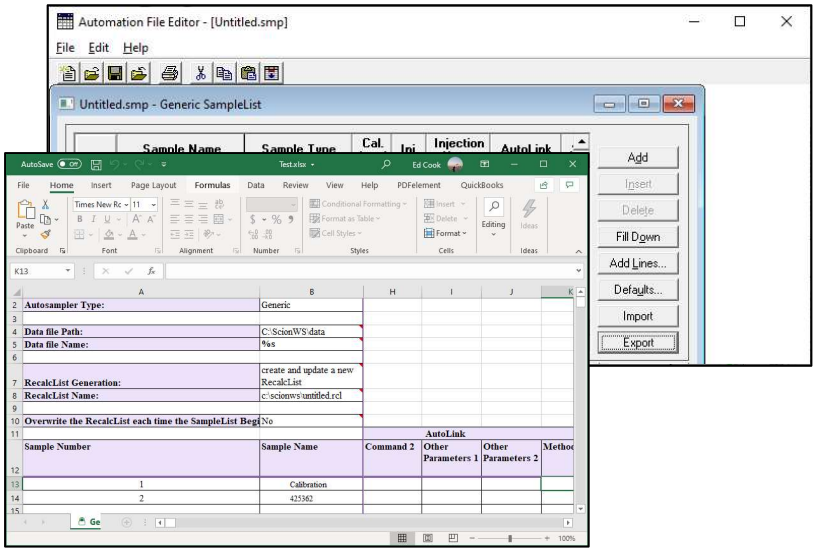
44. View multiple methods side-by-side on one screen.

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”.

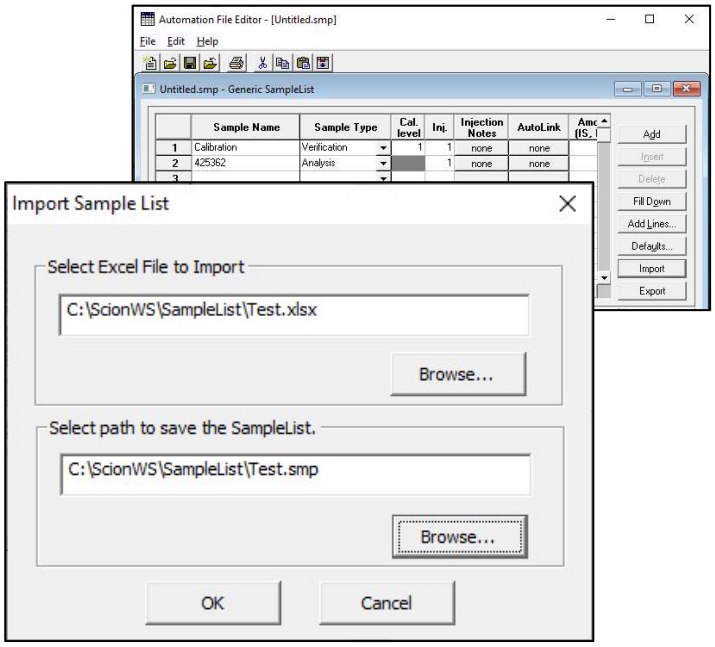




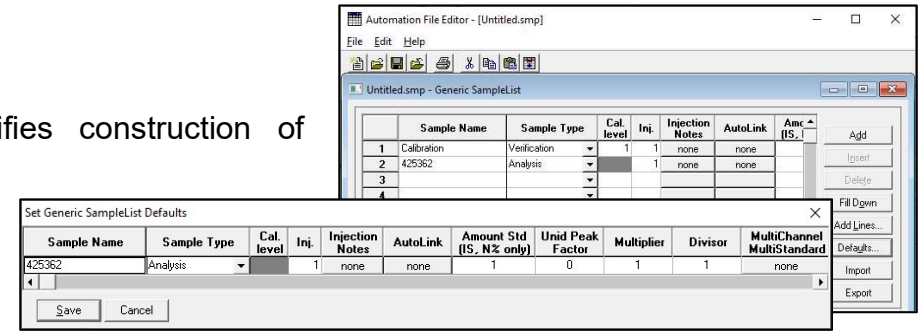
46. Export SampleList to Excel.



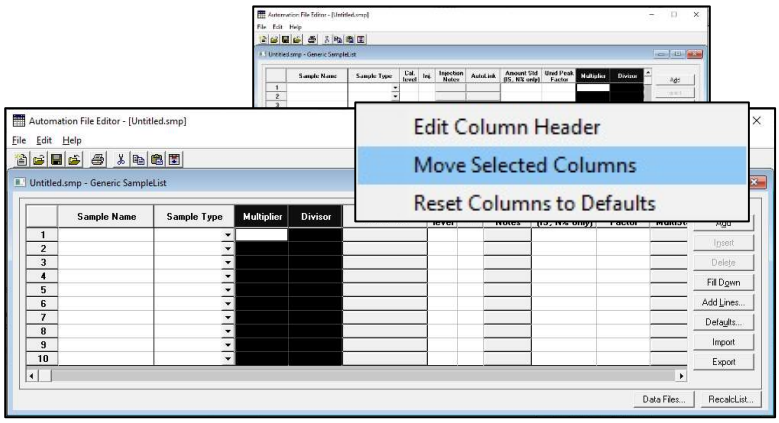
47. Import SampleList from Excel.

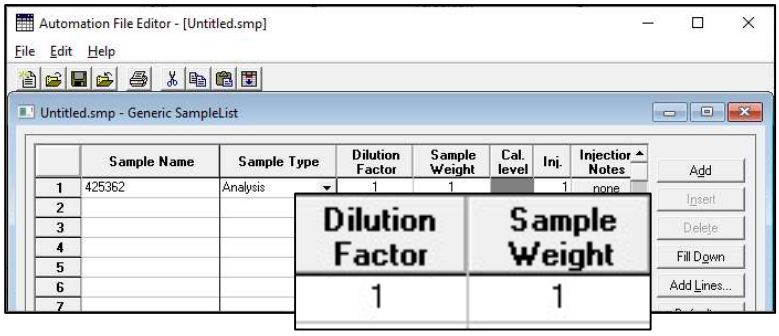


48. Default entries simplifies construction of SampleList.



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





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”.

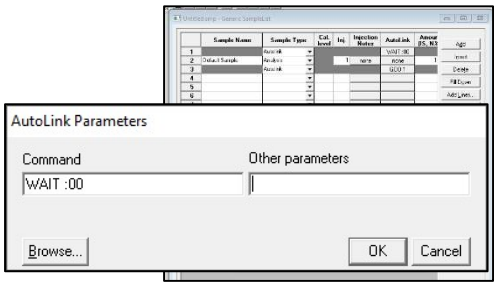
53. SampleList AutoLink commands:

- 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

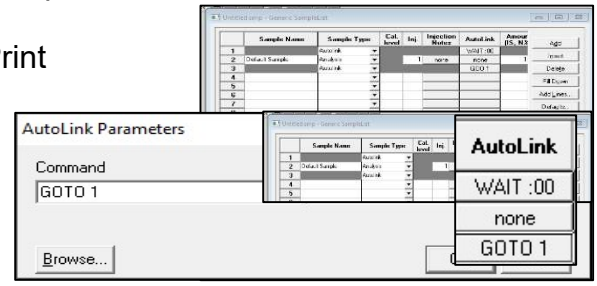


  For example, WAIT 15:03:56 will wait for 3:03:56 PM, unless this time is already passed, in which case there will be no wait. Fields can be omitted. In this case, tailing fields are defaulted to zero, while leading fields are interpreted as the next matching hour or minute. The following examples illustrate 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

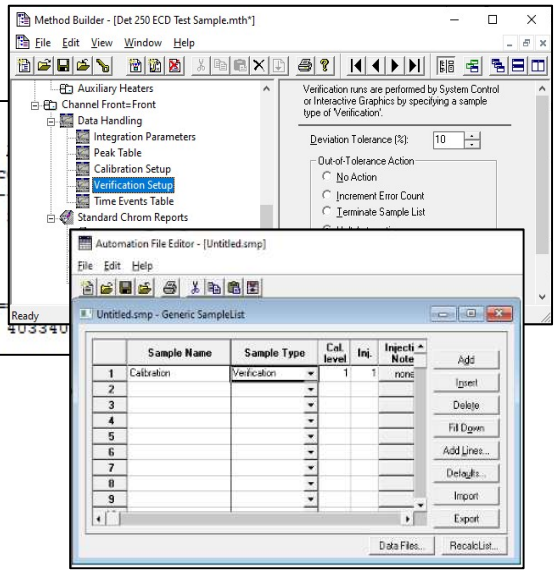
- GOTO - This application jumps to another line of the sample list or log. Use the following syntax in the AutoLink field in a Sample List or Recalc List:
  Command: GOTO <line-number>
  Other-parameters: Inject or Recalc or Print

- 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.

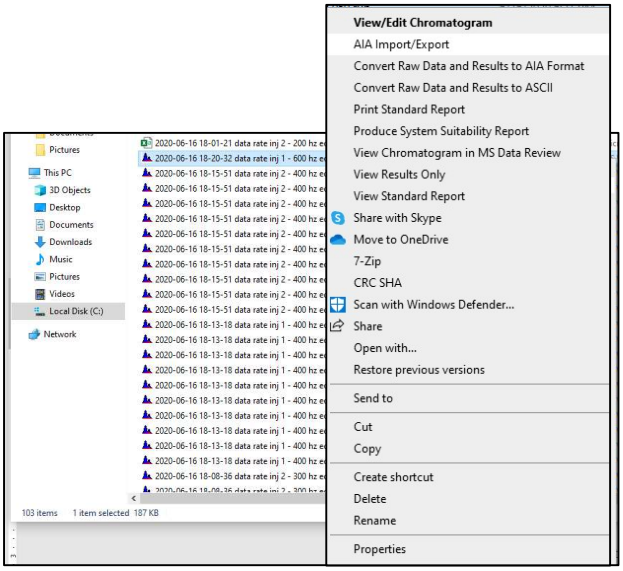


54. "Verification" run type – Reported results compared to values in a calibration level.

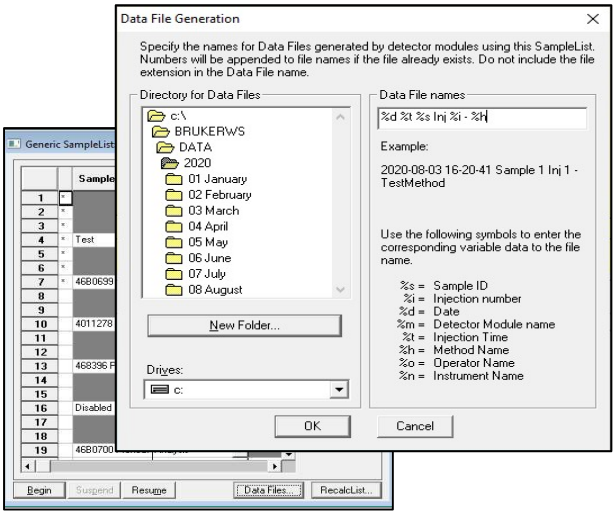
Peak No.	Peak Name	Expected Result ()	Calculated Result ()	Dev. %	Ret. Time (min)	Time Offset (min)	(c
1	Hydrogen	125.8000	126.0991	0.2	5.980	-0.010	
2	Oxygen	25.1500	27.3469	8.7	6.457	-0.009	
3	Nitrogen	49.9400	49.9810	0.1	7.230	-0.011	
4	Methane	24.8600	24.8167	0.2	8.182	-0.011	
	Totals:		228.2437			-0.041	



55. Access data file actions from Windows Explorer.

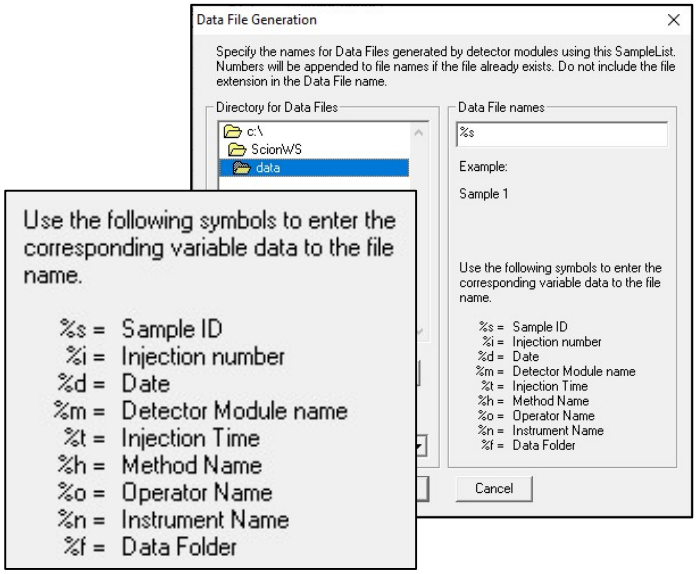


56. Specify/Create data file directory from Sample List.

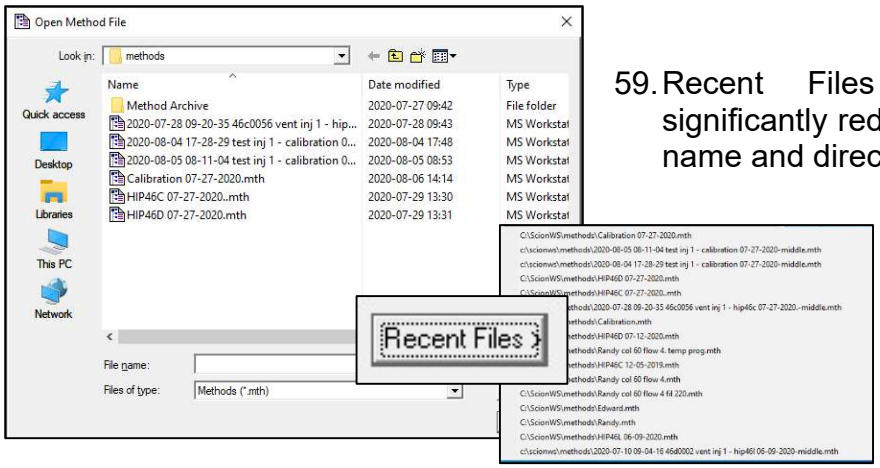


57. Automatic data file naming with tokens.

58. Data file names can have up to 255 characters.

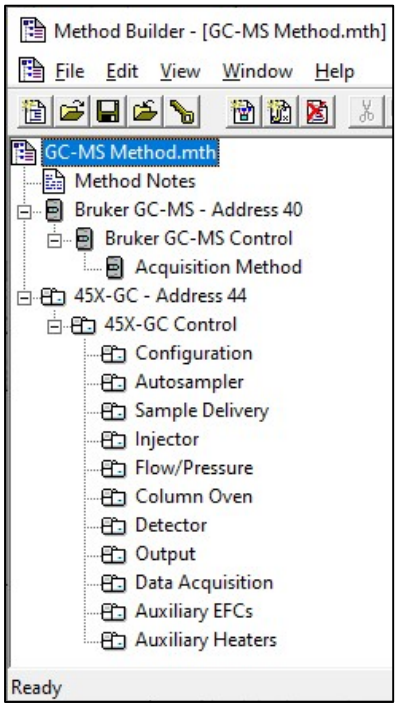


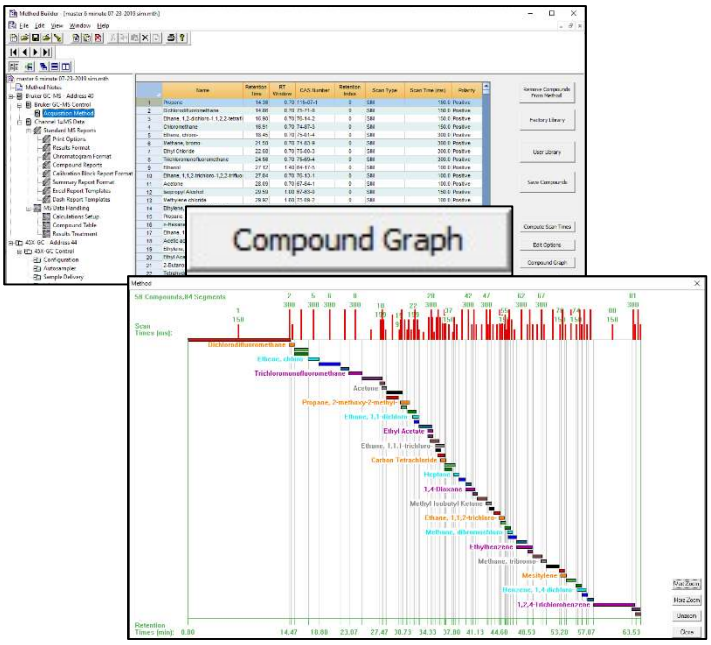
59. Recent Files button. This action significantly reduces errors in entry of file name and directory path.



Suggestions for operations with .XMS data files

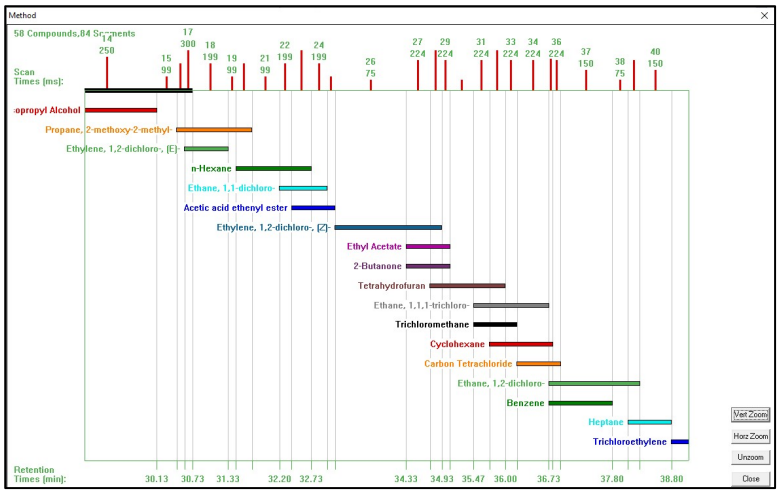
60. Single method for full control of both MS and GC detectors.



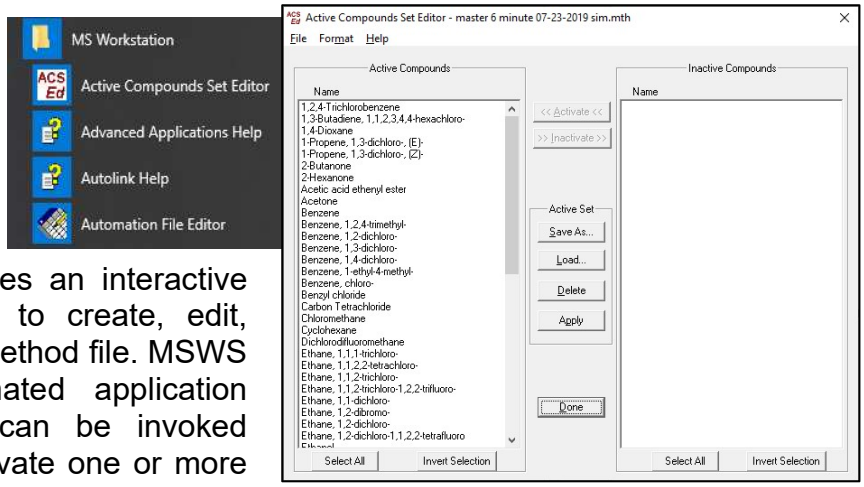


61. Compound Graph illustrates scan times and effects of peak window overlap.

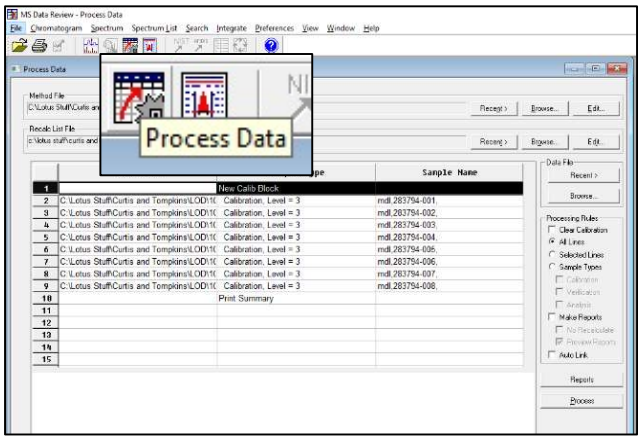
62. Expanded view of portion of Compound Graph.



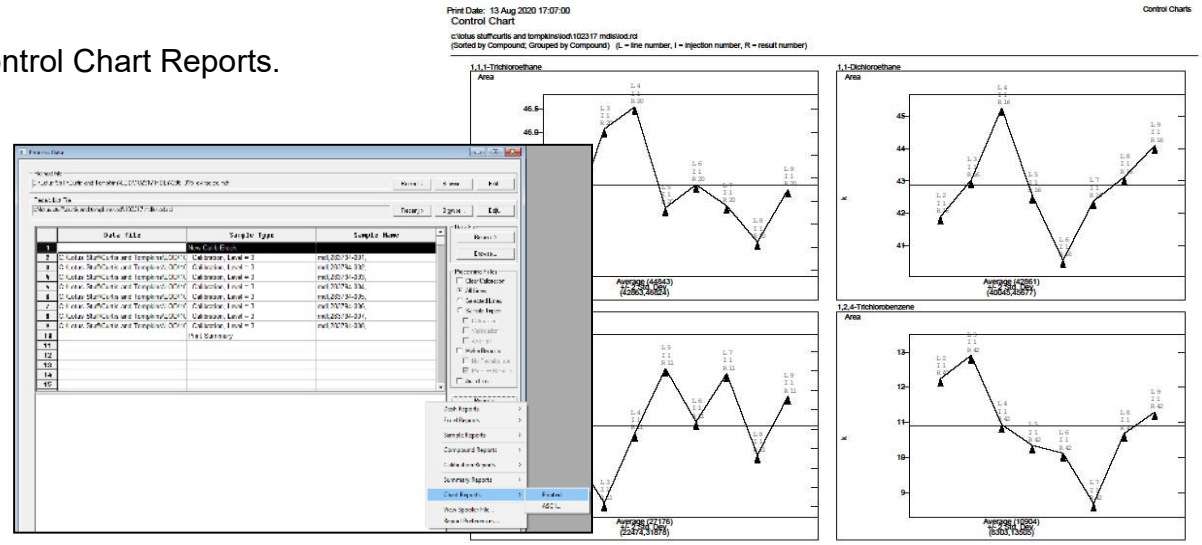
63. Active Compounds Set Editor - ACS is a list of compounds, representing a subset of the Compound Table, which can be saved in a method, and activated during automation. MSWS includes an interactive application (ACTIV2.EXE) to create, edit, delete such sets within a method file. MSWS also includes an automated application (ACTIVATE.EXE) which can be invoked within a sample list to activate one or more sets in the active method.



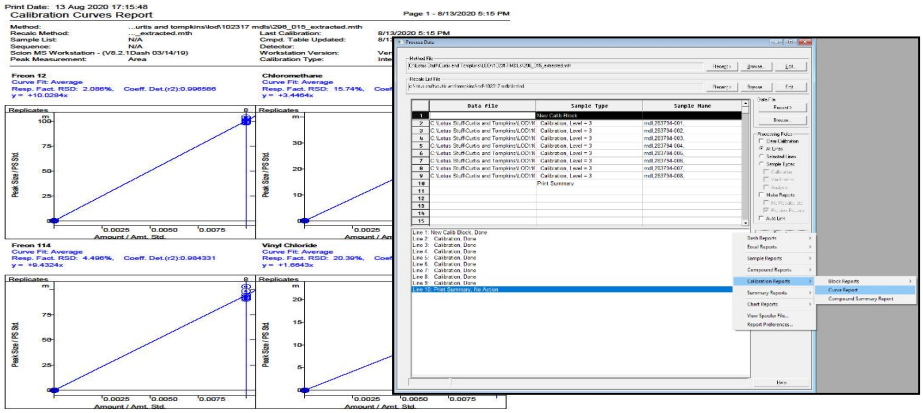
64. Process Files.



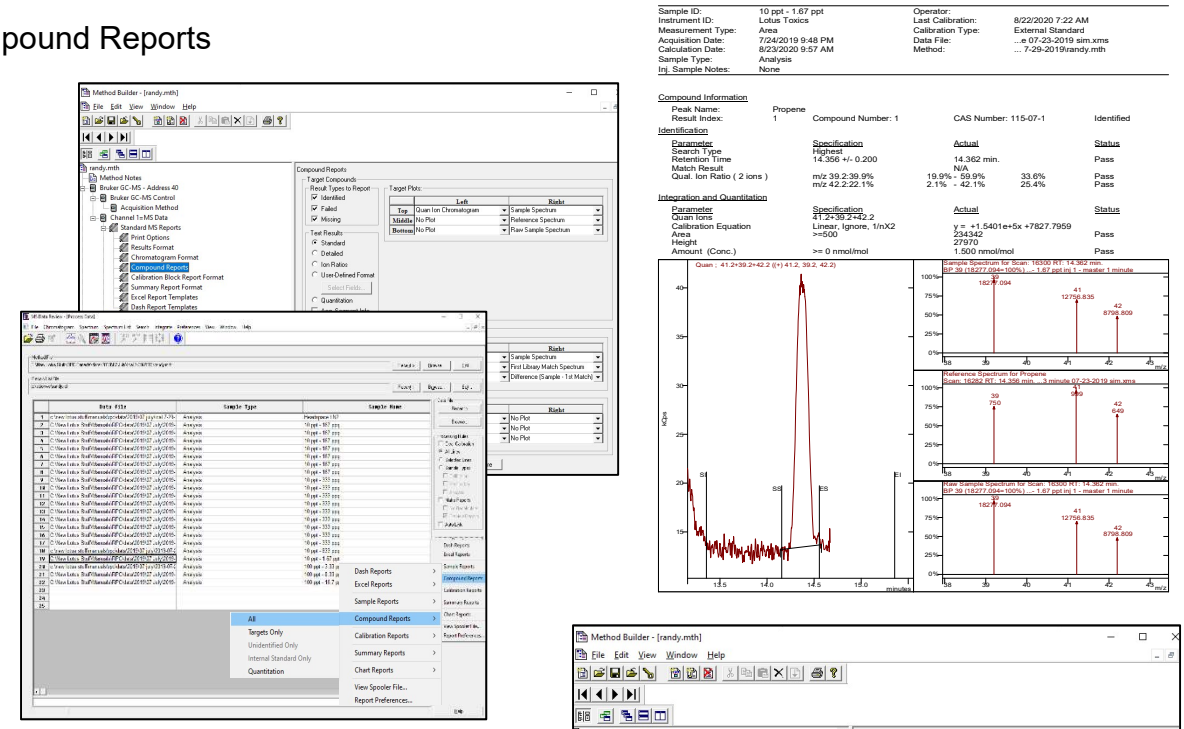
65. Control Chart Reports.



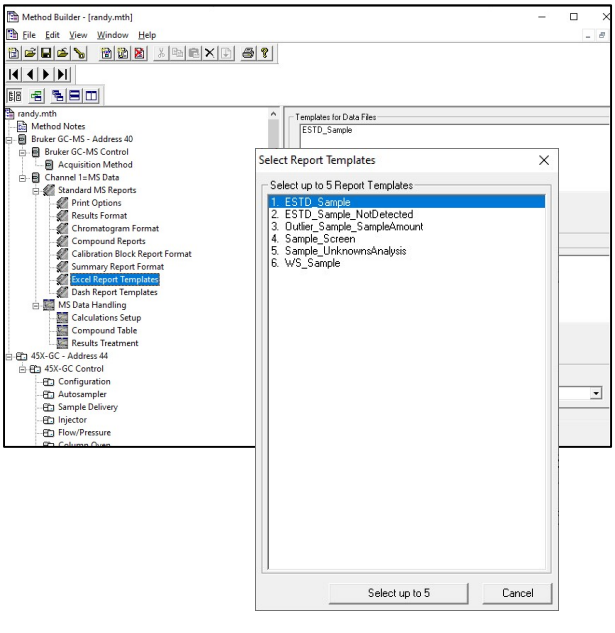
66. Calibration Reports.



67. Compound Reports

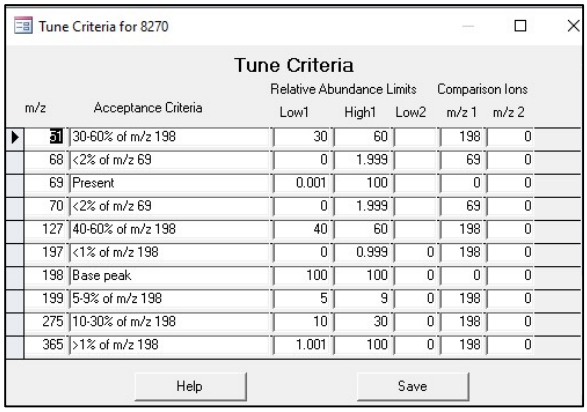


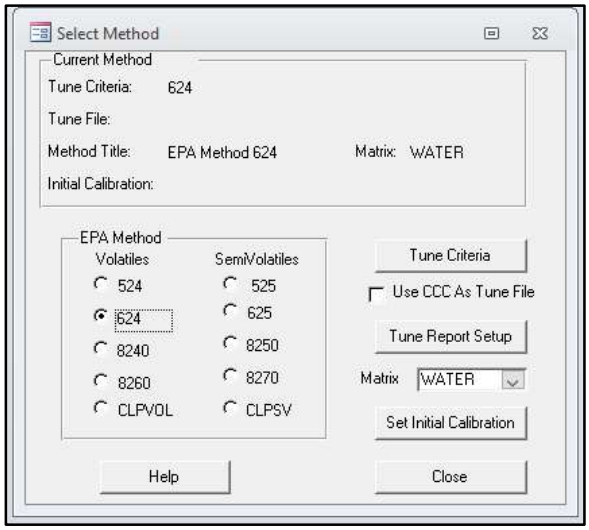
68. Excel Report Templates



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.

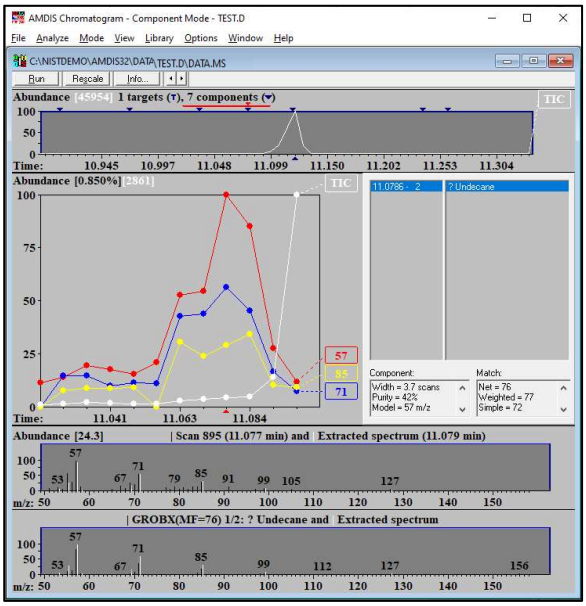


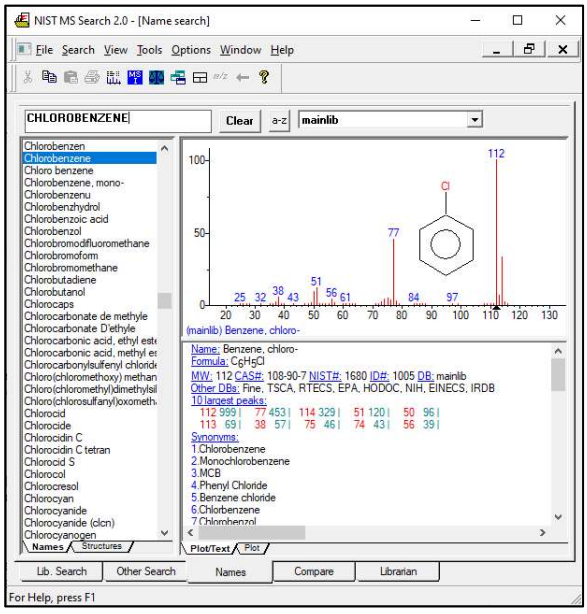


71. Multicompound Software - 19 templates allow various displays of target compounds, tentatively identified and unknown compounds in 1) graphic and text, 2) graphics only and 3) text only configurations.

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.

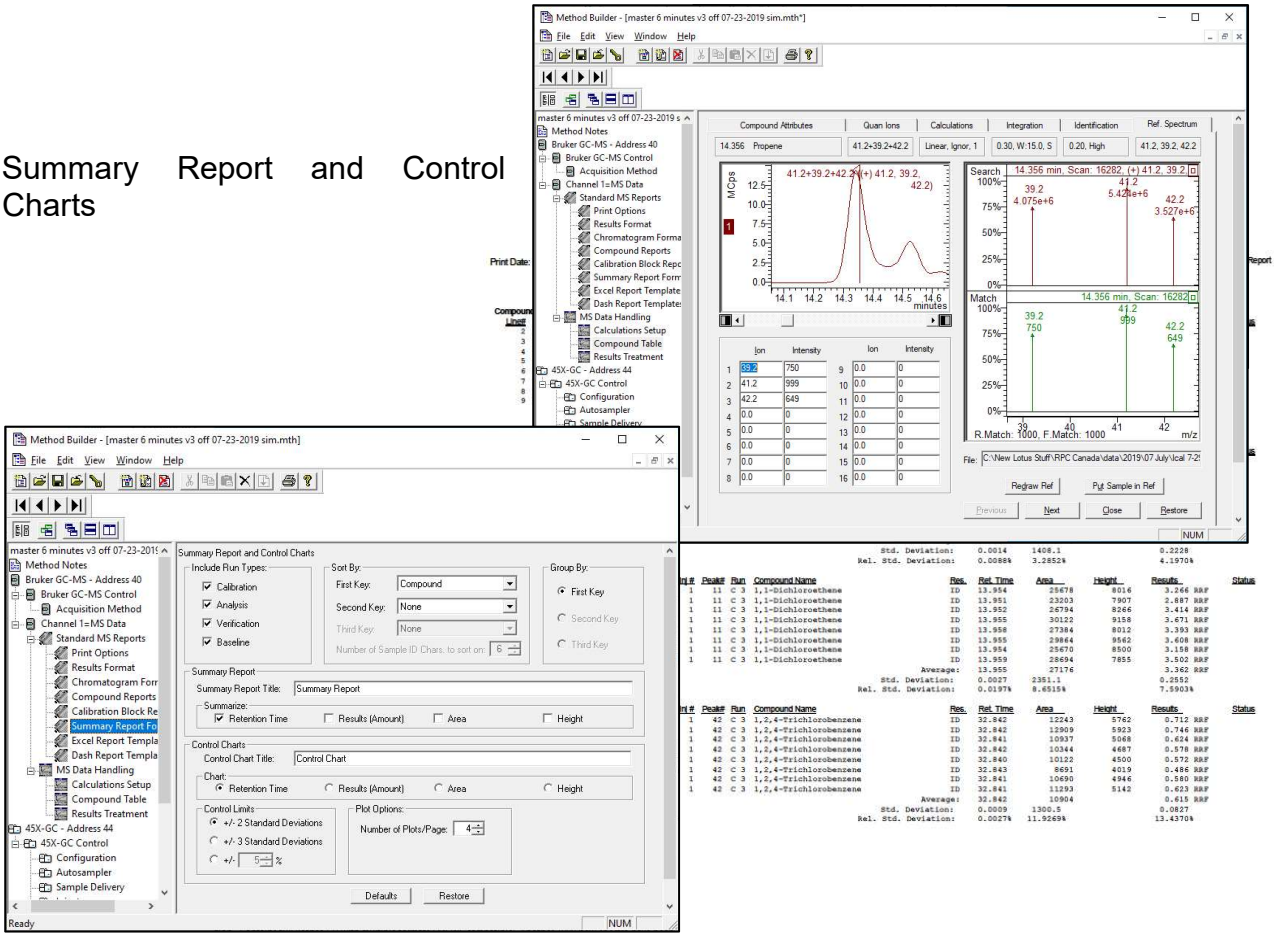
73. NIST Automated Mass Spectral Deconvolution and Identification System - AMDIS - allows users to automate the complex process of extracting data from GC/MS data file. AMDIS works by finding all of the ions that rise and fall at the same time and associating them to a single component. Once it has found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





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.

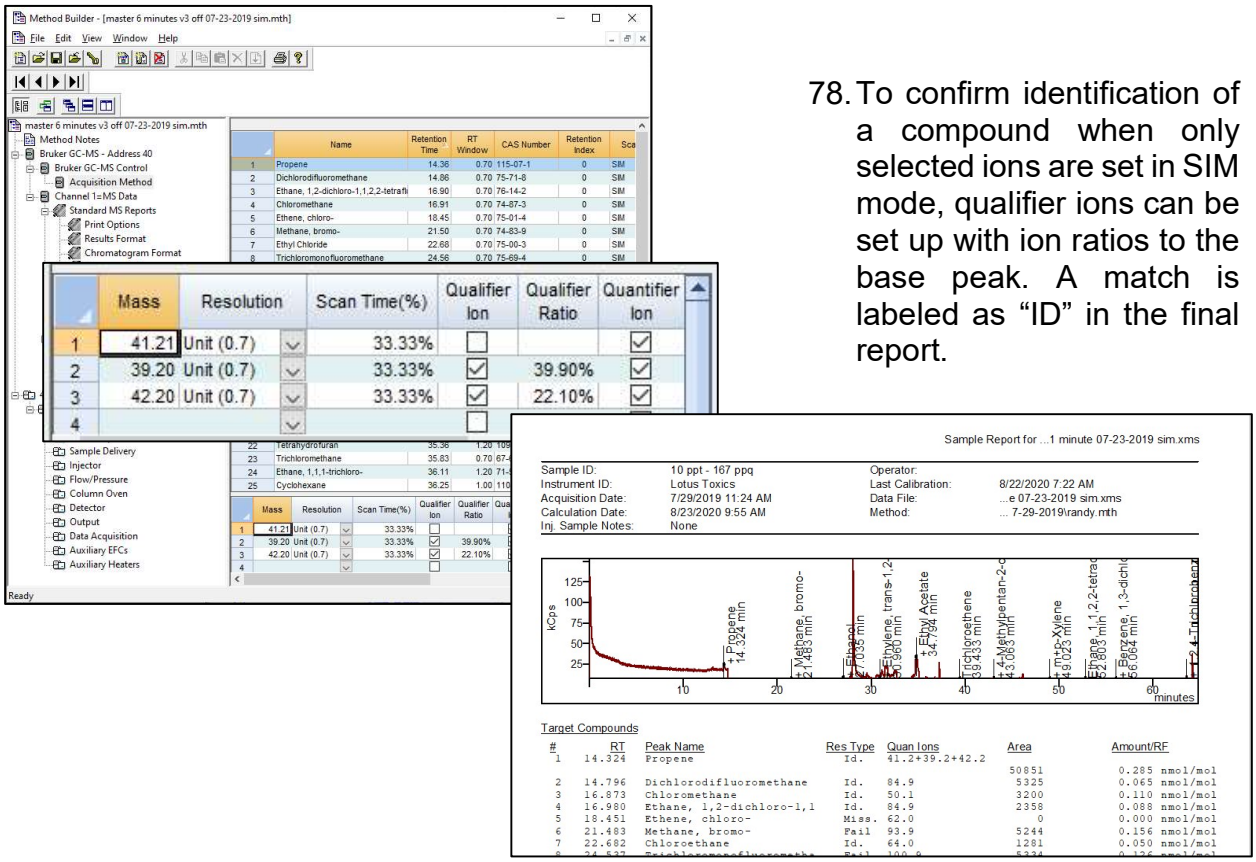
75. Summary Report and Control Charts



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**S** Monitoring (SIM) – Data from multiple ions can be collected to provide positive matching to reference spectrum with use of multiple characteristic ions for compounds.



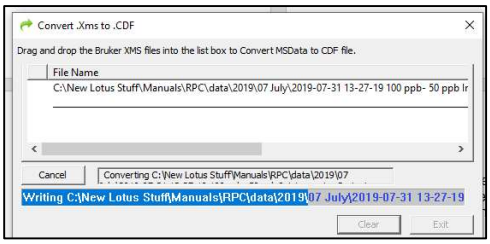
78. To confirm identification of a compound when only selected ions are set in SIM mode, qualifier ions can be set up with ion ratios to the base peak. A match is labeled as “ID” in the final report.

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.

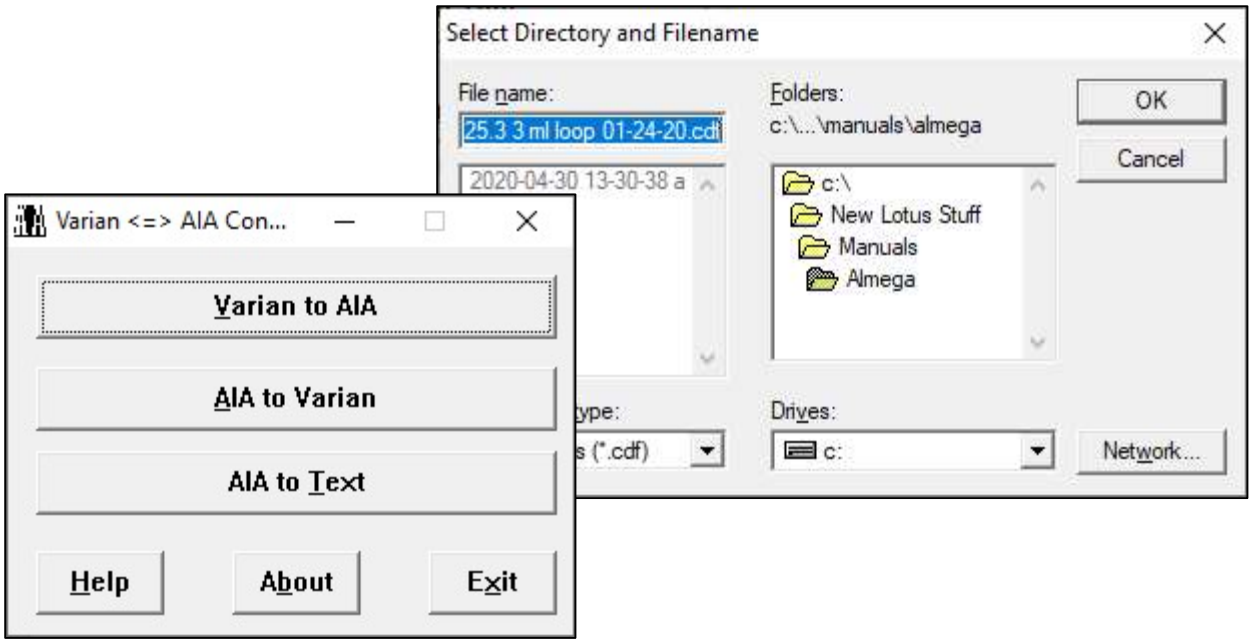
80. Maurer, Pfleger, Weber Library, 2016 Edition - includes novel designer drugs and a broad range of AIDS therapeutics, for a total of over 8,800 clinically relevant substances, including more than 3,500 metabolites.

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 XML-based data format.

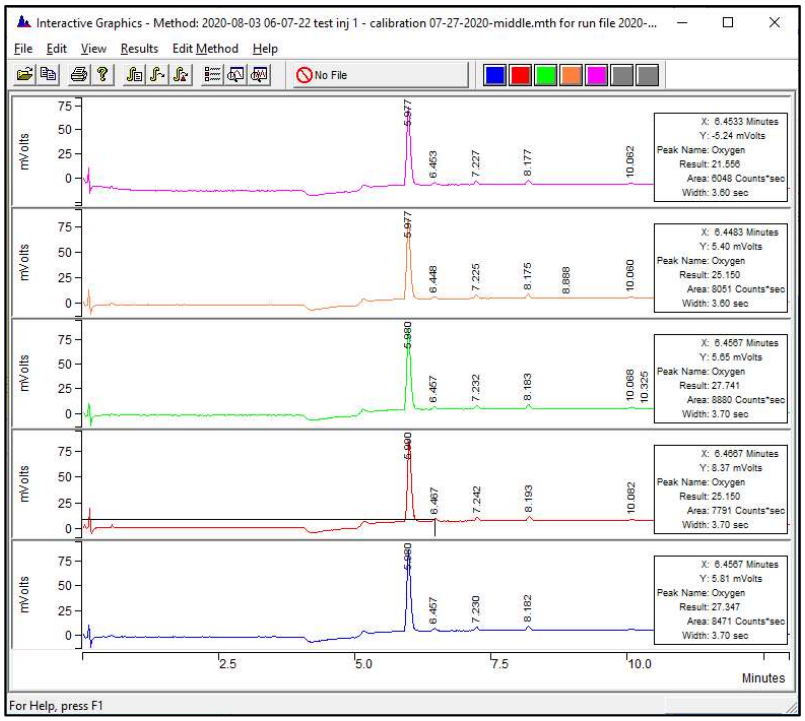


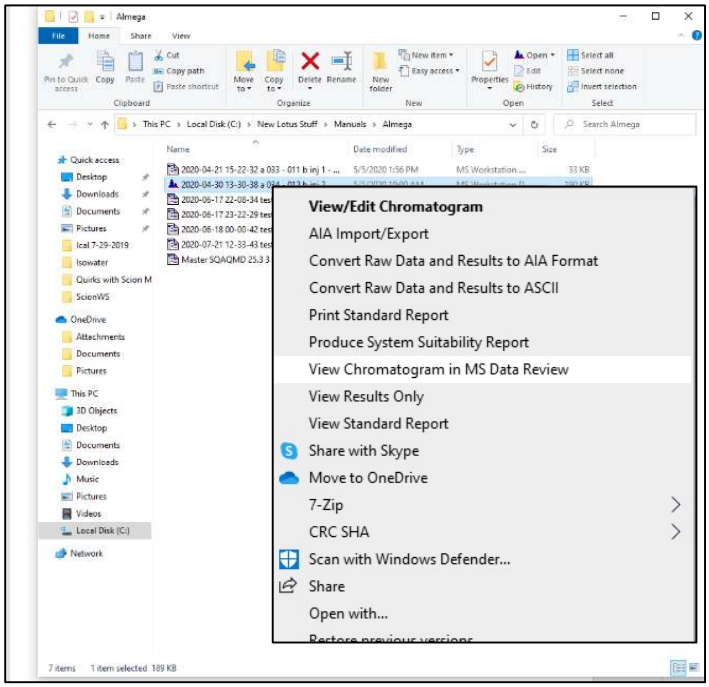
83. ASTM E1947 - 98(2014) Standard Specification for Analytical Data Interchange Protocol for Chromatographic Data. This app generates .CDF files that can be exported/imported in other brands of chromatography software compatible with AIA format.



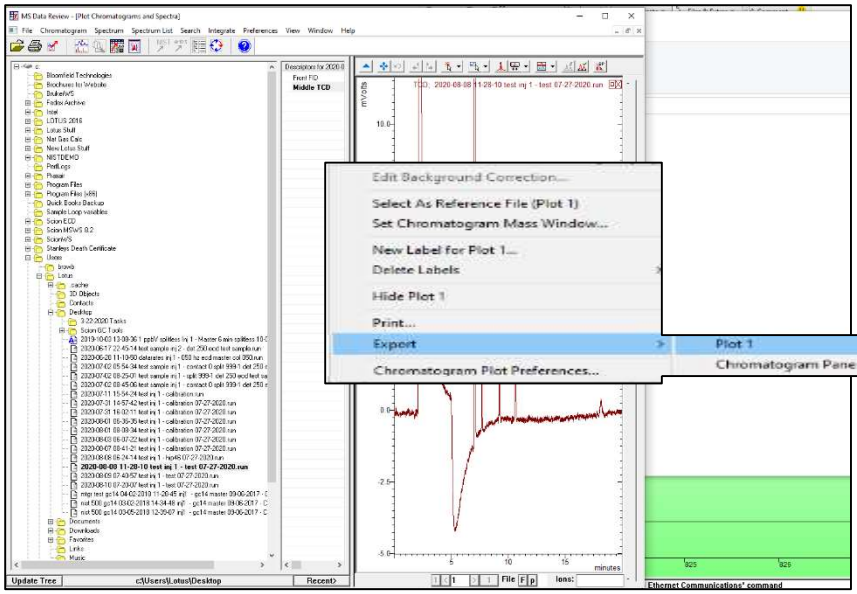
Hints with operations with GC detector .RUN data files

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

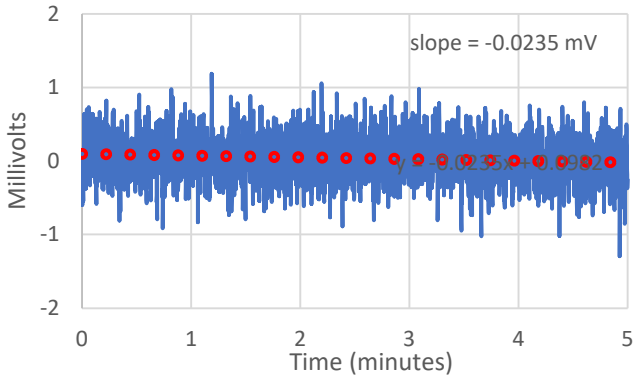




85. Insert .RUN data file into MS Data Review from Windows Explorer by right-clicking on desired data file.

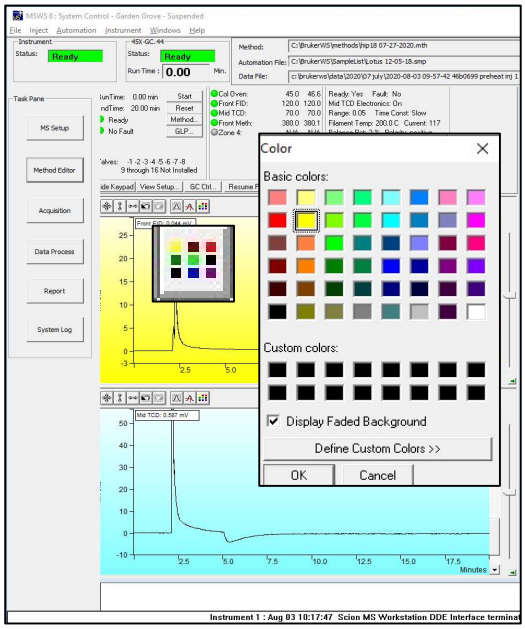


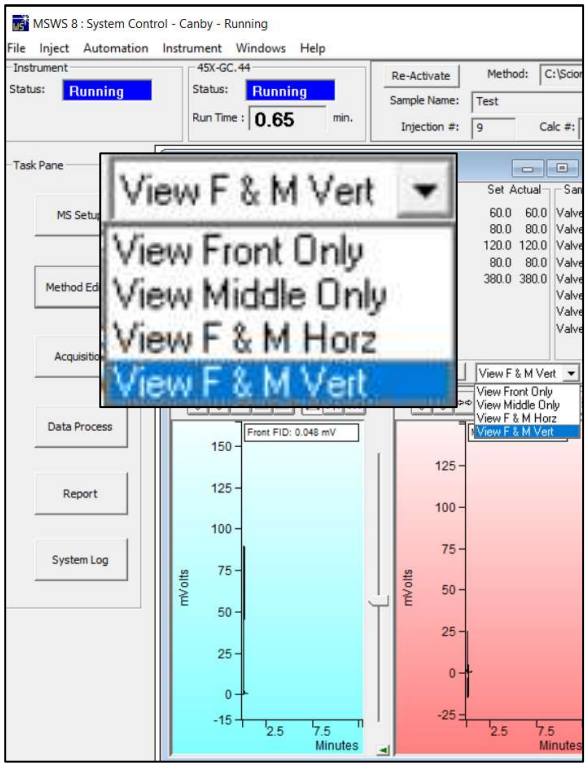
86. ASCII conversion of raw .RUN data points through MS Data Review - right-click on chromatogram.



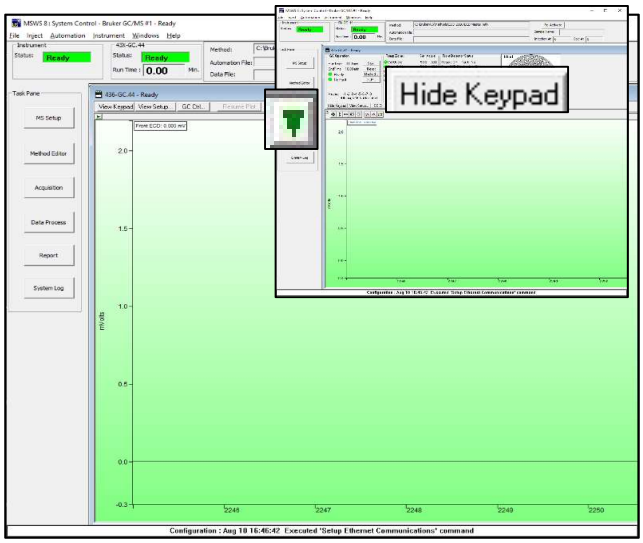
87. Detector signal drift computed through Trend Line of ASCII data points via Excel.

88. Change colors of displayed live chromatograms.

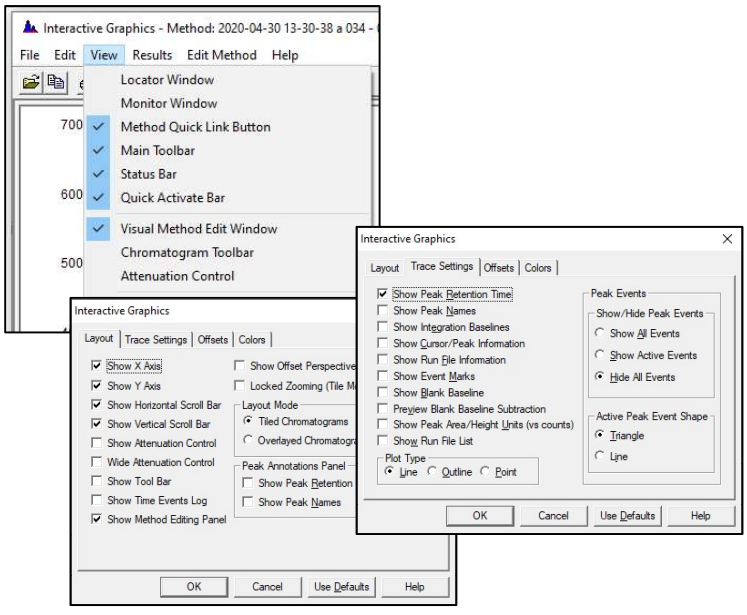




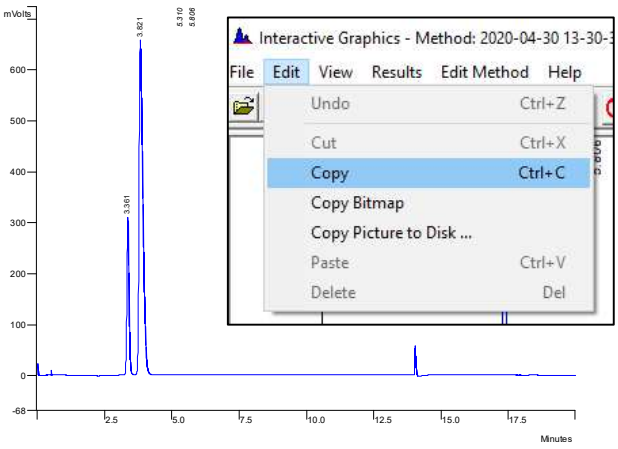
89. Display of live chromatograms in System Control – single, double or triple, and horizontal or vertical.



90. Set chromatogram display for full screen.

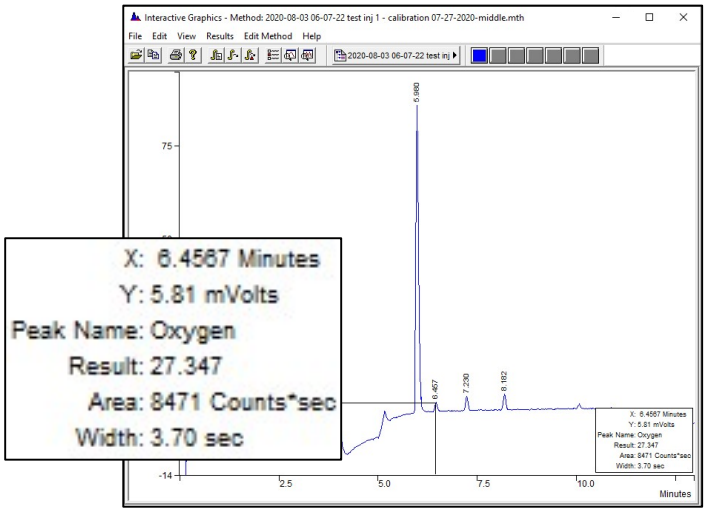


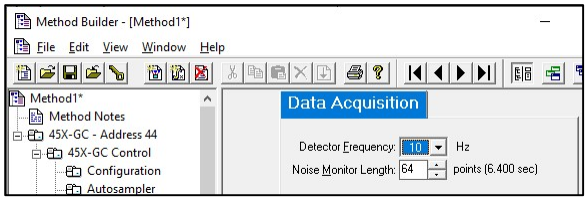
91. Add/remove extra notations on displayed chromatogram in Interactive Graphics.



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.

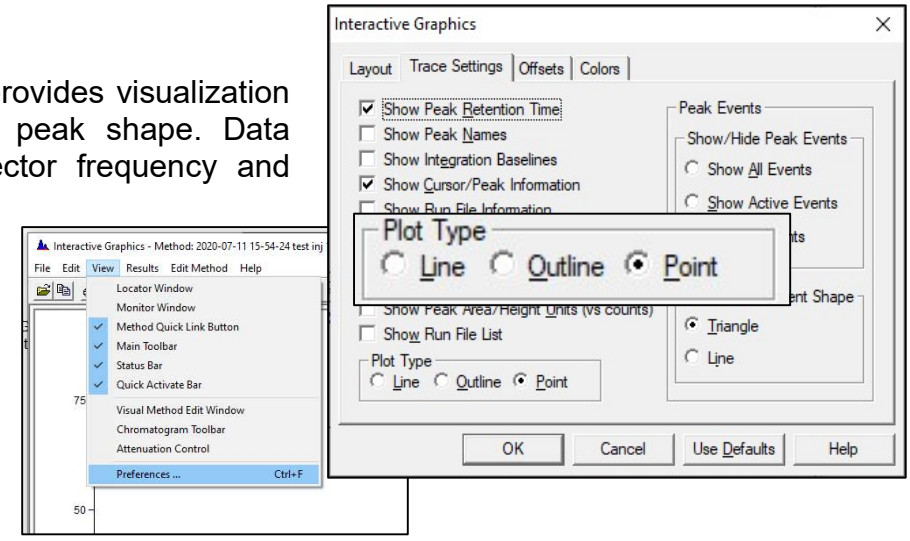
93. Interactive Graphic display of retention time to 0.0001 minutes.

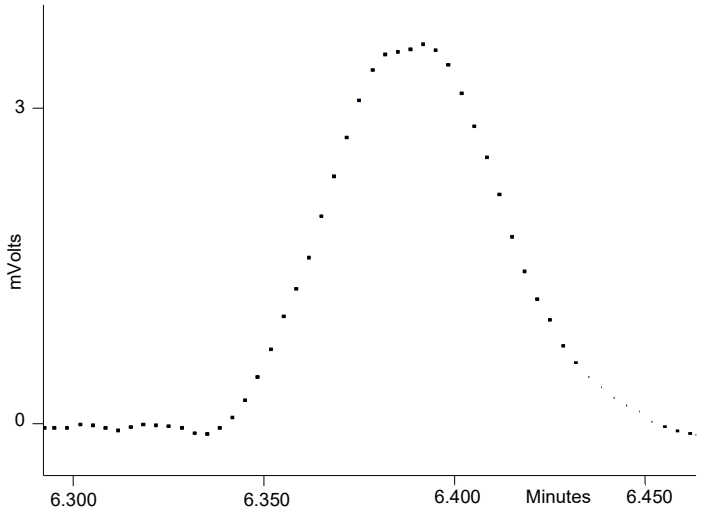




94. Detector frequency. This parameter impacts data collection with number of data points to define the peak and with noise level.

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



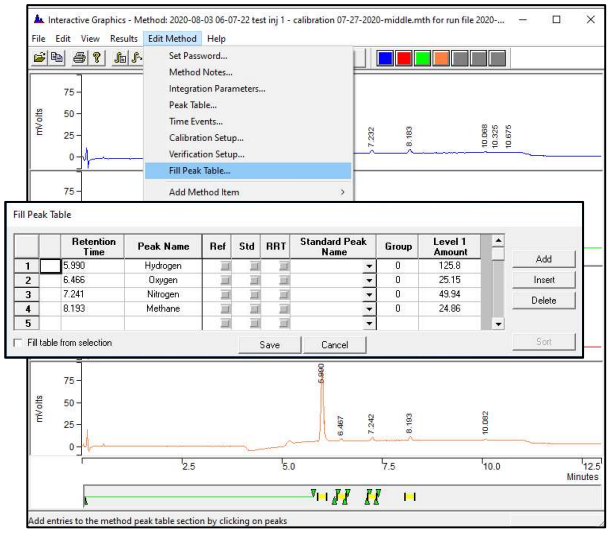


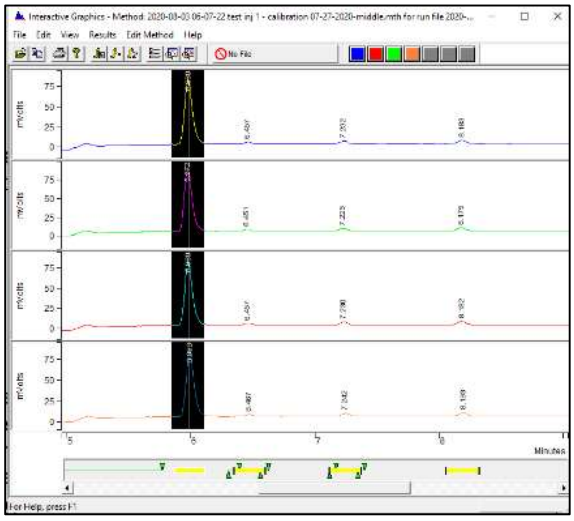
96. Single method possesses:
- Full set of parameters for control of GC
- Full set of parameters for computation of results
- Calibration data points
- Formatting for chromatograms and reports
- Baseline subtract data points

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.

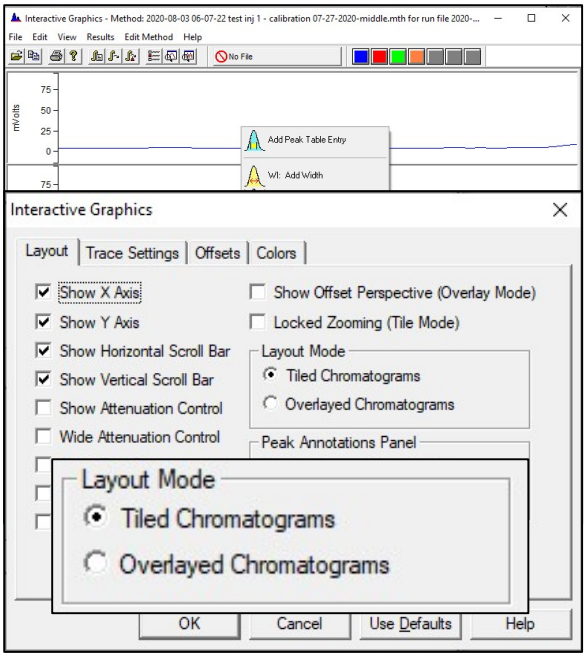


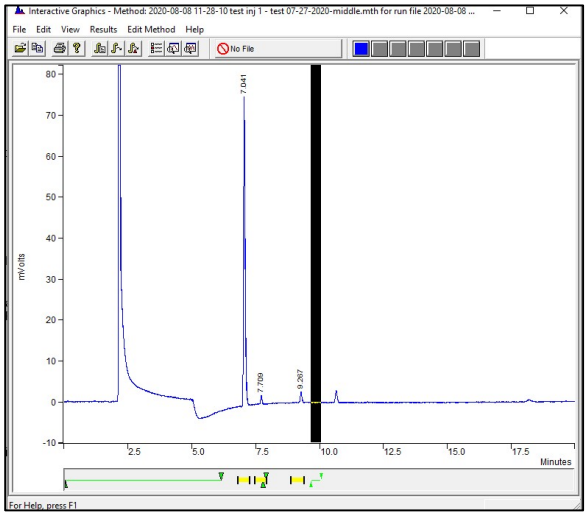


99. Graphically relocate retention times in Peak Table by right-clicking on yellow window under peak and move to adjust.

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.

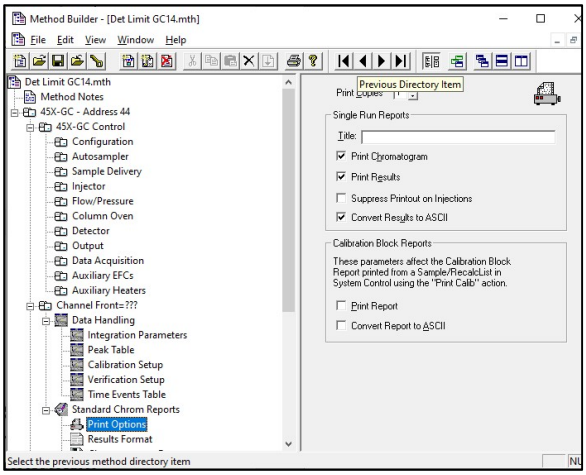


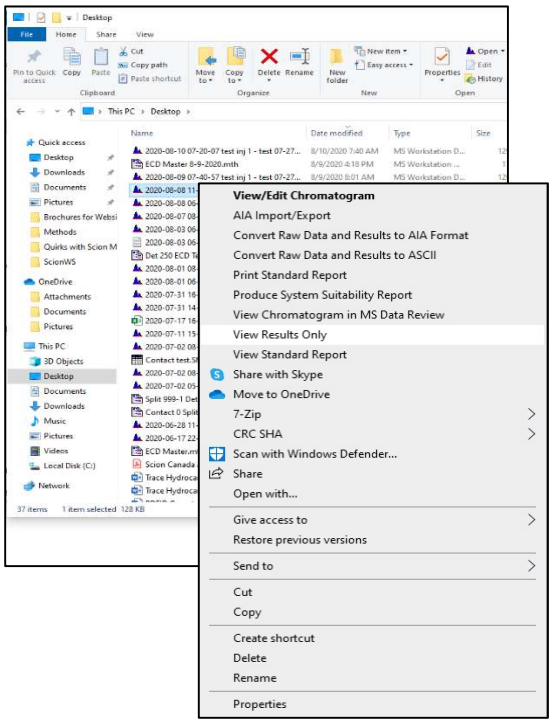


102. Graphically relocate time events with mouse.

103. Reporting of Results:

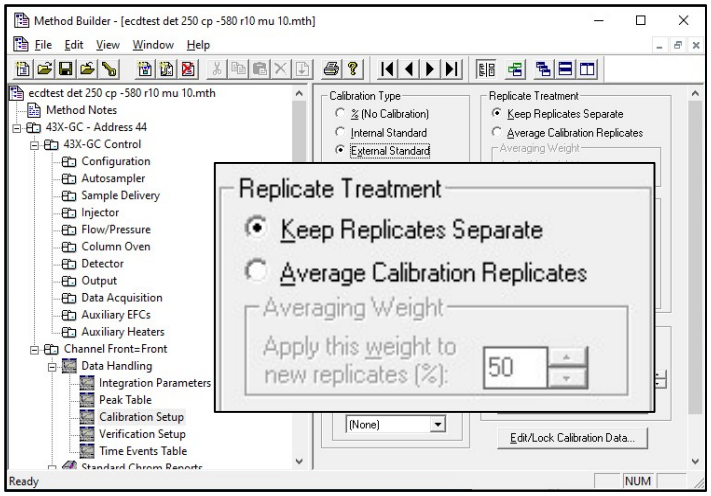
- Set up for automated printing at run end with Automated Printing enabled.





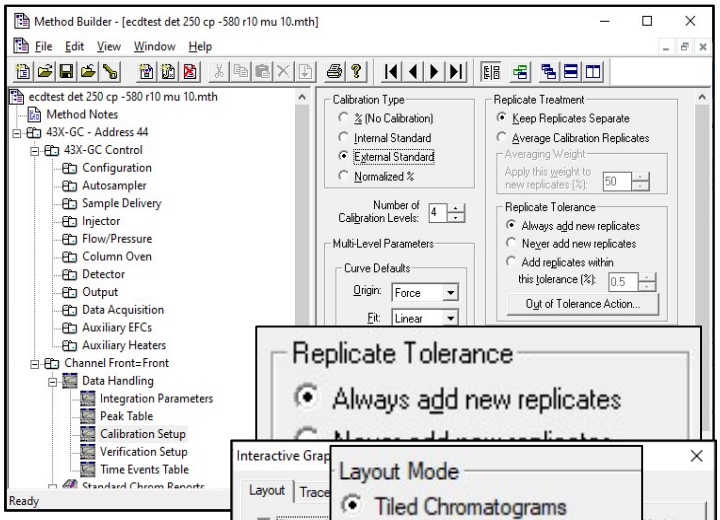
- Set up printing parameters in method.

- Access data files from Windows Explorer.

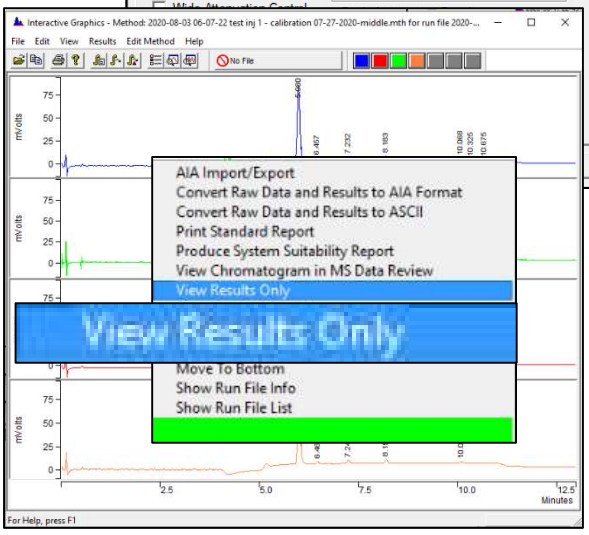


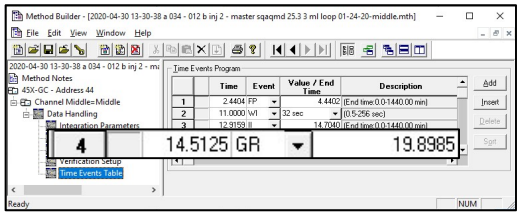
- Interactive Graphics allows up to seven chromatograms to be displayed. If chromatograms are displayed in “tile” mode, as specified in Interactive Graphics > View > Layout, then right-click with mouse in any of them offers its report to be displayed or printed.

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”.

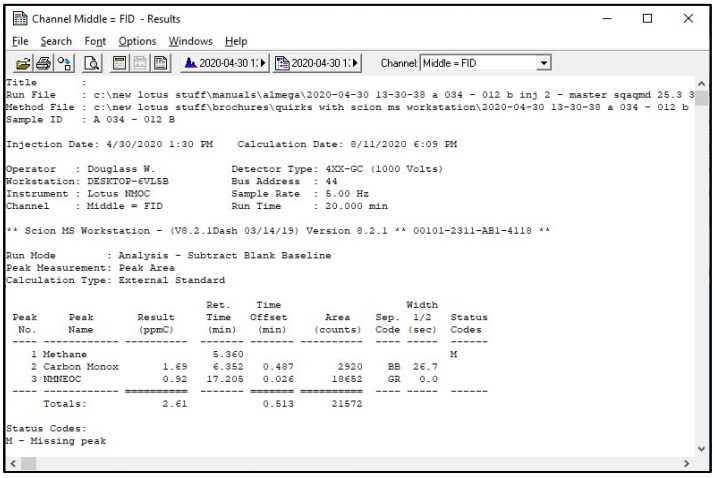


105. Replicate Tolerance in Method Builder - Preset value is set to add replicates within a tight tolerance of 0.5%. Better choice is either to widen the tolerance or “Always add new replicates”.

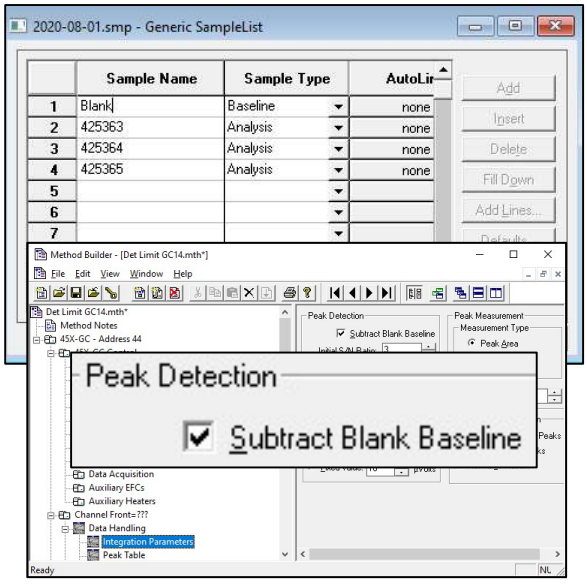




106. Baseline Subtraction - The baseline run is a reduced set of 257 to 512 data points across the chromatogram run time by a bunching process, is stored within the method used for its collection and is subsequently subtracted from sample runs prior to peak detection. Baseline Subtraction is activated 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".

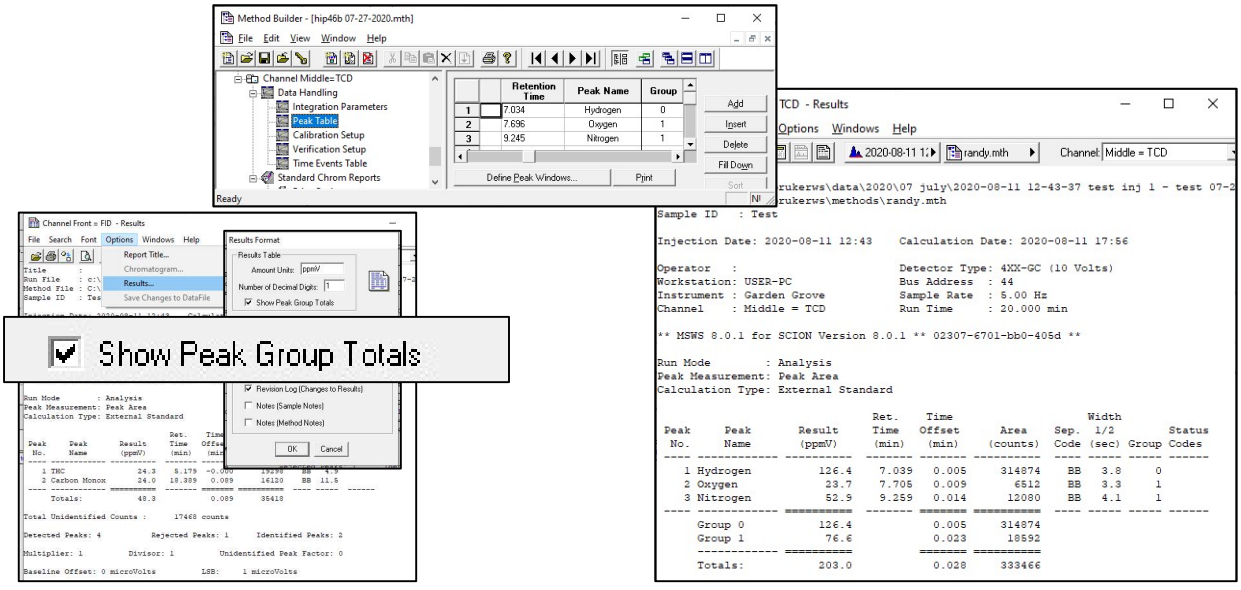


107. Grouping by time interval – detector response can be grouped over a user-selectable time interval. This process is often used for grouping non-methane hydrocarbons in EPA Method 25, and for summing up all hydrocarbons in natural gas for Hexane+. Assigned retention time for the group is the midpoint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

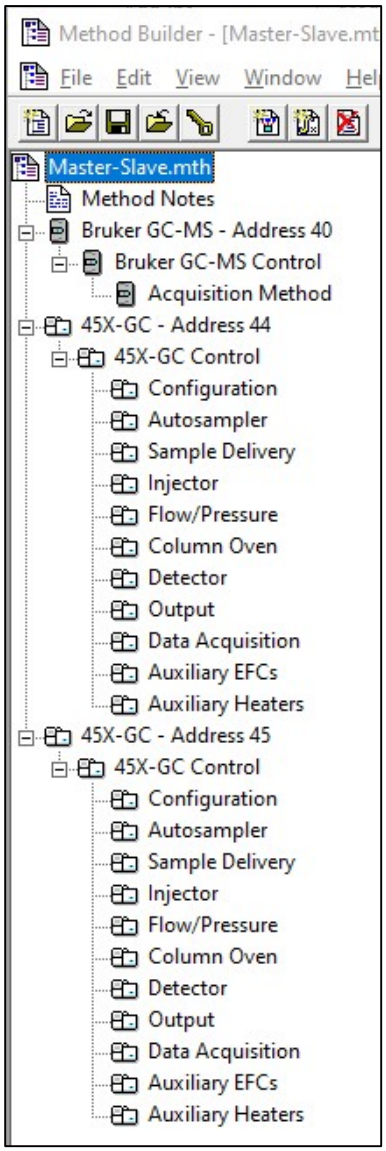


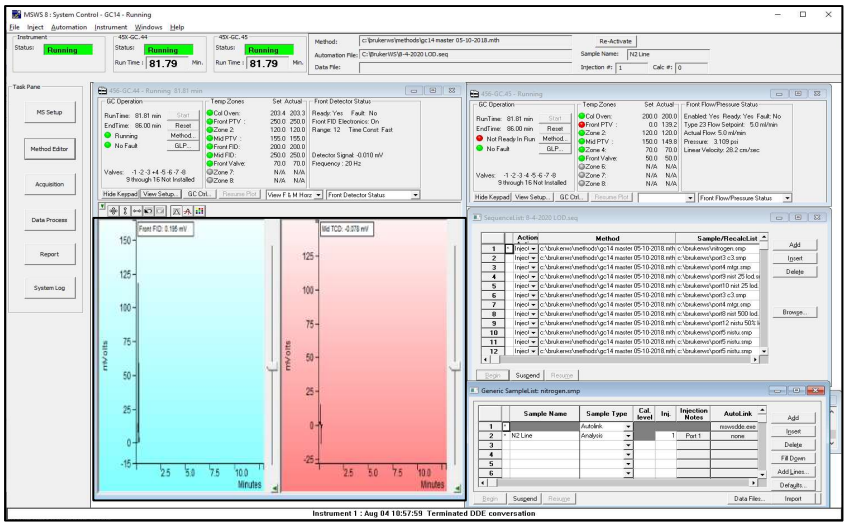
108. Grouping by peak label – After computations are perfomed for peak

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



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





chromatographs.

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