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

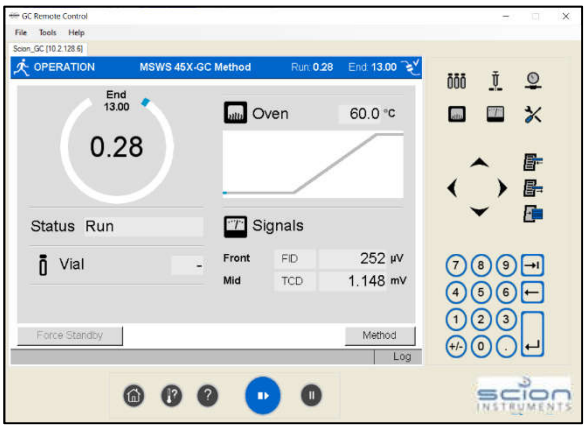
Routine operations with Scion MS Workstation are quite easy to set up parameters for data collection and report generation . The following is a discussion of hidden quirks that may not be obvious as to their usefulness. This discussion assumes that the operator is familiar with basic operations in MS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

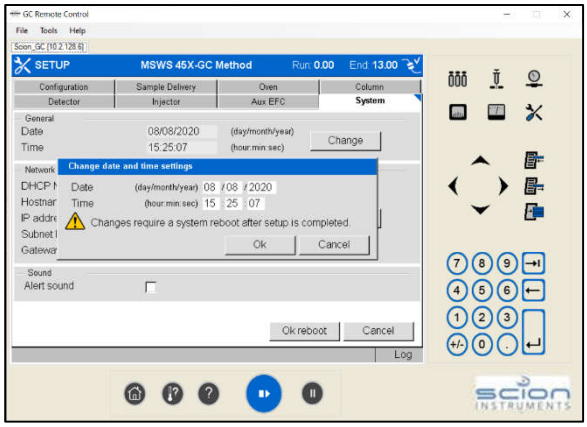
Operations Involving Control of Scion 436/456 Gas Chromatographs.

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.

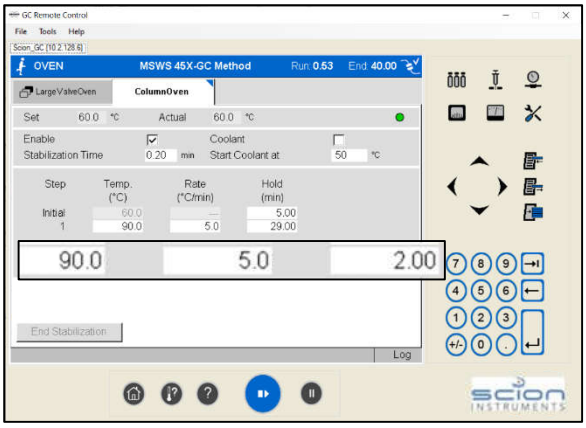
3. **GC Remote Control** - allows view of status of gas chromatograph from a remote computer, typically through Team Viewer or similar app. (C:\Program Files\Scion GC Tools\GC Remote Control). Access is through Taskbar icon:



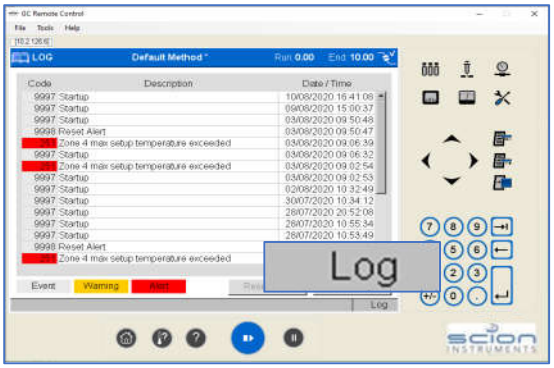


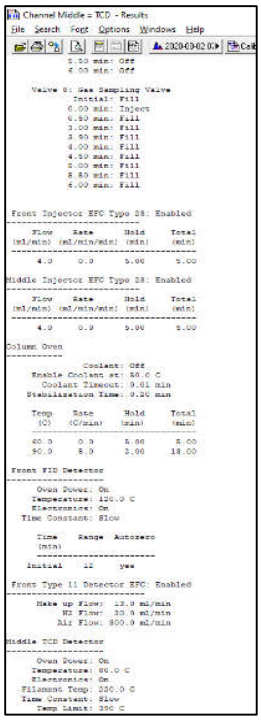
4. **Reboot gas chromatographs through GC Remote Control** by setting a minor change to System Time through Setup > System.

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

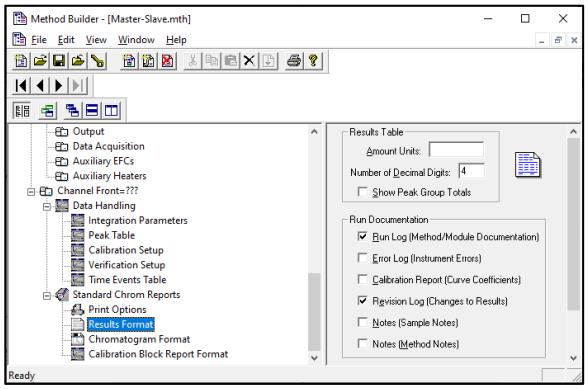


6. **Instrument Log** – lists activities for the instrument, including faults with time/date stamp. Historical logs are available at C:\ScionWS\MSLOG.



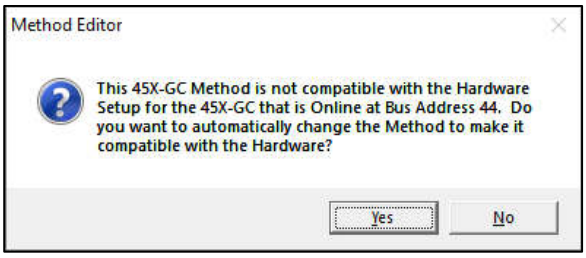


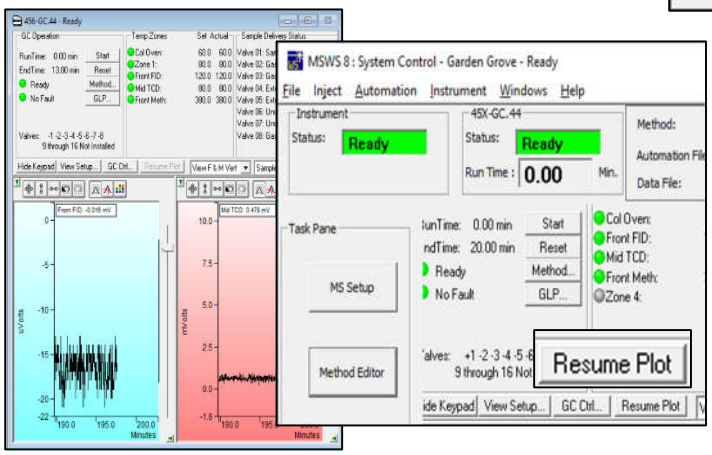
7. **Runlog** - documents all actual run conditions on GC in every .RUN file for full recovery at a later time, even changes made during the run.



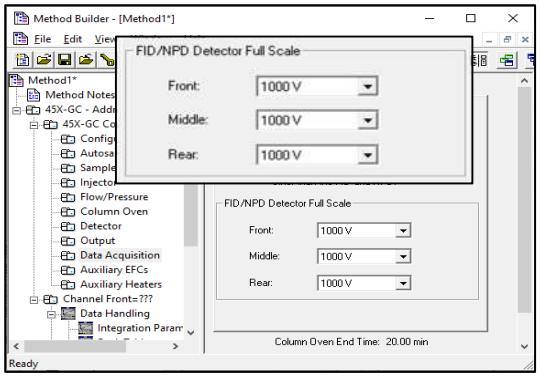
8. **Access any method** – even if it does not match current Setup.

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

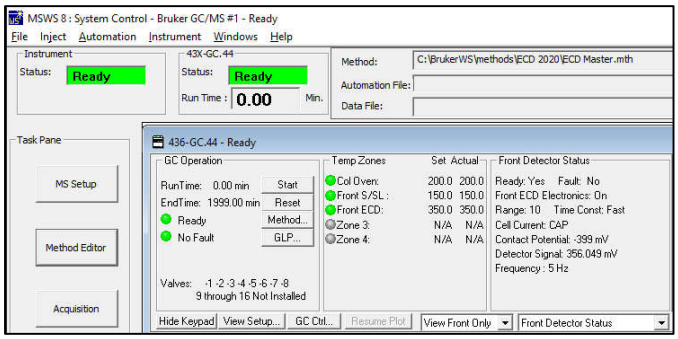




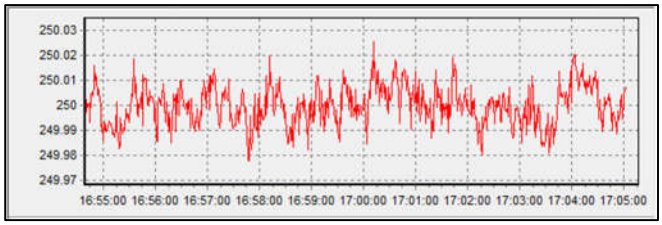
10. **Resume Plot** - permits visible display of active baseline drift and noise without starting a run.



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.

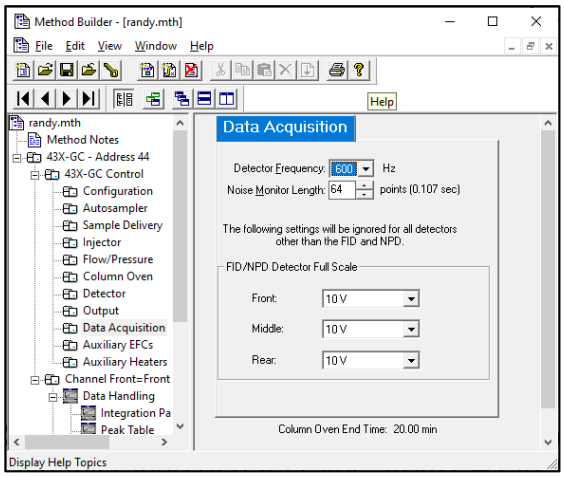


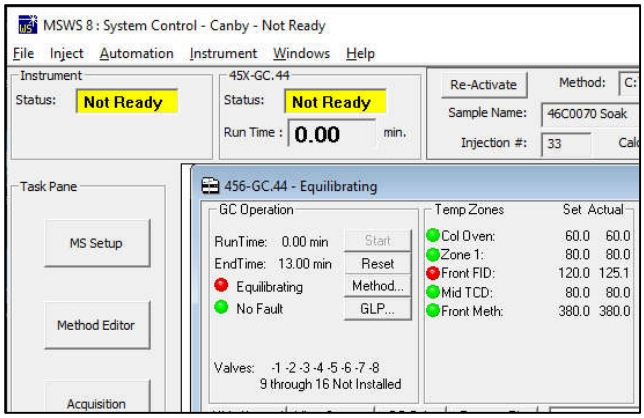
12. **Entry and display of temperature zones in 0.1 ºC increments**.



13. **Stability of temperature zones** - temperature variation over 10 minutes for Electron Capture Detector. Average is 250.015 ± 0.006 ºC.

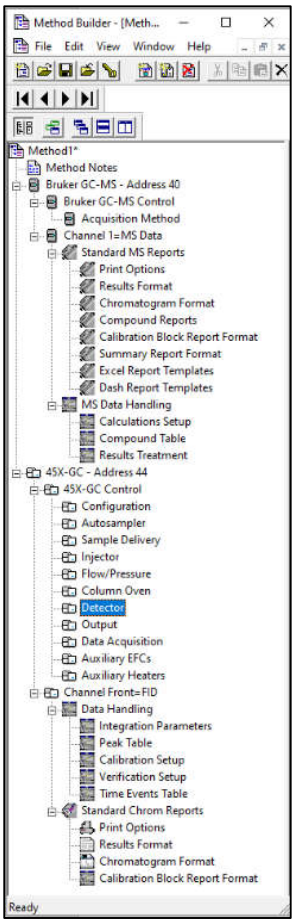
14. **Data Rates for GC Detectors** – All detectors, including Electron Capture Detector (ECD), have full range of data rates, from1 Hz to 600 Hz, in 12 steps.





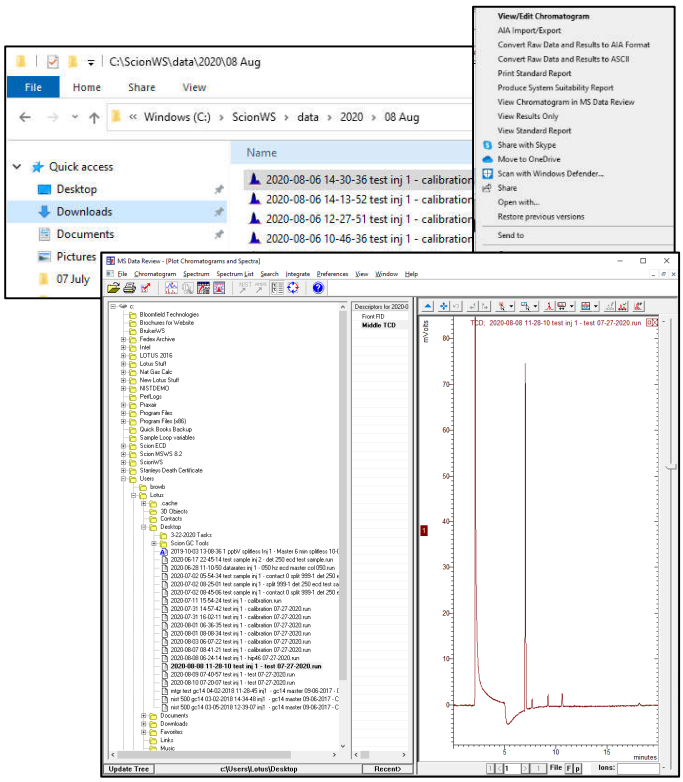
15. **Ready "Green"/Not Ready "Red" status lights.**

Common Hints for Both MS and GC Detector Operations

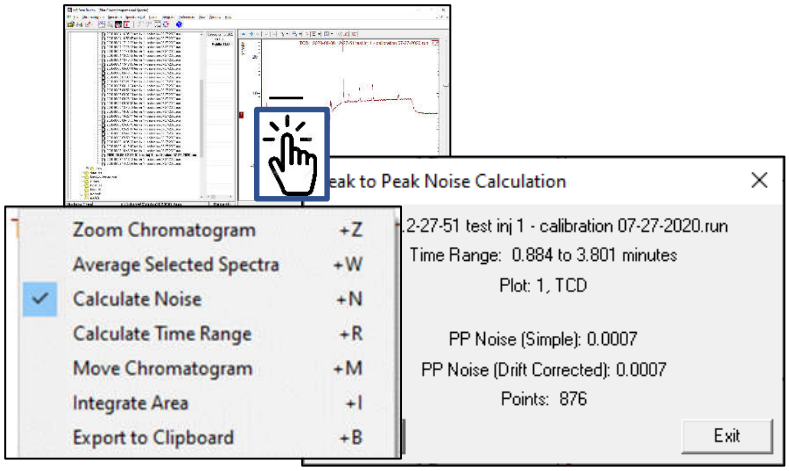


16. **Concurrent instrument control and data collection** for MS and GC with single Method.

17. **Concurrent data collection** for MS and GC with single SampleList.

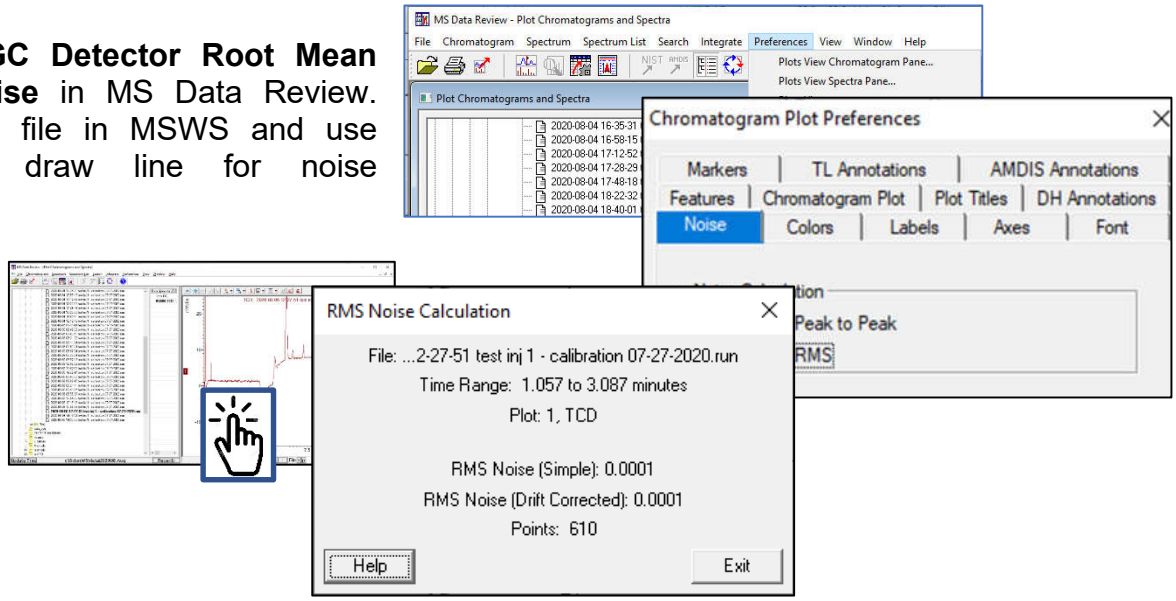


18. **GC chromatogram can be displayed in MS Data Review**, by right-clicking on .RUN file in Windows Explorer.

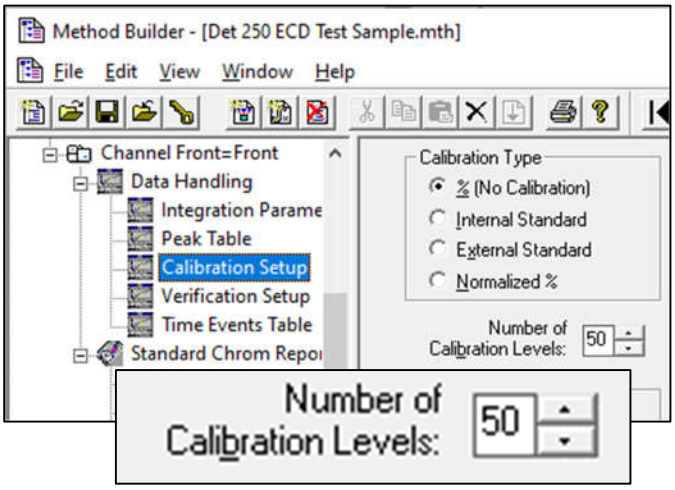


19. **Compute GC Detector Peak-to-Peak Noise in MS Data Review**. Use mouse to draw line for noise calculation.

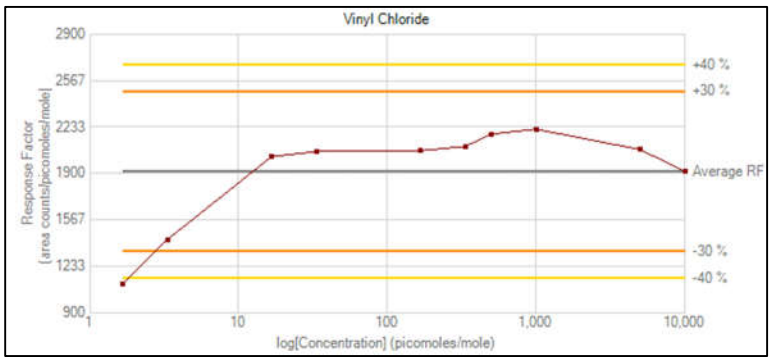
20. **Compute GC Detector Root Mean Square Noise** in MS Data Review. Open .RUN file in MSWS and use mouse to draw line for noise calculation.



21. **Up to 50 calibration levels**.

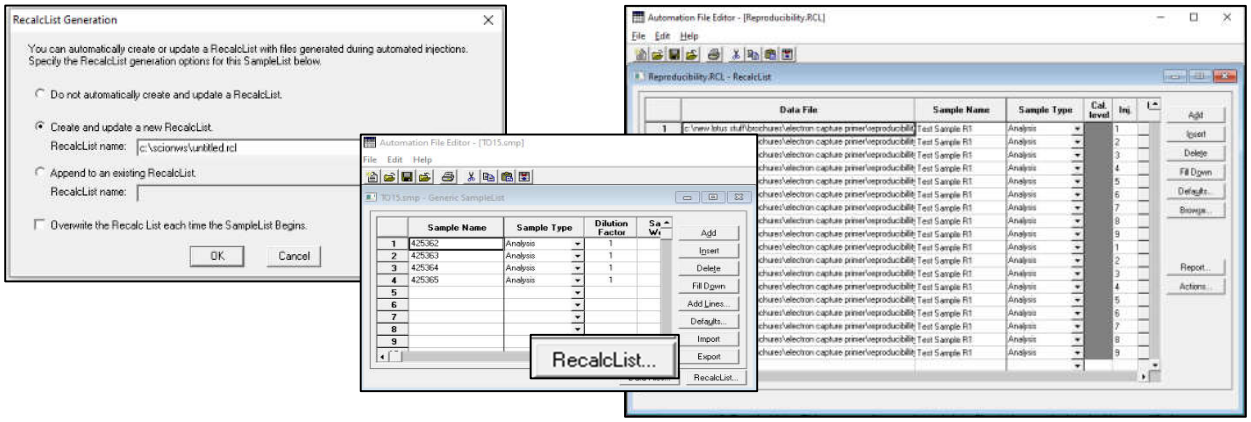


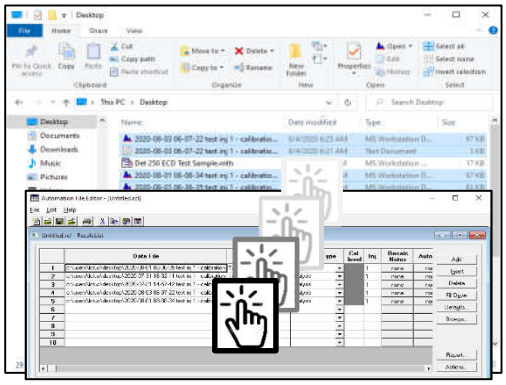
22. **Calibration plots of response factor versus log[concentration]** - from Lotus Consulting. Conventional plots of detector response versus concentration does not provide good visibility of linearity over wide concentration ranges. Results displayed as a semilog plots allows easy validation of linearity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



23. **Response factors computed as** $\frac{\textbf{Area}}{\textbf{\textit{Concnetration}}}$, 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.

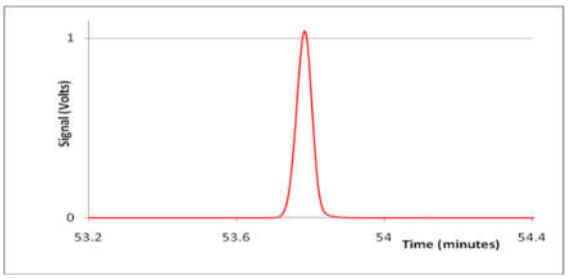


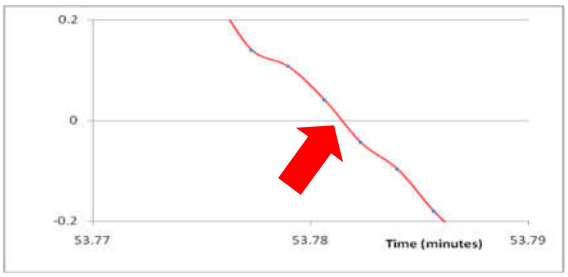


25. **Drag/drop data files into Recalc list.**

[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.





27. **Retention Time reported in 0.001 minute increments.**

28. **Peak Width at ½ height reported in seconds.**

Channel Front = FID - Results

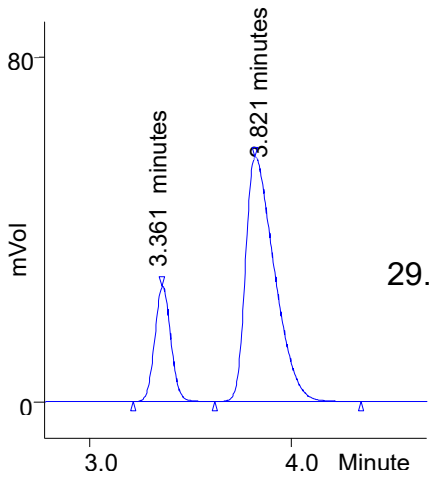
File Search Font Options Windows Help

2020-04-30 1 | Master SQAQ | Channel: Front = FID

```
Title       :
Run File    : c:\new lotus stuff\manuals\almega\2020-04-30 13-30-38 a 034 - 012
Method File : C:\BrukerWS\methods\Master SQAQMD 25.3 3 ml Loop 01-24-20.mth_TCD_
Sample ID   : A 034 - 012 B

Injection Date: 4/30/2020 1:30 PM    Calculation Date: 5/4/2020 12:19 PM

Operator    : Douglass W.            Detector Type: 4XX-GC (1000 Volts)
Workstation: DESKTOP-6VL5B           Bus Address  : 44
Instrument : Lotus NMOC              Sample Rate  : 5.00 Hz
Channel     : Front = FID            Run Time     : 20.000 min

** Scion MS Workstation - (V8.2.1Dash 03/14/19) Version 8.2.1 ** 00101-2311-AB1-

Run Mode         : Analysis
Peak Measurement: Peak Area
Calculation Type: External Standard
```

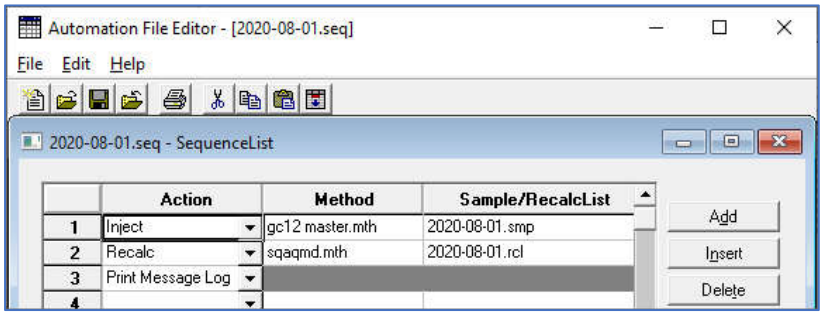
Peak No.	Peak Name	Result (ppmC)	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	Air/CO	0.0000	2.539	0.026	2205	PB	2.5	
2	Carbon Dioxi	500.2108	3.745	0.305	4597272	BB	16.3	
3	Ethane		7.376					M
	Totals:	500.2108		0.331	4599477			

```
Status Codes:
M - Missing peak
```



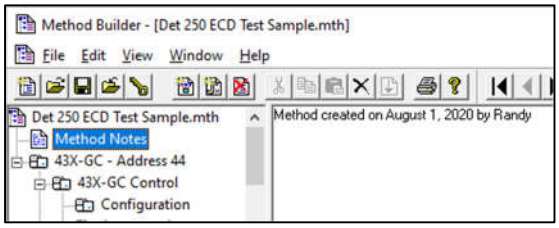
29. **Start and end points for peak integration** are always on the chromatogram tracing.

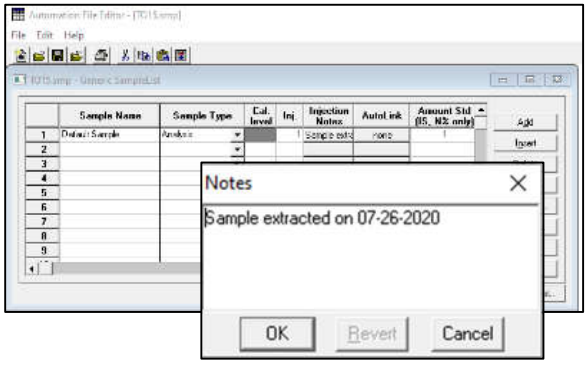
30. **Sequence List** – This screen permits multiple actions related to using a series of methods with multiple SampleLists or RecalcLists. The related MessageLog can be printed to provide documentation of actions.



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

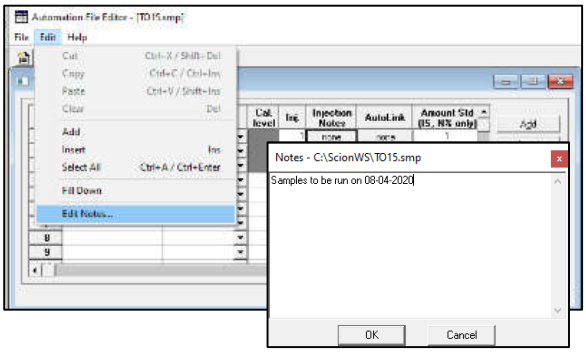
- **Method Notes**.

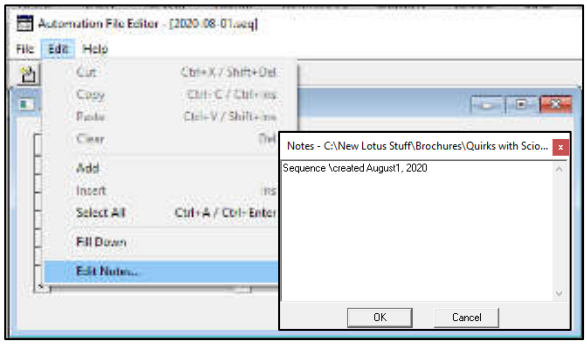




- **Injection Notes**.

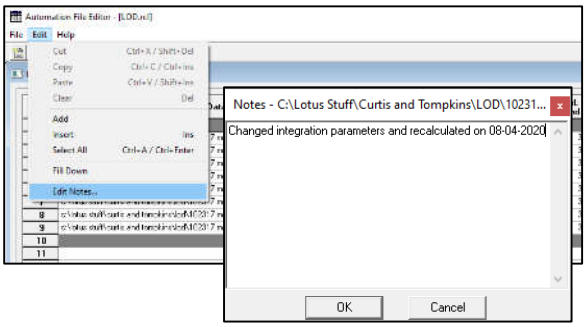
- **Sample List Notes**.



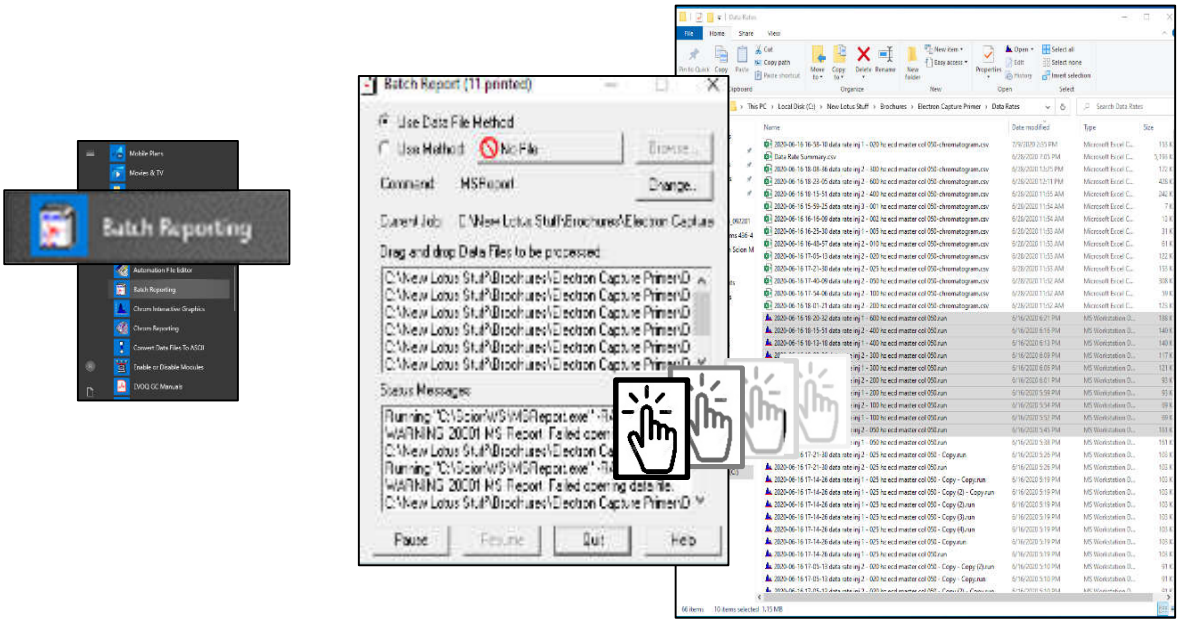


- **Sequence List Notes**.

- **Recalc List Notes**.

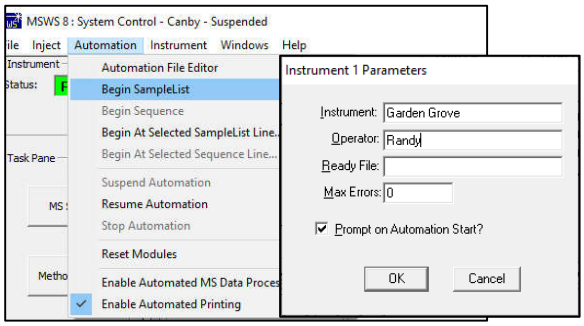


32. **Batch Processing** - icon accessible at Start > MS Workstation > Batch Reporting. Easy and quick approach to reprocess lots of similar data files by highlighting desired data files in Windows Explorer and drag-drop into window.



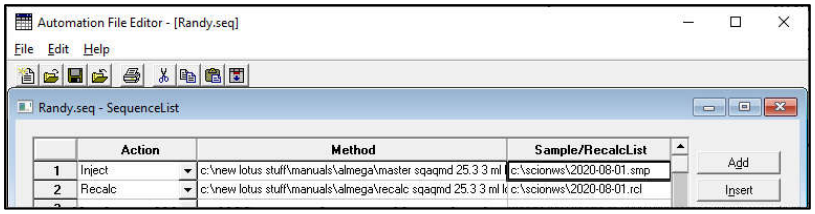
33. **Sample injection time/date and sample name are locked** at time of data collection and cannot be changed postrun.

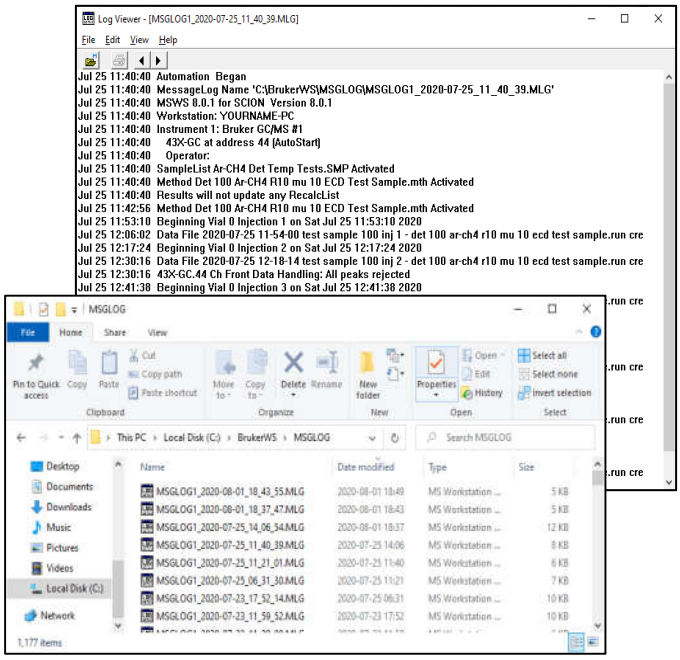
Title :
Run File : c:\users\lotus\desktop\2020-07-31 14-57-42 test inj 1 - calibration 07-27-2020.run
Method File : C:\ScionWS\methods\Calibration 07-27-2020.mth
Sample ID : Test
Injection Date: 7/31/2020 2:57 PM Calculation Date: 7/31/2020 3:10 PM
Operator : Detector Type: 4XX-GC (10 Volts)
Workstation: Windows Bus Address : 44
Instrument : Canby Sample Rate : 1.00 Hz
Channel : Middle = TCD Run Time : 13.000 min



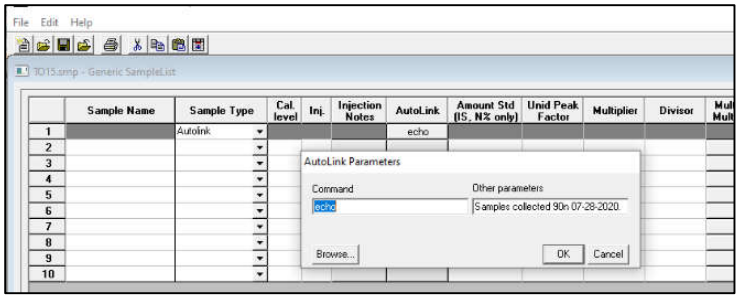
34. **Name of Operator can be entered** when a SampleList of Sequence is initiated and cannot be changed postrun.

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.





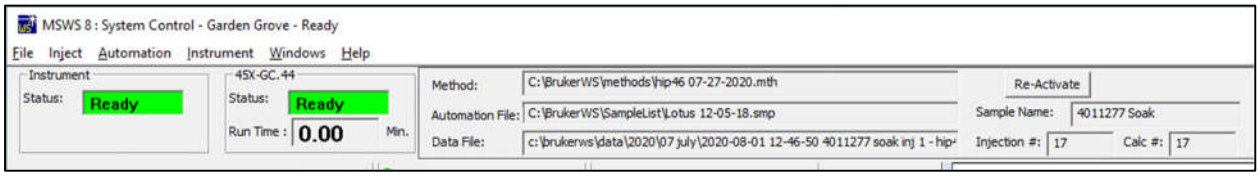
36. **MessageLog** lists all system control activities, documented with time/date of injection, sample labeling, data file label and location, and errors. These logs are available for recall later.



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:

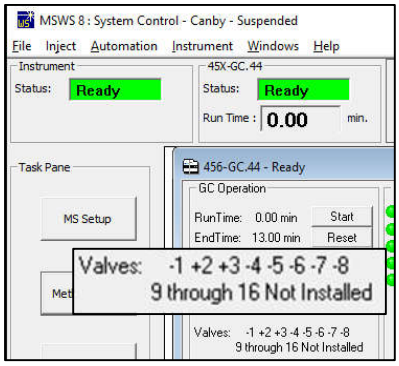
command-line: echo
other-parameters: <descriptive text to be "echoed" in the Message Log>

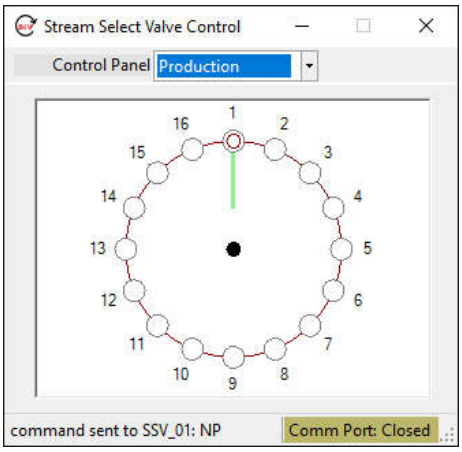
38. **Header block in System Control**:



- 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

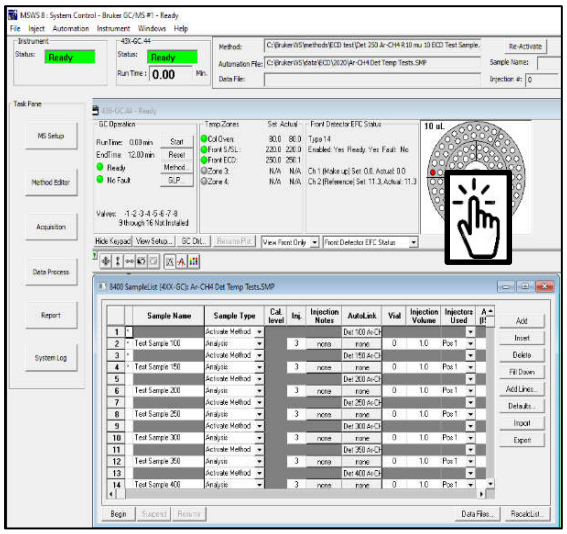
39. **Live display of all valve activities** on System Control screen.

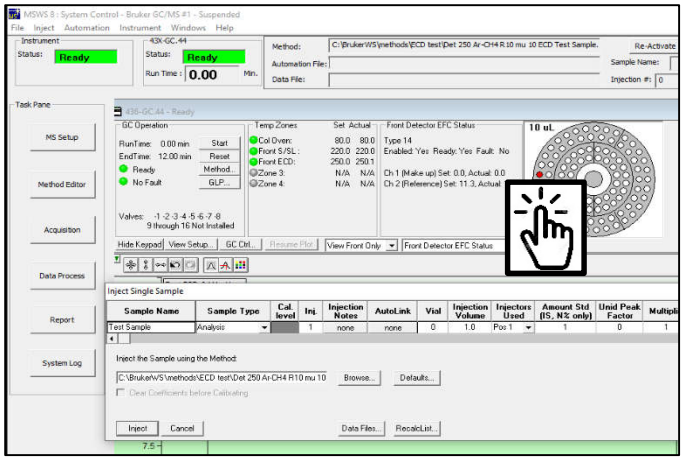




40. **Stream Selector Valve Controller** – from Lotus Consulting. Control of sampling position for loading gas samples is set through SampleList. Access is with Task Bar icon:

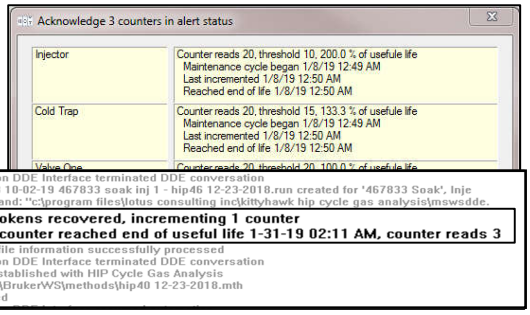
41. **Direct access to SampleList from 8400 display** by clicking on center of carousel.

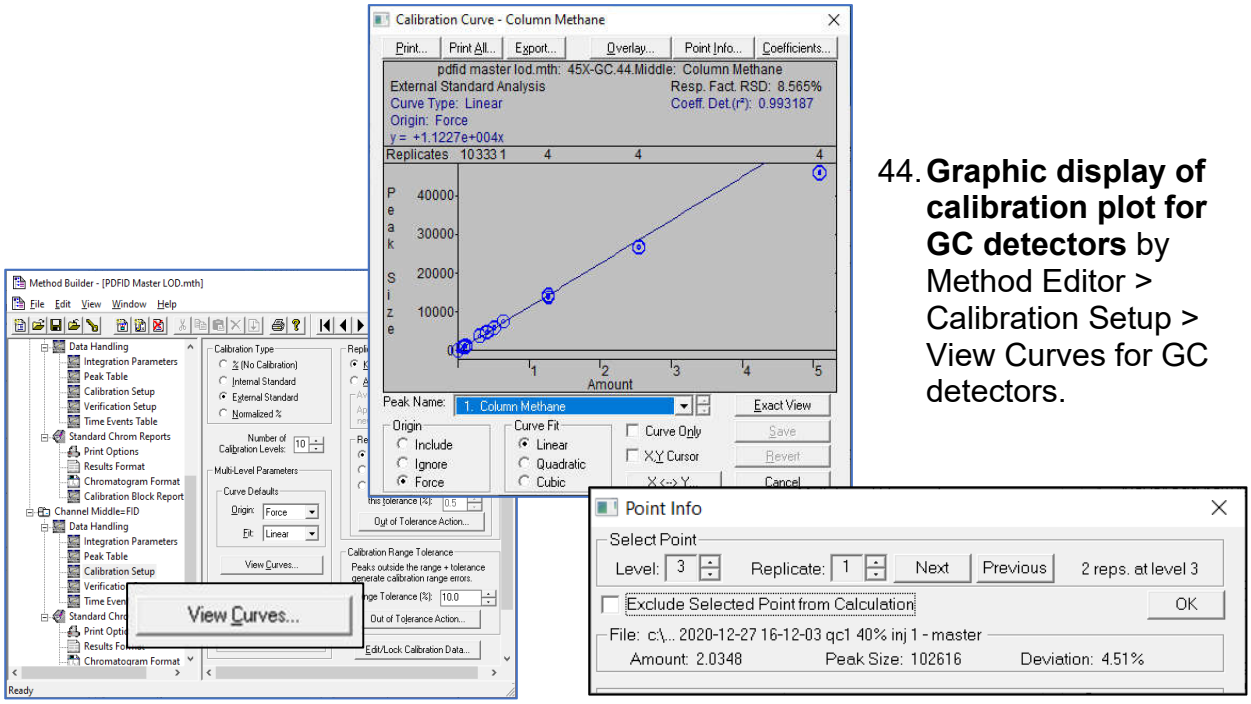




42. **Direct access to Inject Single Sample** by clicking on vial position in 8400 display.

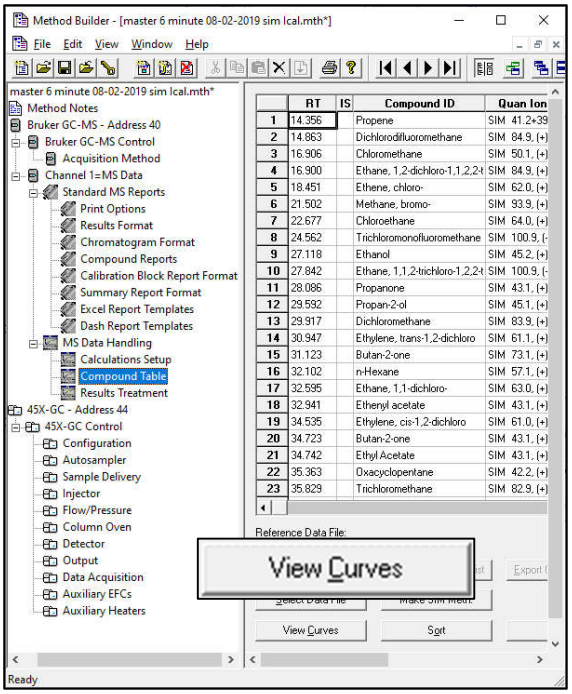
43. **Run Counter** - available from Lotus Consulting. It is designed to complement MS Workstation, adding the ability to track the maintenance lifetime of one or more components. Run Counters increments a cycle counter for designated components each sample run, providing a message log entry and on-screen alert when the configured lifetime has been reached. Additionally, counter details can be reviewed including percentage of useful lifetime and predicted end-of-life

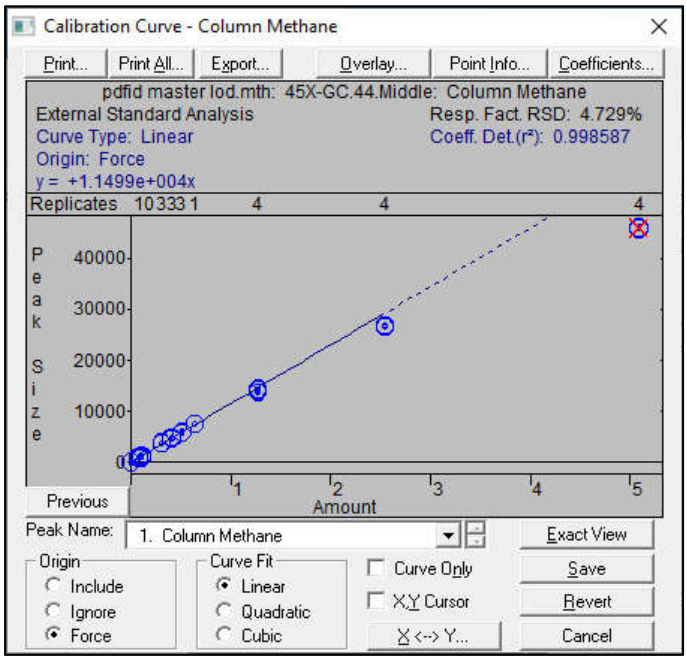




44. **Graphic display of calibration plot for GC detectors** by Method Editor > Calibration Setup > View Curves for GC detectors.

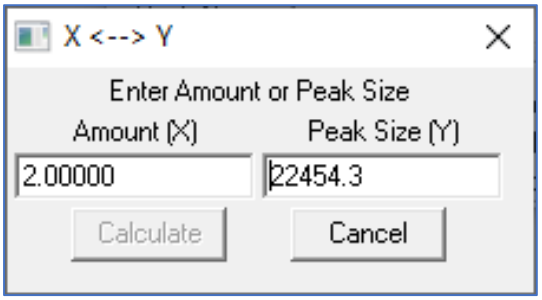
45. **Graphic display of calibration plot for MS data** through Method Editor > Channel 1=MS Data > MS Data Handling > Compound Table > View Curves.

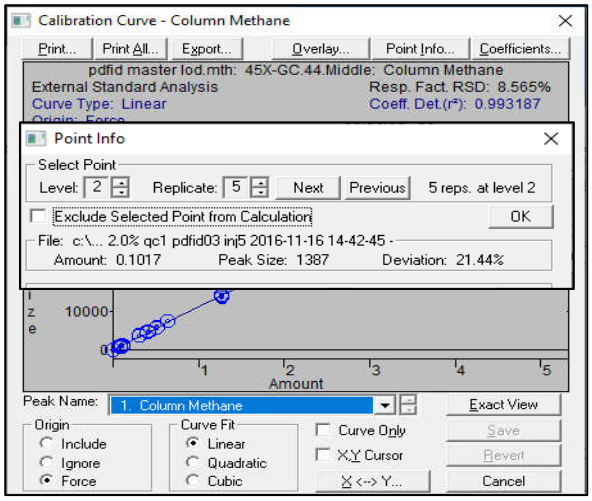




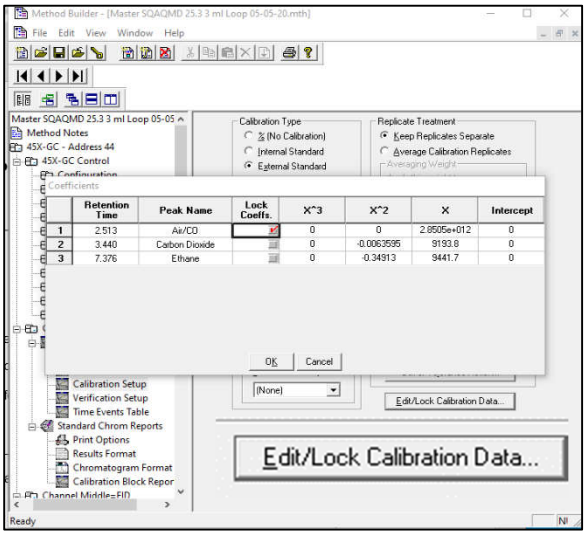
46. **Edit out obviously invalid data points** in calibration plot by right clicking on specific points. Excluded points are indicated in red.

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





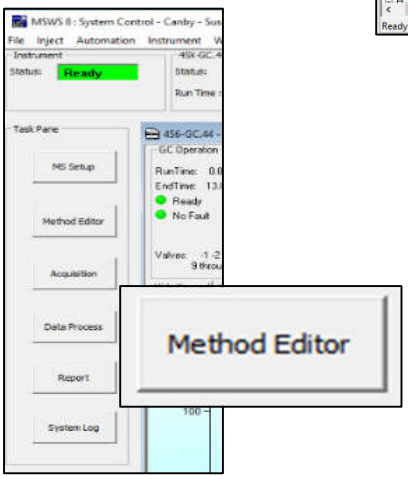
48. **Source of calibration data point** with Calibration Curve > Point Info.



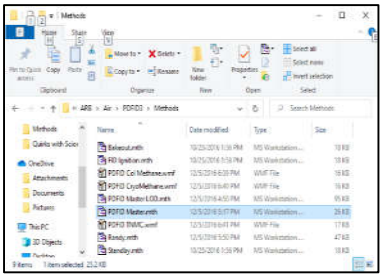
49. **Edit/Lock Coefficients** - When multiple standards with differing analytes are used, coefficients need to be locked after they are calibrated so that the next mixture does not alter them. In addition, coefficients from related analytes can be manually entered. For example, the response values for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

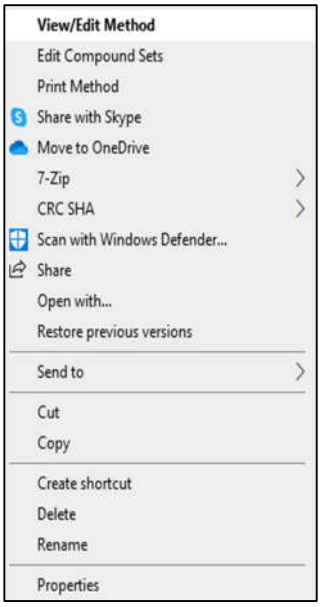
50. **Approaches to opening method:**

- **Task Pane**

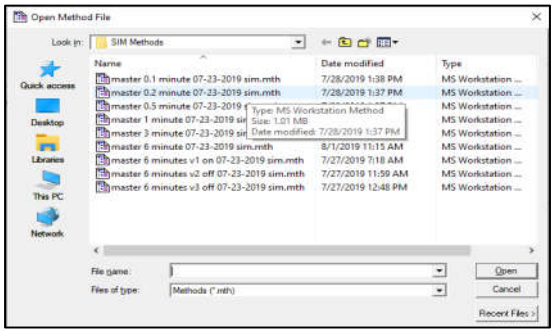


- **Windows Explorer**

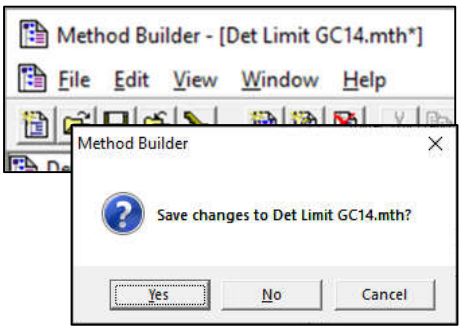


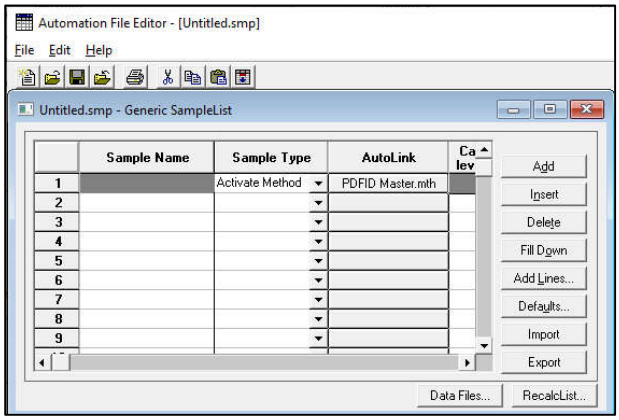


- **Method Builder icon on Task Bar**.



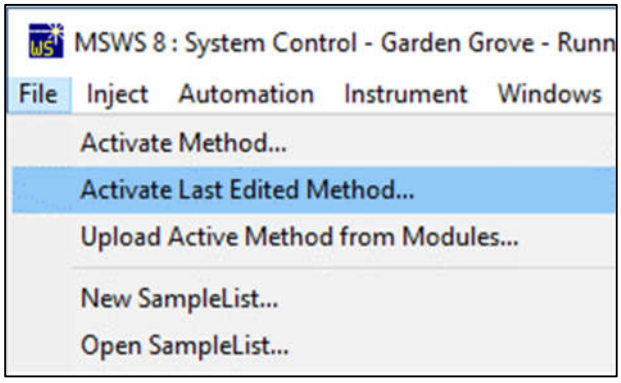
51. **Indication that Method file has not been saved** with an asterisk after the file name in the header. If not manually saved, a prompt will appear for saving.

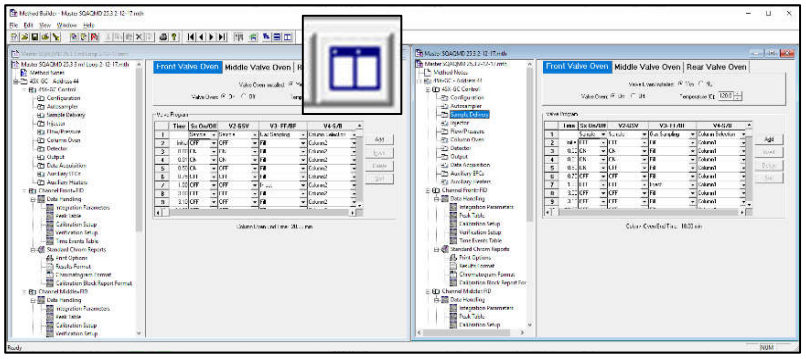




52. **Activate method through SampleList.**

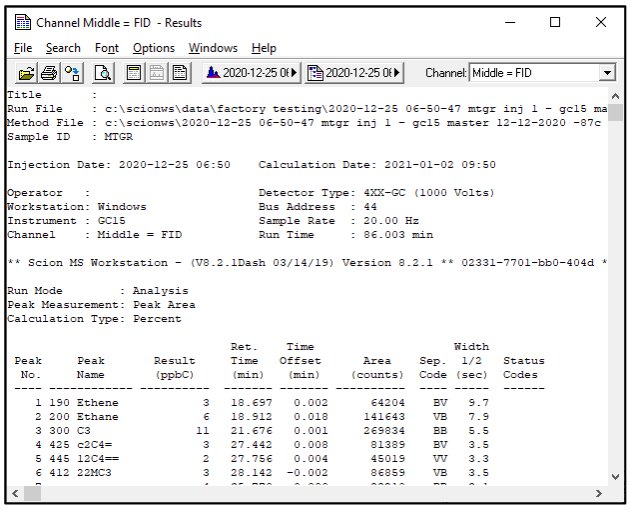
53. **Activate “Last Edited” method.**





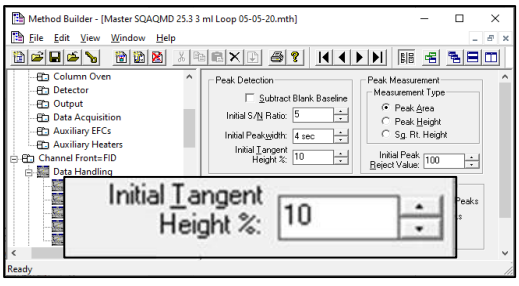
54. **View multiple methods side-by-side** on one screen.

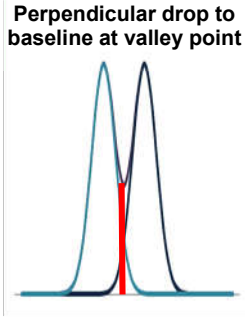
55. **Sep Codes** - indicated in reports.

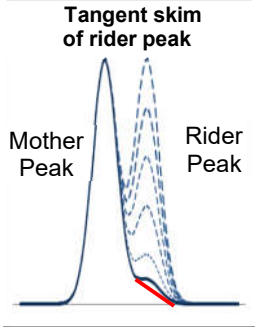


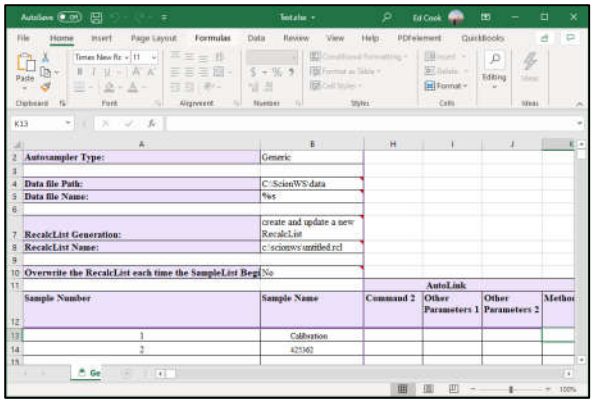
SepCodes	Peak Onset	Peak End
BB	Baseline	Baseline
BV	Baseline	Valley
VV	Valley	Valley
VB	Valley	Baseline
TF	Tangent Fused	
TS	Tangent Skim	
PB	Perpendicular Drop	Baseline
BP	Baseline	Perpendicular Drop
PB	Perpendicular Drop	Baseline
VP	Valley	Perpendicular Drop
PV	Perpendicular Drop	Valley
GR	Grouped Peaks by Time	
HF	Horizontal Baseline Forward	
HB	Horizontal Baseline 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”.

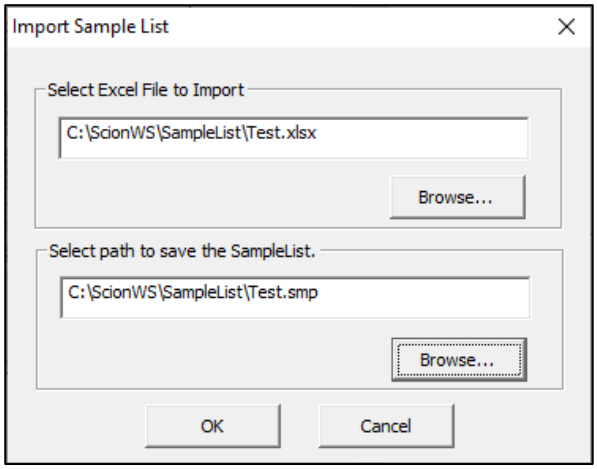






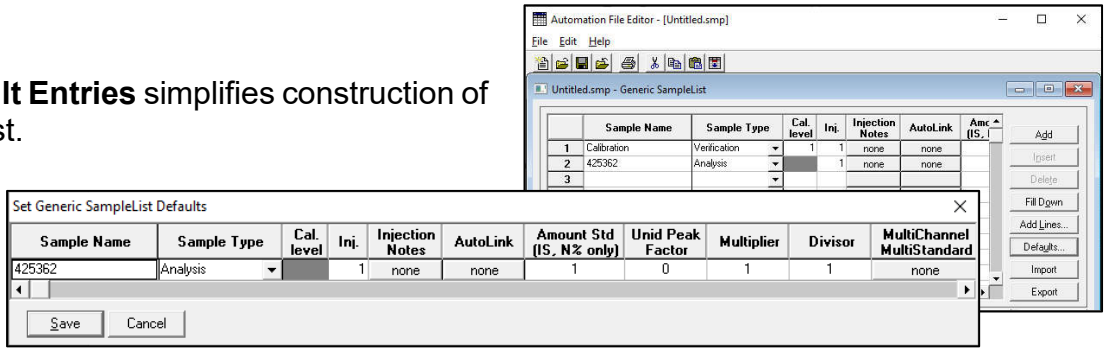


57. **Export SampleList to Excel**



58. **Import SampleList from Excel**.

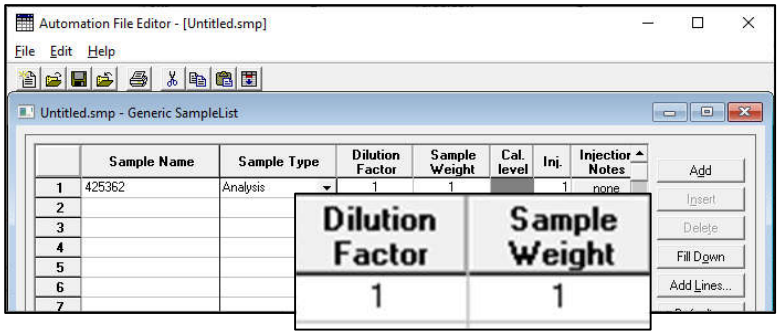
59. **Set Default Entries** simplifies construction of SampleList.

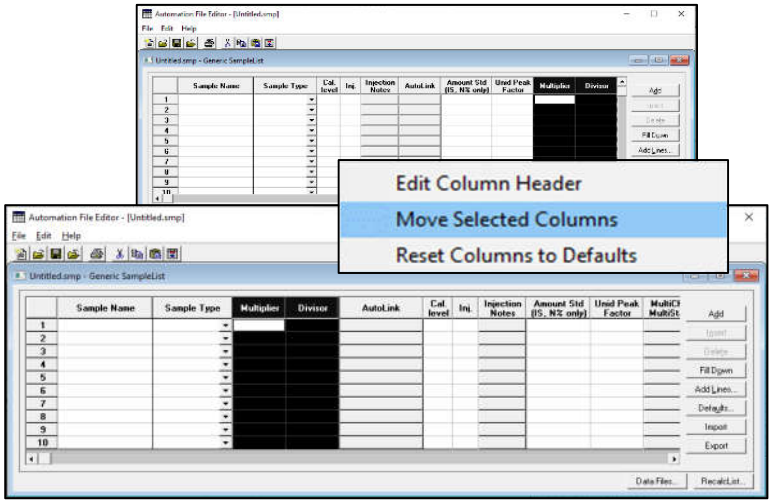


60. **Copy/paste lines in SampleList with “Shift – c” and then “Shift - v”.**

61. **Copy/paste lines in RecalcList with “Shift – c” and then “Shift - v**”.

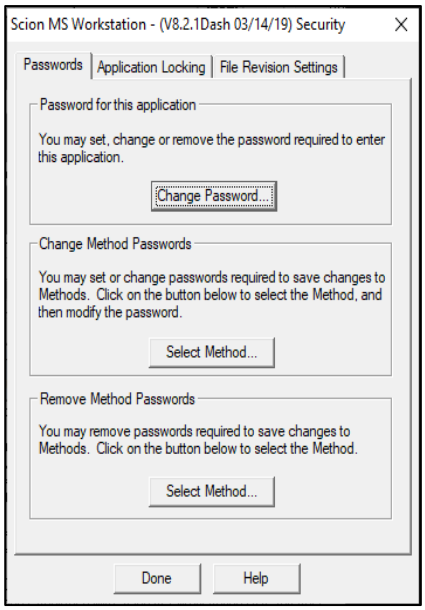
62. **Move columns in SampleList** by right-clicking in header.

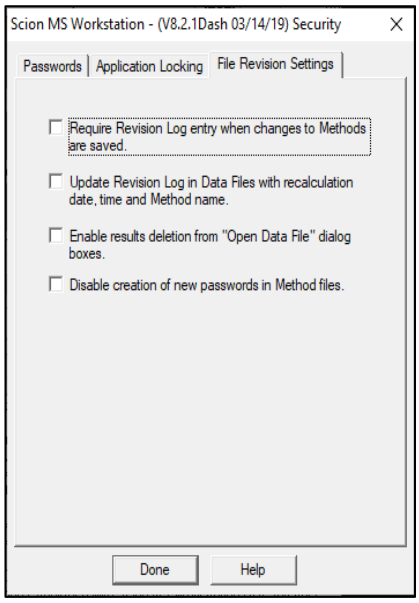


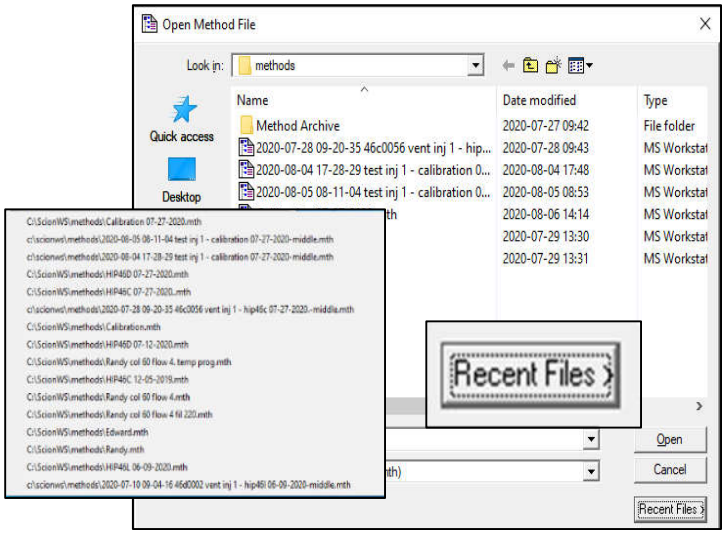


63. **Relabel column header** in SampleList.

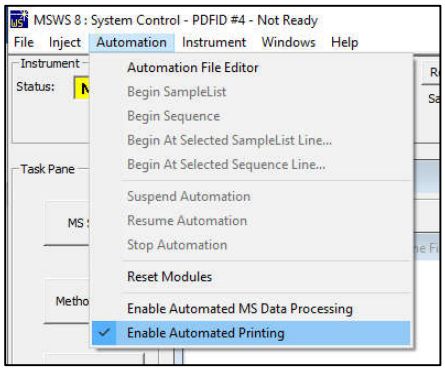
64. **Security** – Passwords, Application Lock and File Revision Settings. Details displayed with “Help”.





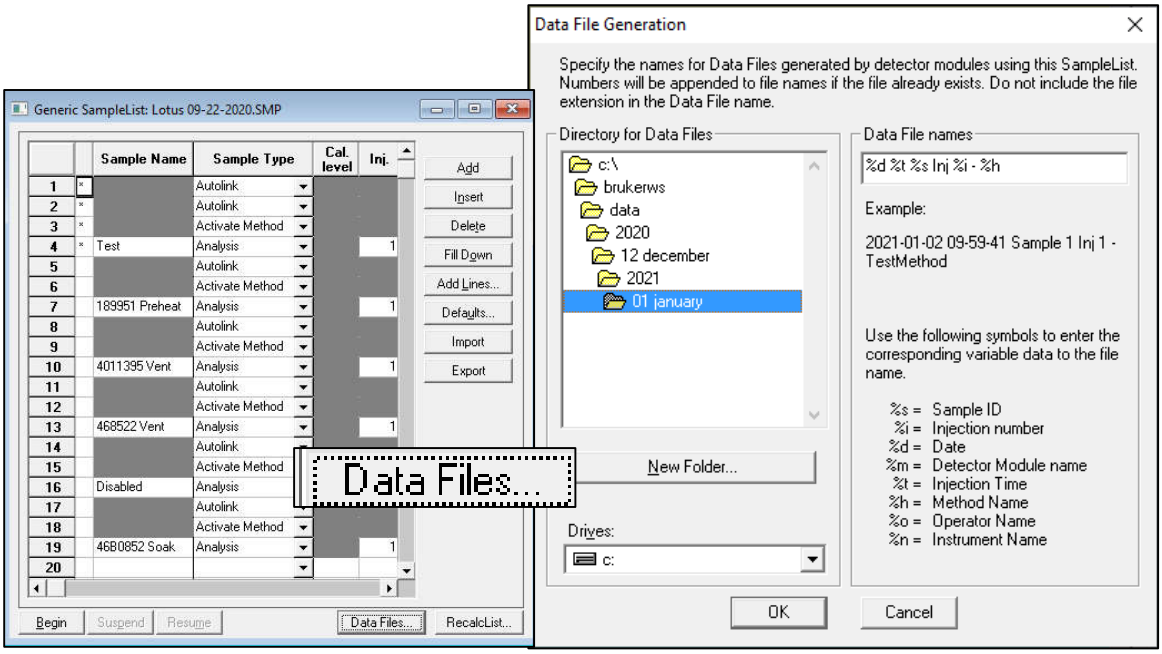


65. **Recent Files button** - This action significantly reduces errors in entry of file name and directory path.



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

67. **Specify/Create data file folder from SampleList.**



68. **Status/Error Codes**

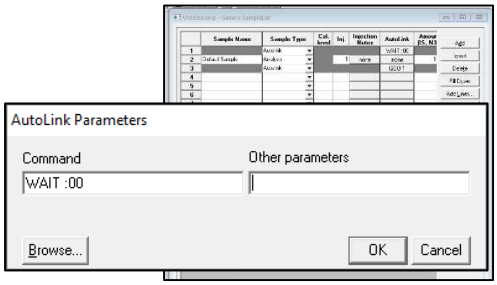
```
    Compounds
        S - Internal Standard Peak
        R - Reference Peak
        T - Relative Retention Peak
        NA - Not Active

    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.
     O : 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.
     l : Too many similar spectra. Search may be incomplete.
     m : Too few points to quantitate. Check time range.
     p : Peak < Size Threshold. Check Integration params.
     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

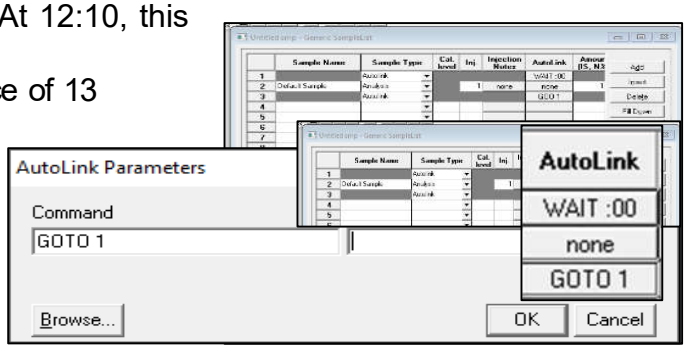
  

  For example, WAIT 15:03:56 will wait for 3:03:56 PM, unless this time is already passed, in which case there will be no wait. Fields can be omitted. In this case, tailing fields are defaulted to zero, while leading fields are interpreted as the next matching hour or minute. The following examples illustrate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

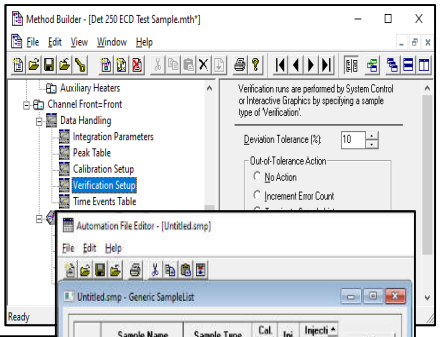
  13: taken as 13:00:00.
  13:10 taken as 13:10:00.
  :13 taken as the next occurrence of 13:00 minutes after the hour. At 12:15, this command would wait for 13:13. At 12:10, this command would wait for 12:13.
  ::13 taken as the next occurrence of 13 seconds after the minute

- **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:

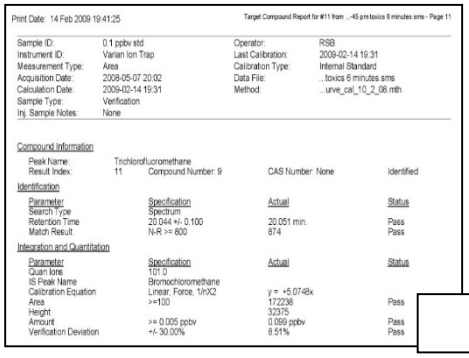
  Command: GOTO <line-number>
  Other-parameters: Inject or Recalc or Print

- **WAIT and GOTO** can be used to create an infinite loop to perform an injection every preset time interval to monitor a process stream.

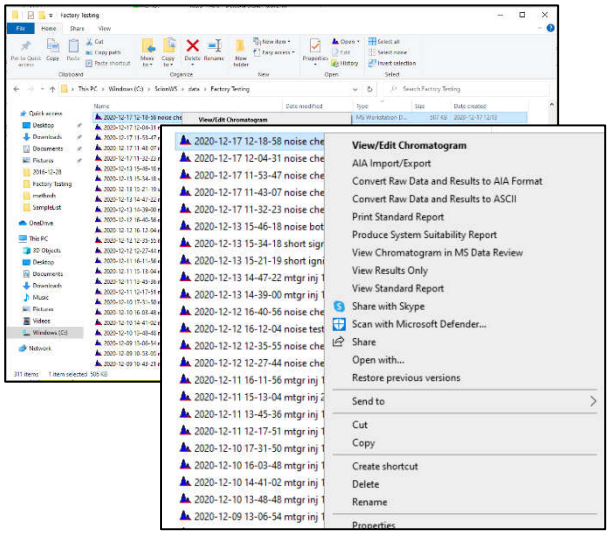
70. **"Verification" run type** - reported results compared to values in a calibration level.

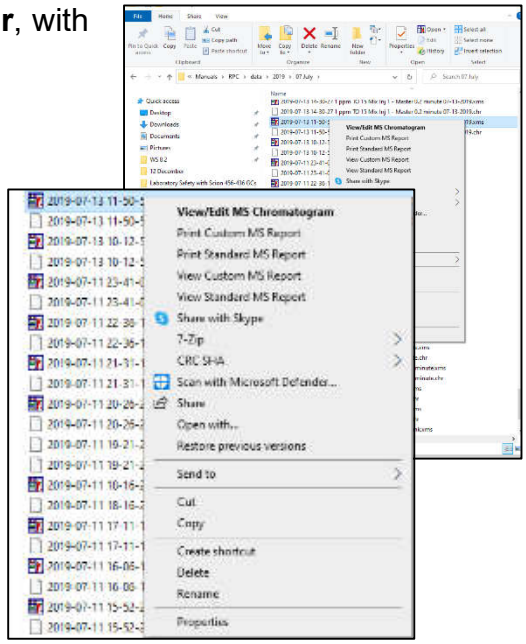
  

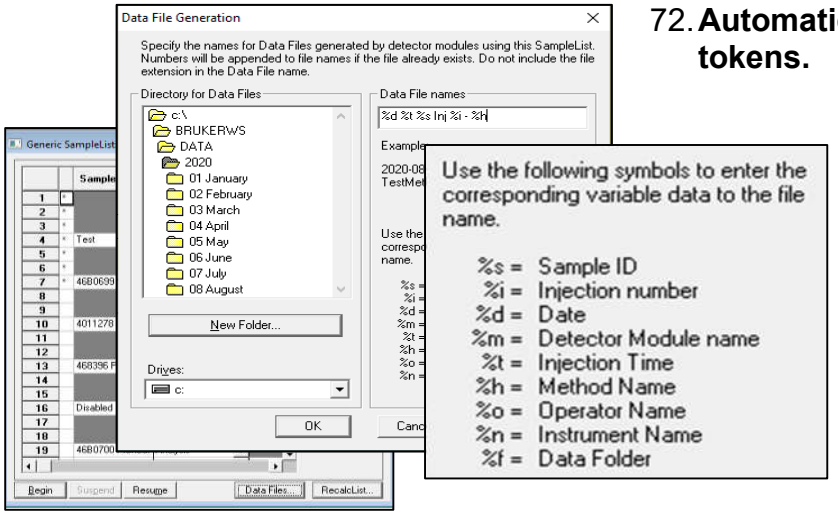
Peak No.	Peak Name	Expected Result ()	Calculated Result ()	Dev. %	Ret. Time (min)
1	Hydrogen	125.8000	126.0991	0.2	5.980
2	Oxygen	25.1500	27.3469	8.7	6.457
3	Nitrogen	49.9400	49.9810	0.1	7.230
4	Methane	24.8600	24.8167	0.2	8.182
	Totals:		228.2437		

Amount	>= 0.005 ppbv	0.099 ppbv
Verification Deviation	+/- 30.00%	8.51%

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



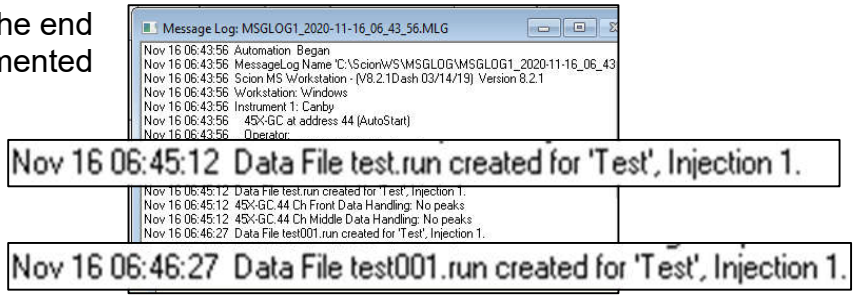




72. **Automatic data file naming with tokens.**

73. **Data file names can have up to 255 characters** (NT File System - contrast to Virtual File Allocation Table 8.3).

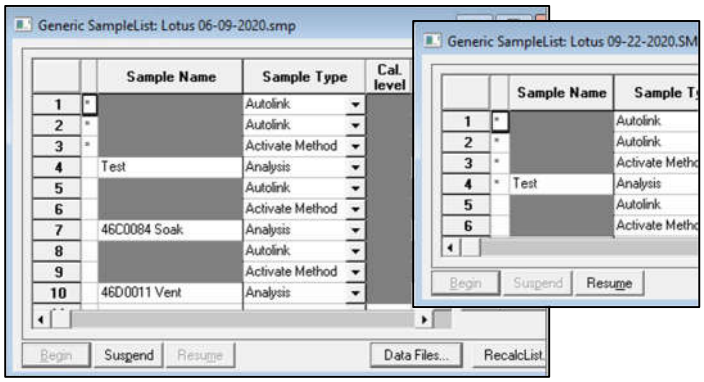
74. **Cannot overwrite data files.** - If new data name matches an existing file in the same folder, then three digits are automatically appended to the end the name and incremented thereafter

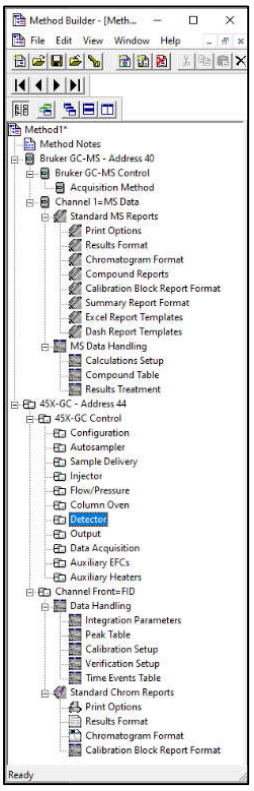


Suggestions for Operations with .XMS data files

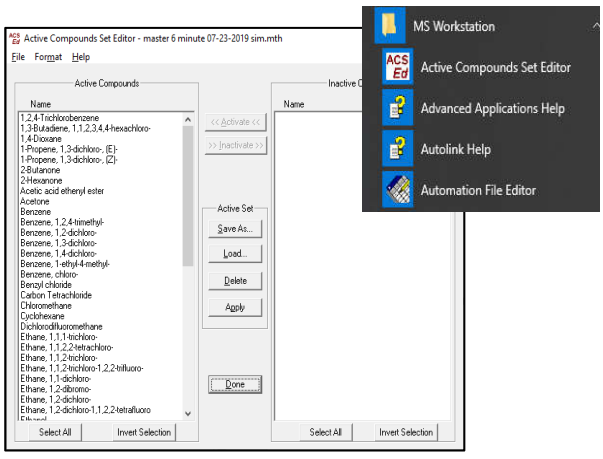
75. **Peak processing for chromatograms for .XMS files** is discussed in Peak Detection with Varian MS Workstation: http//lotusinstruments.com/wp/wp-content/uploads/Peak-Detection-with-Varian-MS-Workstation.pdf

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**.

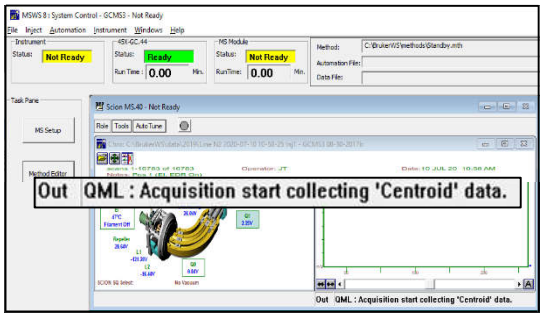


78. **Active Compounds Set (ACS) Editor** - ACS is a list of compounds, representing a subset of the Compound Table, which can be saved in a method, and activated during automation. MSWS includes an interactive application (ACTIV2.EXE) to create, edit, delete such sets within a method file. MSWS also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

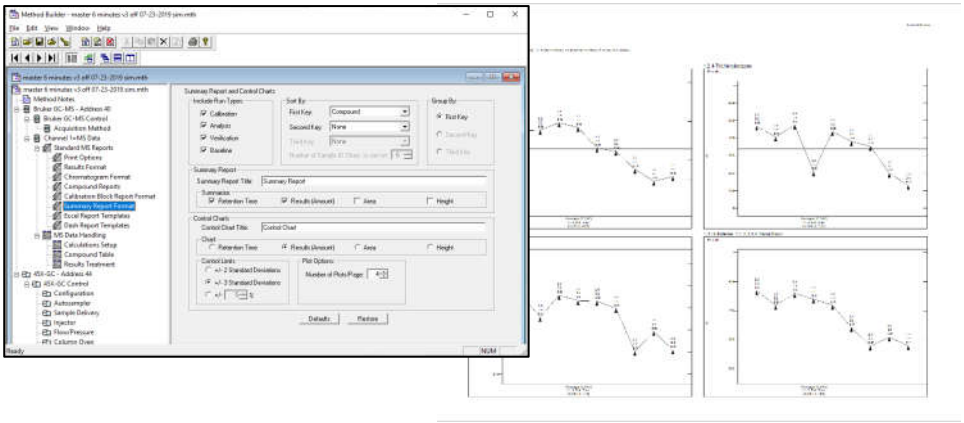
79. Hot Keys in MS Data Review

```
------------------------------------------------------------------------
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
        l - 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
        up arrow      - Next Spectrum

------------------------------------------------------------------------
Spectra Plot Control
    Single-Click-Actions
        l - 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
    F1 - Help
```

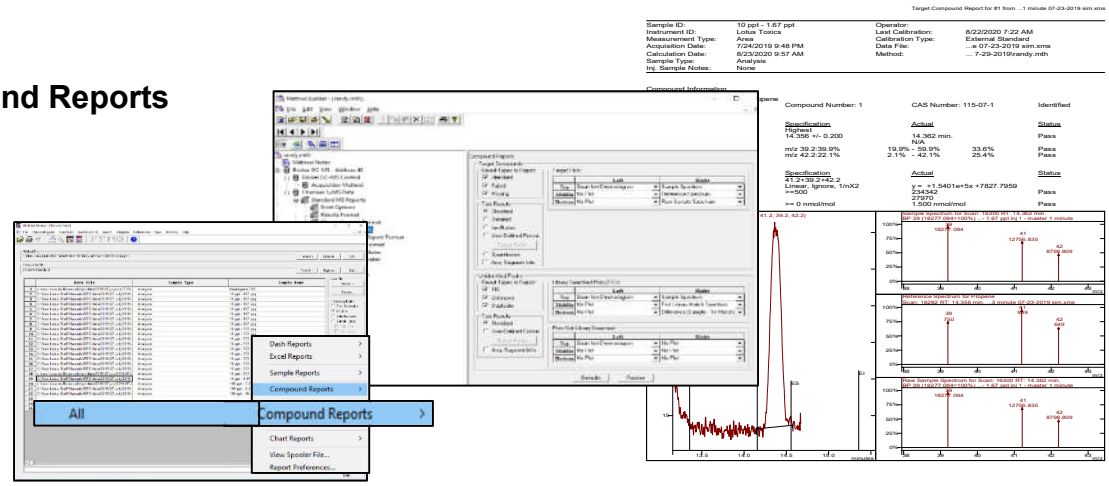
80. **QML Commands** (Quadrupole Macro Language) – reserved for Scion Service operations. This is not intended for user operations.



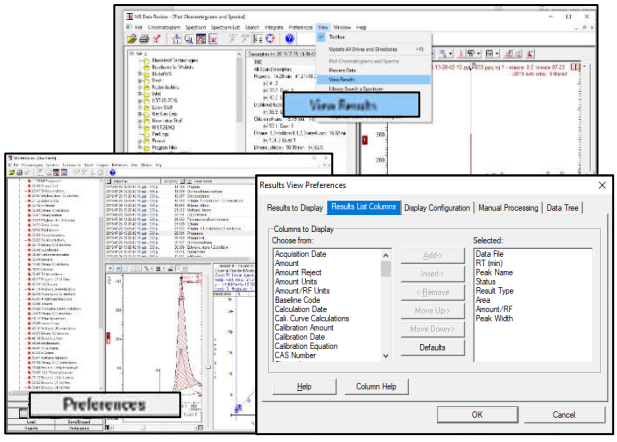
81. **Control Chart Reports**



82. **Compound Reports**

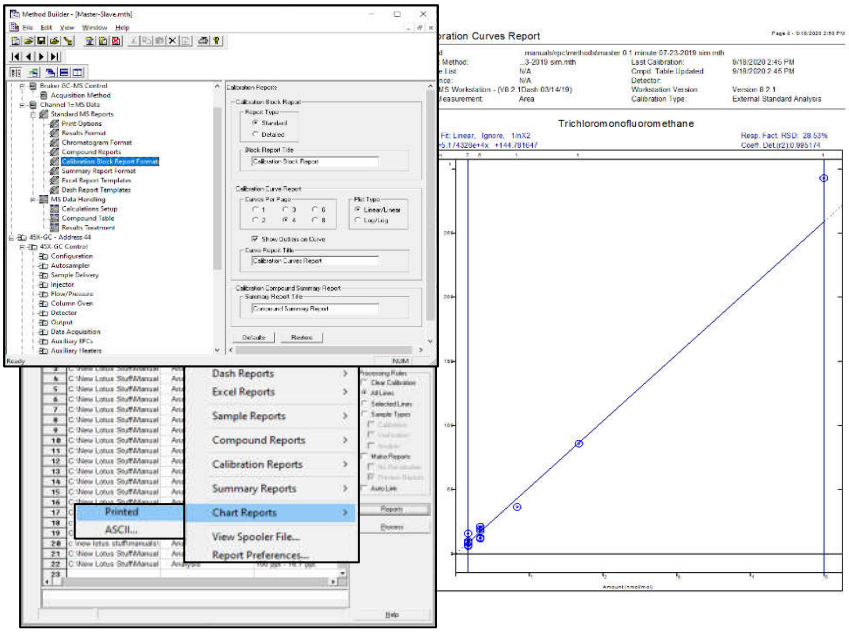


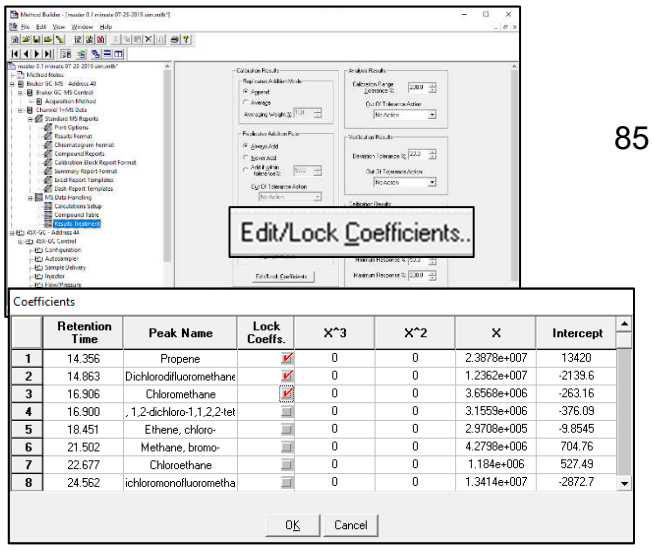
83. **Format in View Results** - report format can be altered with options available through menu from MS Data Review > View > View Results > Preferences > Results List Columns. See following list for choices.



Columns to Display	Description
Acquisition Date	The time and date when data file was created.
Amount	The calculated result. Amounts are calculated from the calibration curve for all files, including Calibration and Verification files. Areas or heights 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 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/RF	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 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 the Internal Standard. When integrated areas or heights are reported for the results, the units are reported as Counts.
Area	The integrated area of the peak. Areas greater than 999999 are reported in scientific notation.
Baseline Code	Two-character codes that specify how peak integration was started, ended, and the type of baseline used. (Select the Results Codes Help menu item for definitions.)
Calculation Date	The time and date when the data file was last quantitated.
Cali. Curve Calculations	The Curve Fit Type, Origin Point, and Regression Weighting used to calculate a calibration curve.
Calibration Amount	The compound Calibration Level Amount that is specified in the method.
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.
Channels	The physical channels on which the scan functions to create the chromatogram were generated. Merged is reported if all available channels are combined. 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 Automation Editor.
IS Height	The baseline-corrected height of the Internal Standard peak used to quantitate an Analyte.
IS Peak Name	The name of the Internal Standard used to quantitate an Analyte.
IS RT (min)	The retention time of the Internal Standard peak used to quantitate an Analyte.
Lbr. #	The library entry number of the match that was reported from the library search of an Unknown Peak.
Library	The name of the library that contains the match reported from the library search of an Unknown Peak.
Match Prob.	The probability that the match reported from the library search of an Unknown Peak is correct, assuming that the correct match is in the database.
Match Result	The Forward or Reverse Match result used to rank the matches from a search. Target Compound Spectrum Match identification always uses Normal-Forward 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 Unknown Peak results will not be reported, and Target Compounds will be designated as Missing.
Peak Type	The peak types other than Analyte that may be specified in the method for a Target Compound: SP: Internal Standard, REF: Reference, RRT: Relative 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 Ions	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 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.
Result #	The line number of the reported result.
Result Type	Compound Result Types are Identified, Missing, or Failed (Failed one or more Ion Ratio specifications). Unknown Peak Result Types are TIC (Tentatively Identified Compound) Duplicate (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 segment. Merged is reported if all available scan functions are combined. Merged is always used to quantitate Unknown Peaks.
Scan Number	The scan number of the apex point of the integrated peak.
Search Type	The search type specified in the method to identify the integrated peak. Target Compounds: Spectrum, Nearest, Highest, First, or Last. Unknown Peaks: Library Search, or None.
Slope 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 rate and the specified Peak Width.
Status	Single character result codes that report status information or problems which occurred when a peak was processed. Error codes are a subset of the Status codes. (Select the Results Codes Help menu item for definitions.)
Tangent %	Peaks on the trailing edge of a peak will be integrated as tangent peaks if their heights are less than the specified percent of the parent peak height.
Threshold	At least one match result must be equal to or greater than this threshold for a Target Compound or an Unknown Peak to be identified.
Top 2 Matches	The top 2 match results that meet the Threshold specification will be reported when an Unknown Peak is library searched.
Top 3 Matches	The top 3 match results that meet the Threshold specification will be reported when an Unknown Peak is library searched.
Top Match	The top match result that meets the Threshold specification will be reported when an Unknown Peak is library searched.

84. **Calibration Reports.**





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.

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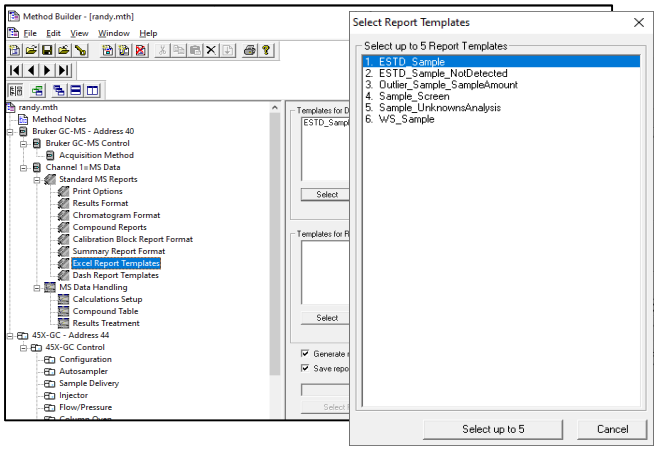
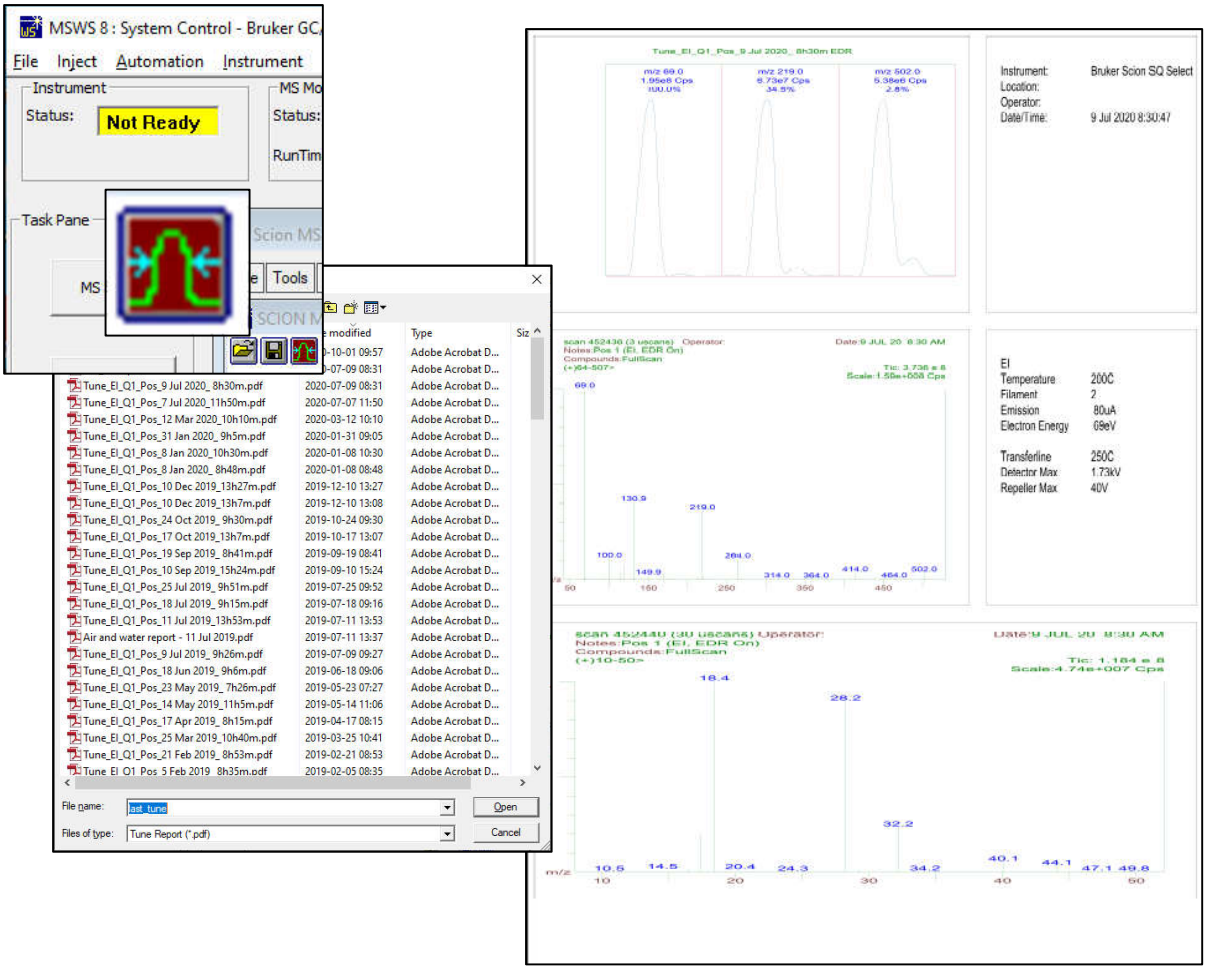
86. **Excel Report Templates.**



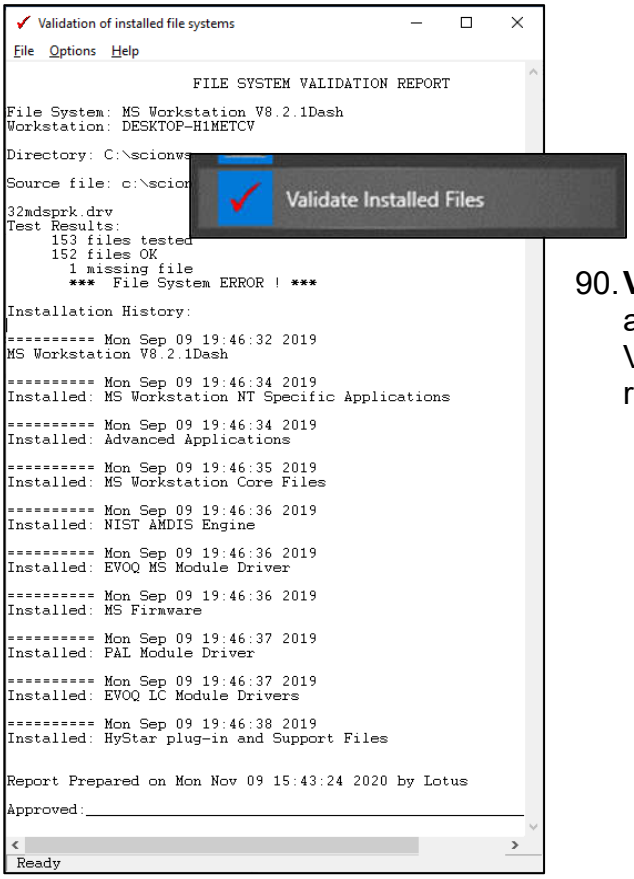
87. **Dash Reporting** - report authoring system that provides tools for designing and generating reports of analytical data from Scion MS Workstation, as well as other relational database sources. The system works by querying the MS Workstation database and applying a report method to the data to produce 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.



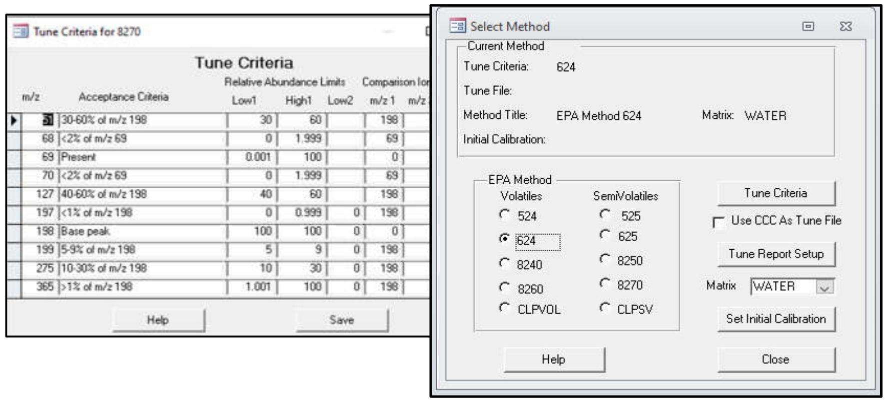
89. **System Suitability -** is a custom report template used to compute and report system suitability indicators from Scion MS Workstation data files. The following types of reports may be generated:

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).
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.

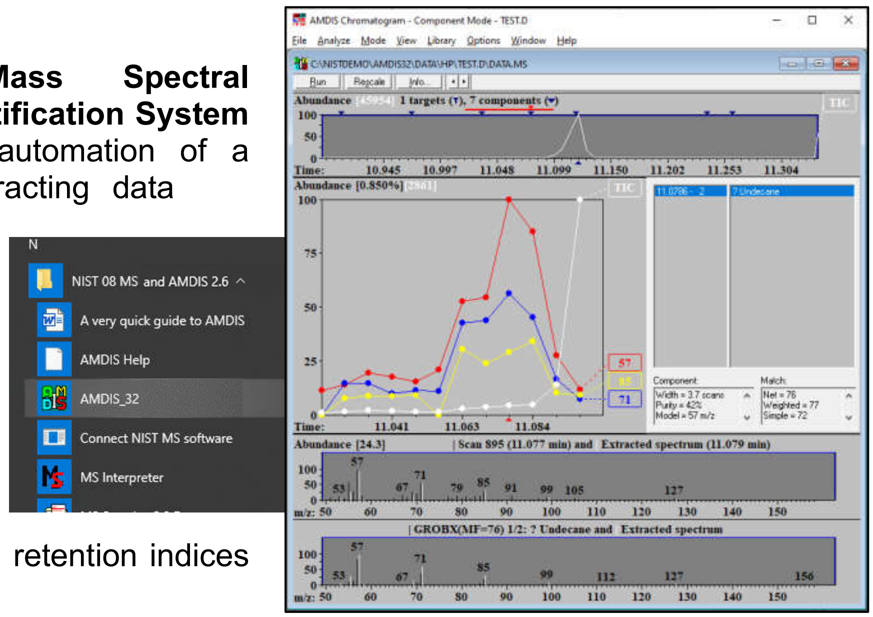


90. **Validation of Installed File Systems** – is accessed through MS Workstation > Validate Installed Files. This action could be required for many laboratory audits.

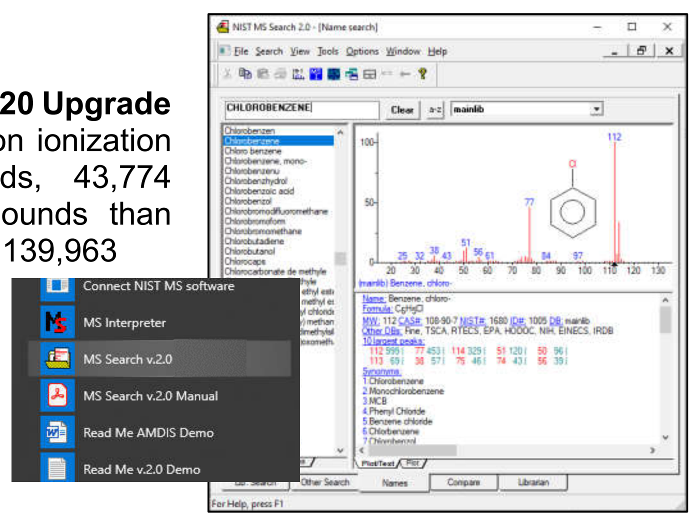
91. **EnviroPro Reporting** - provides detailed information on reporting results for common USEPA methods - 524, 525, 624.625, 8240, 8250, 8260, 8270, 8270, CLPVOL and CLPSV. Tune Reports can be generated.



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 then associating them to a single component. Once it has found this component, it compares it to a library of spectra and retention indices provided.



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.



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.

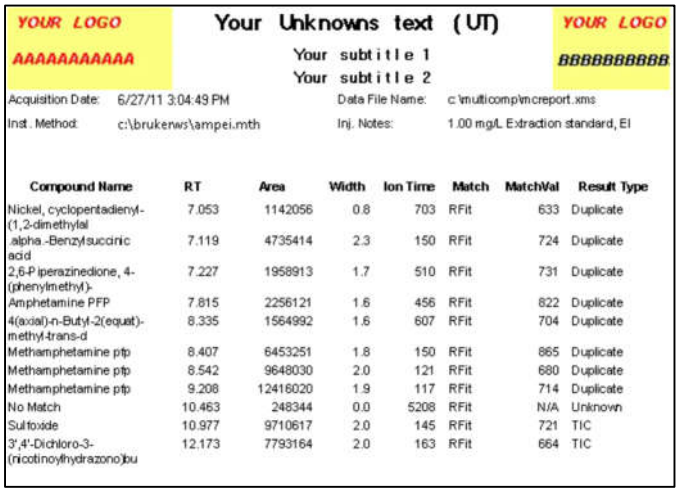
96. **Rosner Mass Spectra Library of Designer Drug** 2019 (Scion P/N 392052102 - is the largest collection of chemical signatures of new psychoactive substances (NPS) and drugs of abuse in the world. This impressive mass spectral library was developed to support forensics and toxicology labs to combat 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 EI 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.



YOUR LOGO — Your Unknowns text (UT) — YOUR LOGO

AAAAAAAAAA — Your subtitle 1 — BBBBBBBBBB

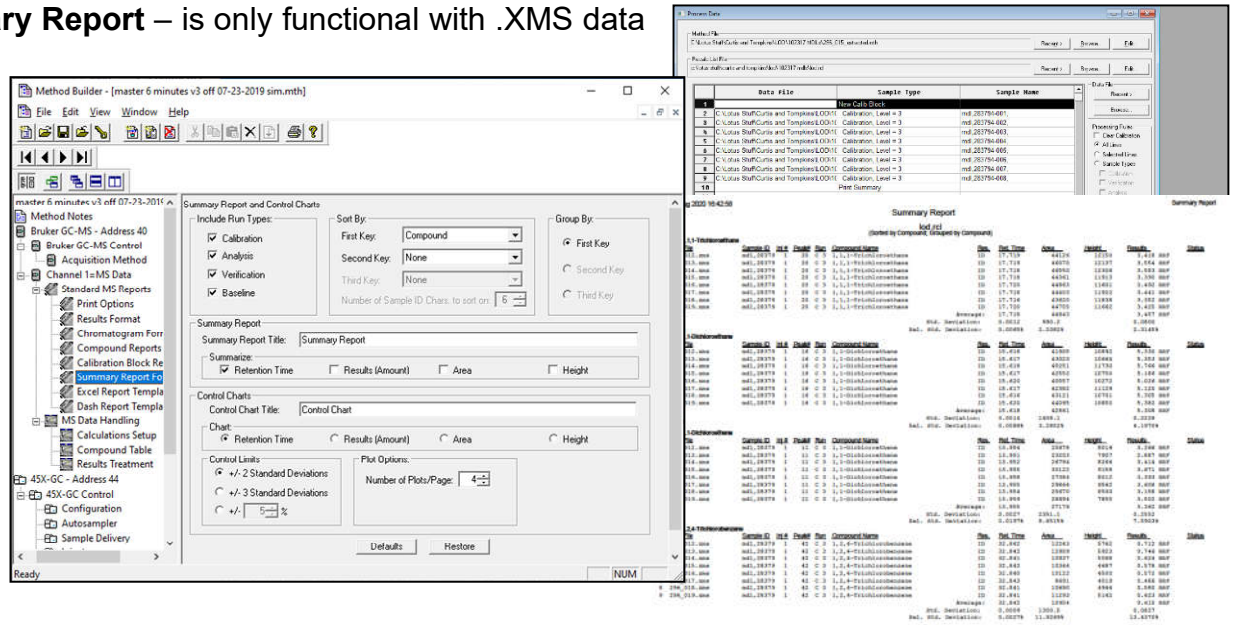
Your subtitle 2

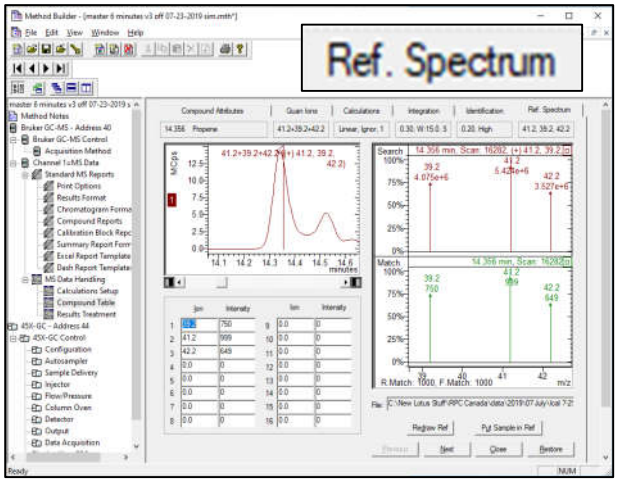
Acquisition Date: 6/27/11 3:04:49 PM — Data File Name: c:\multicomp\mcreport.xms

Inst. Method: c:\brukerws\ampei.mth — Inj. Notes: 1.00 mg/L Extraction standard, EI

Compound Name	RT	Area	Width	Ion Time	Match	MatchVal	Result Type
Nickel, cyclopentadienyl-(1,2-dimethylal	7.053	1142056	0.8	703	RFit	633	Duplicate
.alpha.-Benzylsuccinic acid	7.119	4735414	2.3	150	RFit	724	Duplicate
2,6-Piperazinedione, 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 ptp	9.208	12416020	1.9	117	RFit	714	Duplicate
No Match	10.463	248344	0.0	5208	RFit	N/A	Unknown
Sulfoxide	10.977	9710617	2.0	145	RFit	721	TIC
3',4'-Dichloro-3-(nicotinoylhydrazono)bu	12.173	7793164	2.0	163	RFit	664	TIC

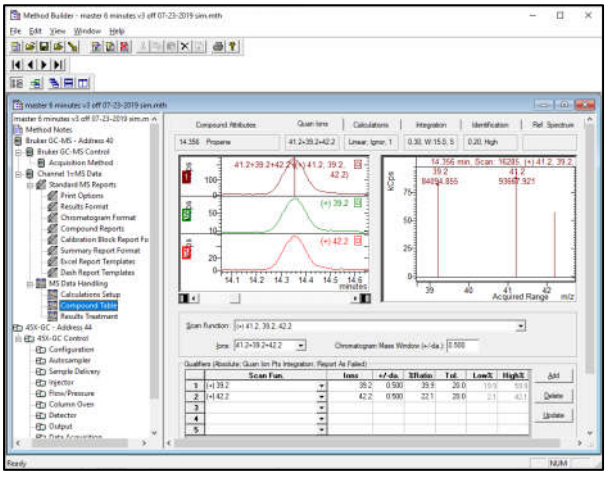
101. **Summary Report** – is only functional with .XMS data files.



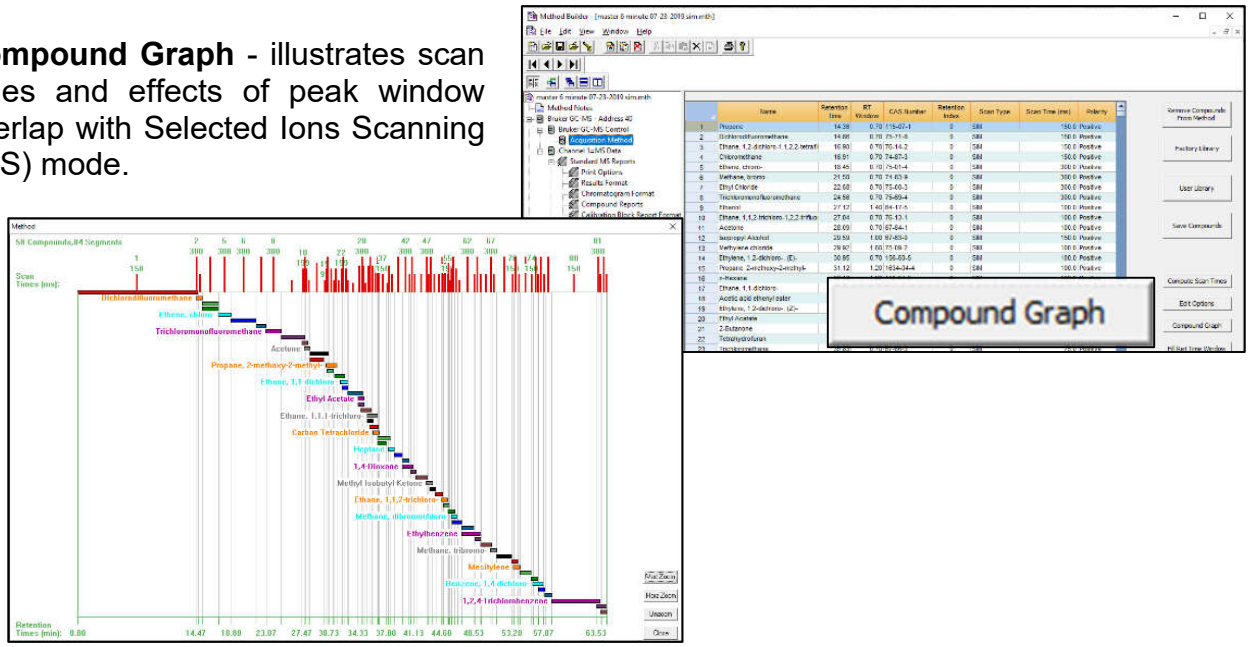


102. **Ref Spectrum** – is used to identify the peak can be set either from a standard spectrum, or from user adjustments of ions and their intensities.

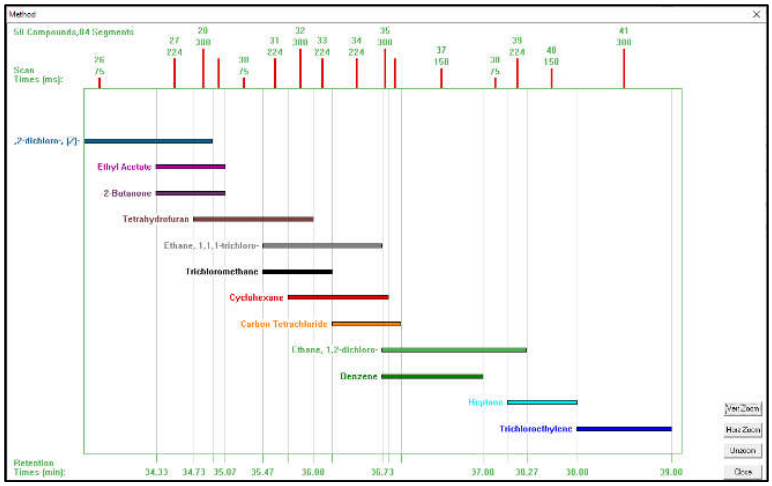
103. **Selected Ions Monitoring (SIM)** – Data from multiple ions can be collected to provide positive matching to a reference spectrum with use of multiple characteristic ions for compounds.

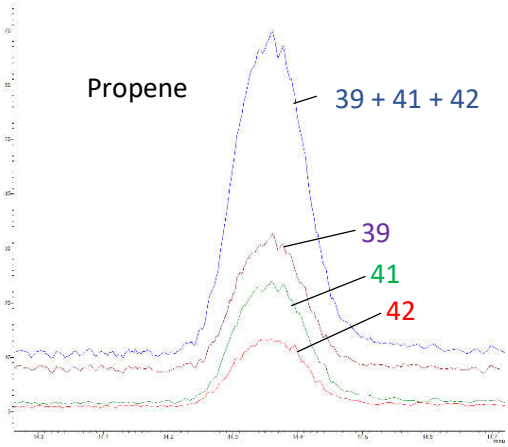


104. **Compound Graph** - illustrates scan times and effects of peak window overlap with Selected Ions Scanning (SIS) mode.



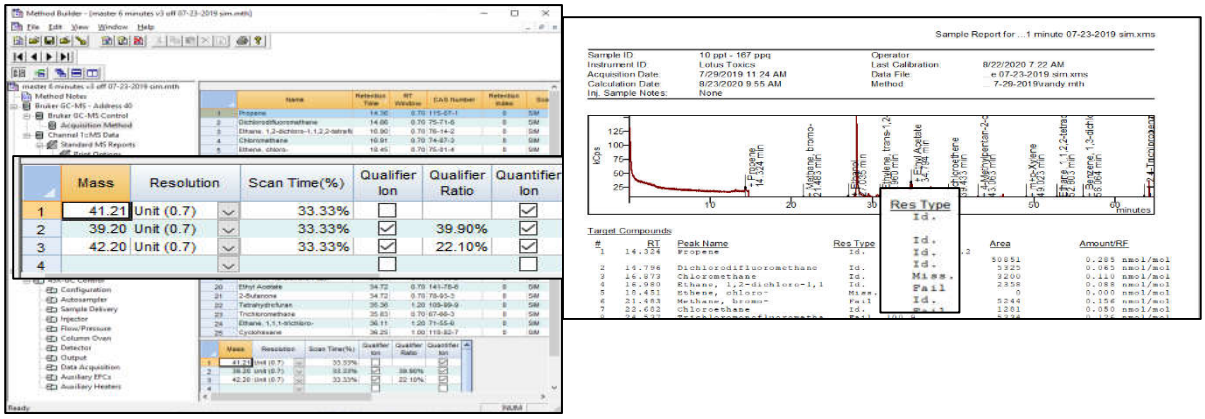
105. **Expanded view of portion of Compound Graph** - allows visual indications of overlapping scan windows. Display area is selected through mouse actions on edges of graph or click/drag inside the presentation. Regions of overlap degrades the quality of the data, especially related to noise levels. 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.



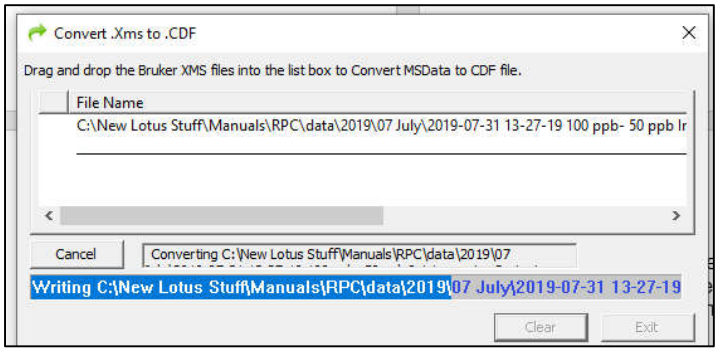


106. **Multiple Quan Ions** – To boost peak response, specially for low responders such as propene and chloromethane, muliple ions can be defined as scan functions to enhance peak detection, especially for SIM mode

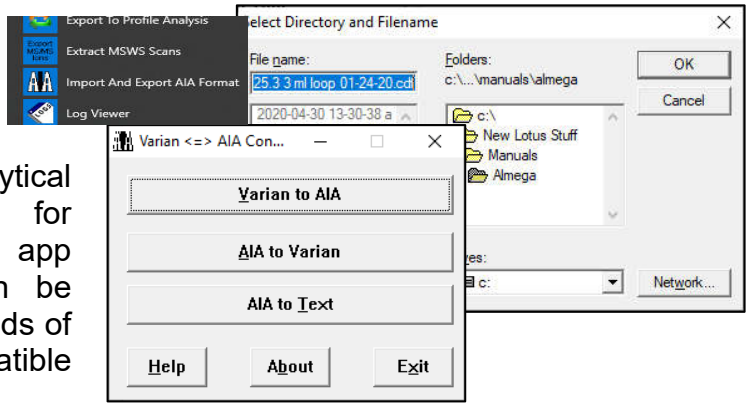
107. **SIM (Selected Ions Monitoring) Peak Confirmation** - To confirm identification of a compound when only selected ions are set in SIM mode, qualifier ions can be set up with ion ratios to the base peak. A match is labeled as “ID” in the final report. Obviously NIST library searches do not apply.



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.

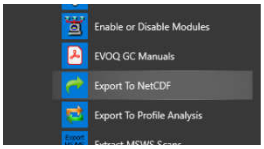


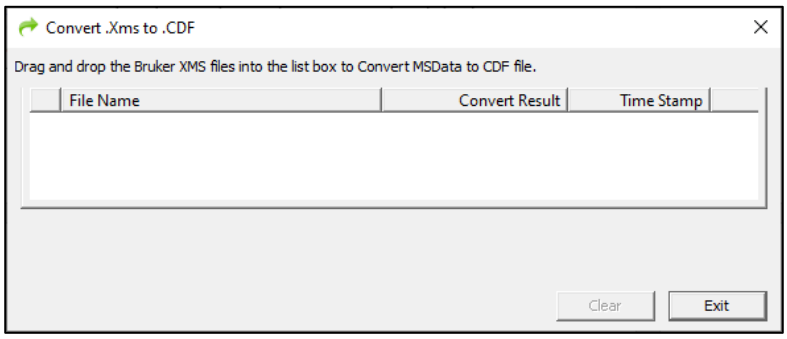
109. **Convert files to AIA** (Analytical Instruments Association)[2] - ASTM E1947 - 98(2014) Standard Specification for Analytical Data Interchange Protocol for Chromatographic Data. This app generates .CDF files that can be exported/imported into other brands of chromatography software compatible with AIA format.



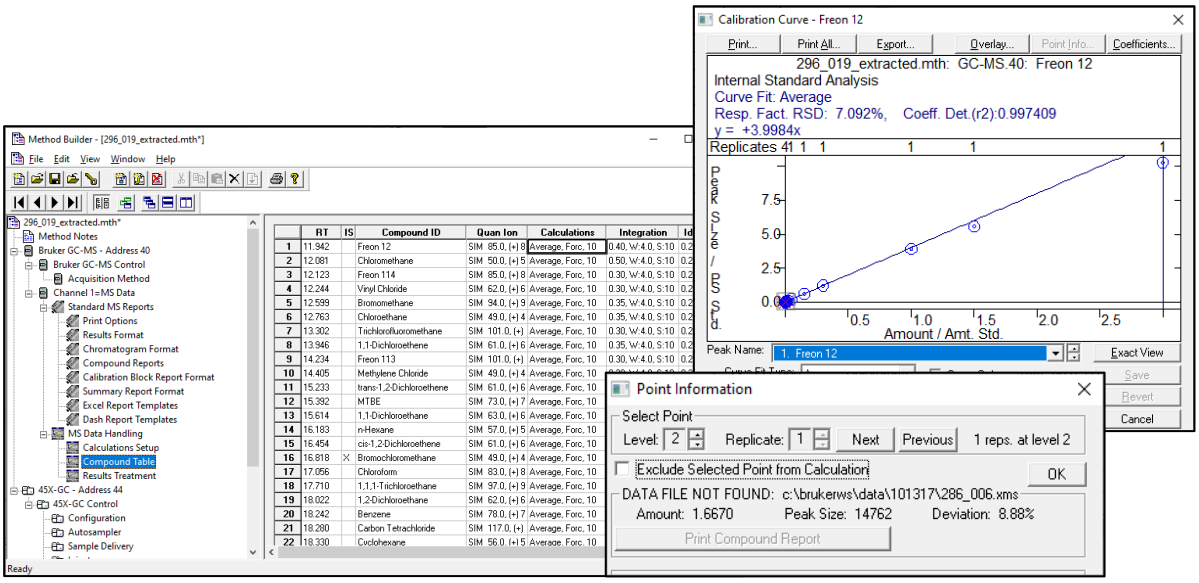
[2] D.C. Nelson, Chemometrics and Intelligent Laboratory Systems, 26 (1994), p. 43. www.sciencedirect.com/science/ article/abs/pii/0169743994900175

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.





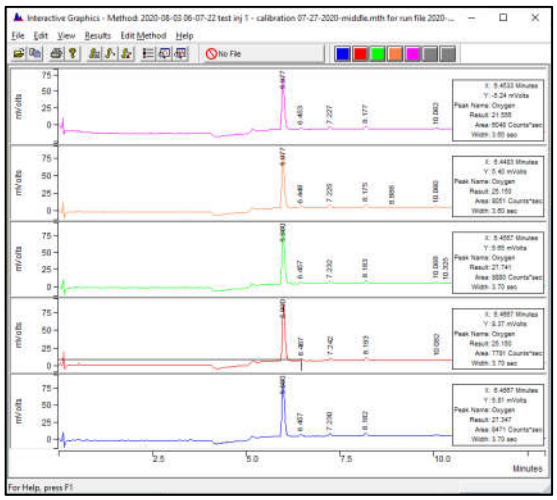
111. .**XMS data files** for MS possess:
- Raw data points
- Last computed results
- Copy of last method used
- Link to original method
- Complete calibration data
  - Response Factors
  - Calibration Point Information
    - Calibration Amounts
    - Calibration Peak Sizes
    - Deviations from Curve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

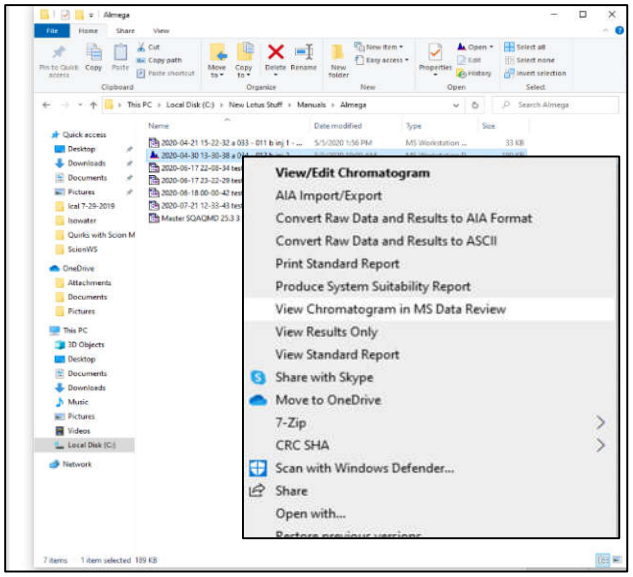


Hints with Operations with GC Detector .RUN Data Files

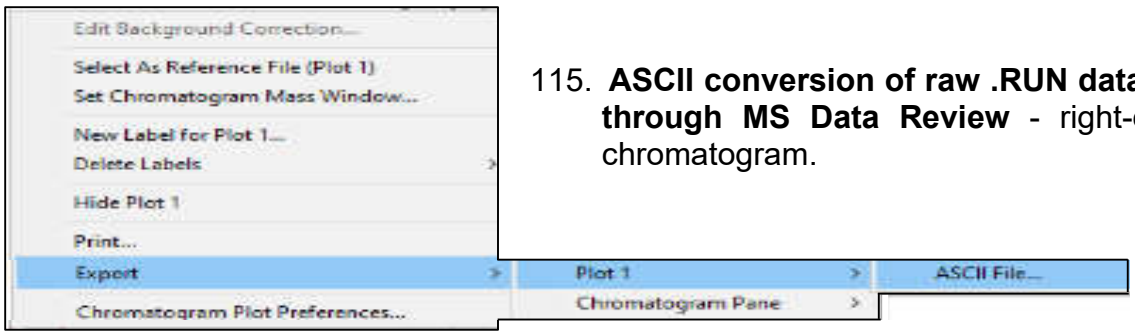
112. **Peak processing for chromatograms for GC detector run files -** are discussed in Peak Detection with Varian Star Workstation. http://lotusinstruments.com/wp/wp-content/uploads/Peak-Detection-with-Varian-Star-Workstation.pdf

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

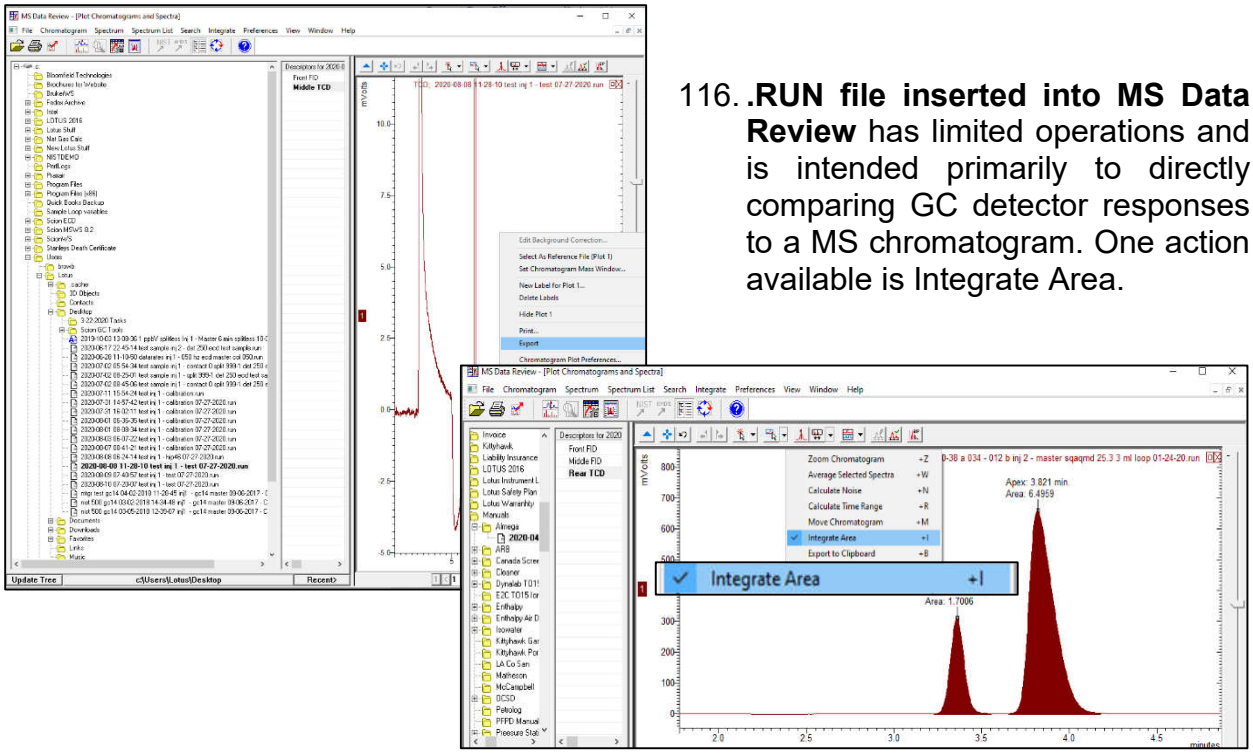




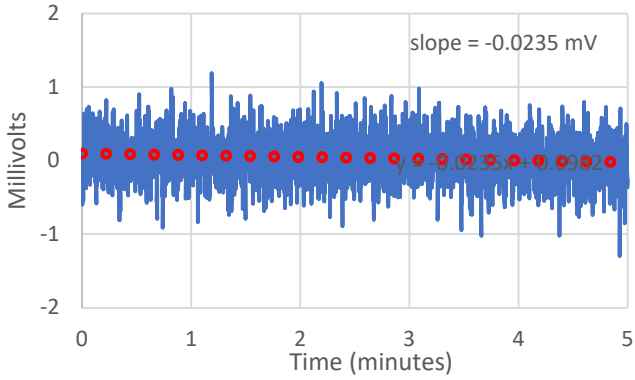
114. **Insert .RUN data file into MS Data Review** from Windows Explorer by right-clicking on desired data file.



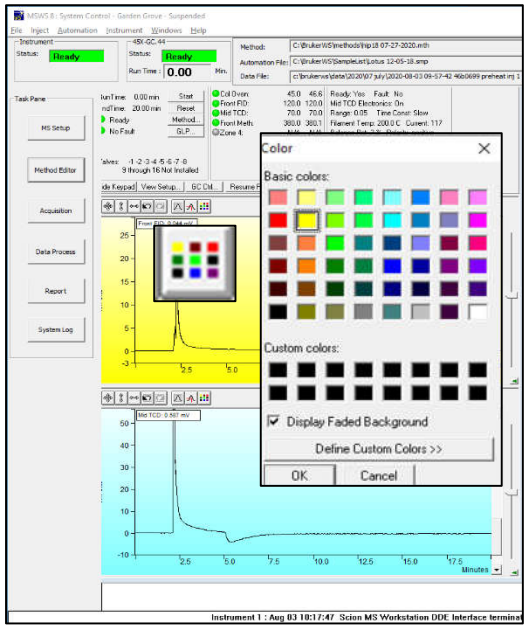
115. **ASCII conversion of raw .RUN data points through MS Data Review** - right-click on chromatogram.



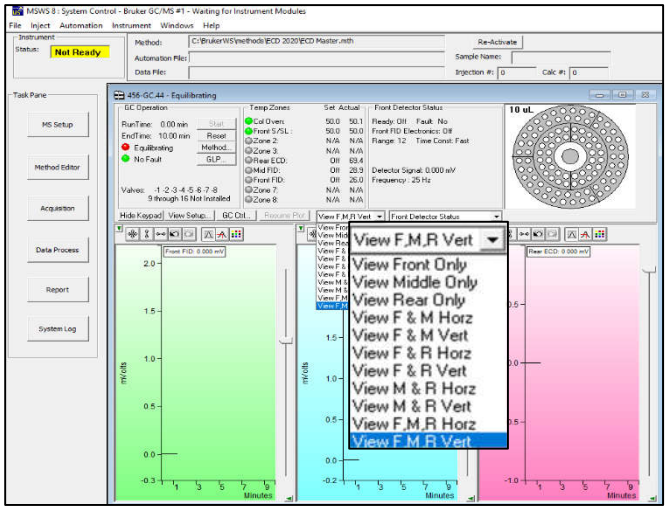
116. **.RUN file inserted into MS Data Review** has limited operations and is intended primarily to directly comparing GC detector responses to a MS chromatogram. One action available is Integrate Area.



117. **Detector signal drift** - computed through Trend Line of ASCII data points via Excel.

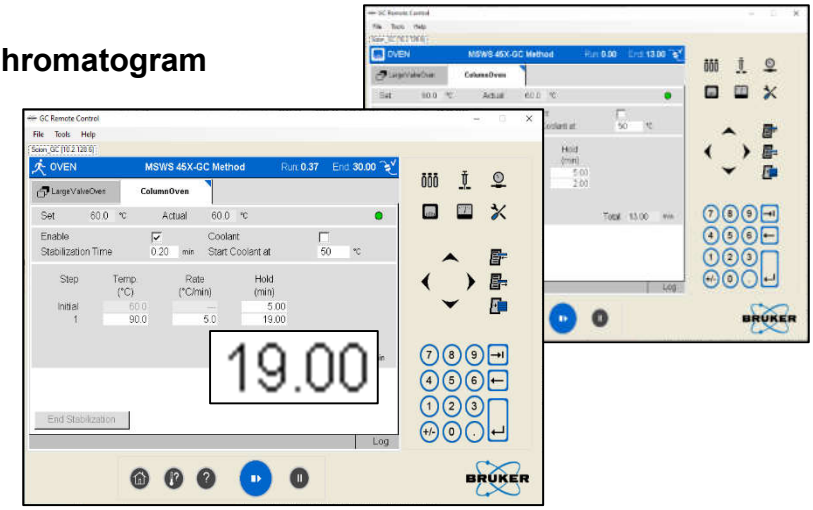


118. **Change background colors** of displayed live chromatograms.

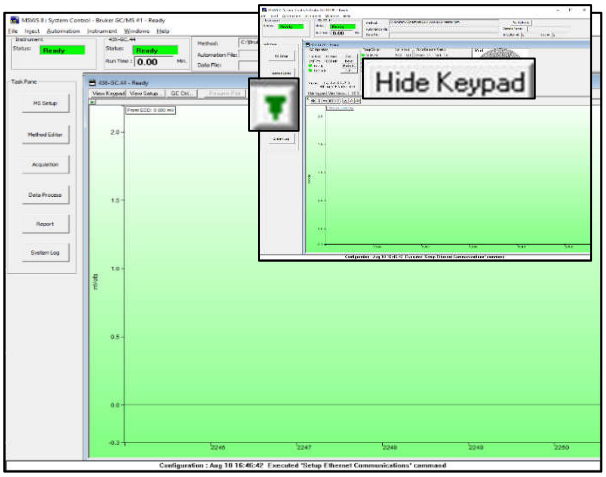


119. **Display of live chromatograms in System Control** - single, double or triple, and horizontal or vertical.

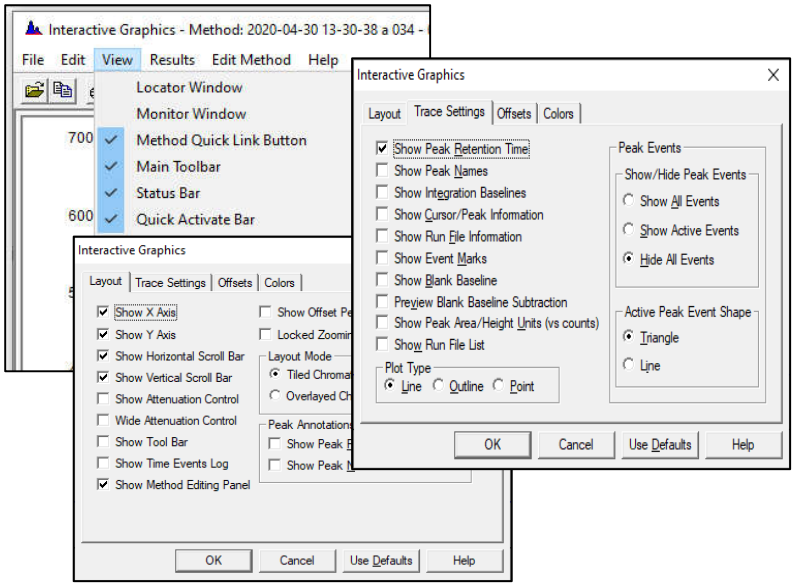
120. **Change Run Time in Active Chromatogram** - Keyboard on Scion 436/456 is active during a run, and the column oven hold time in the final step can be adjusted longer or shorter time to impact both the GC run time and GC detector(s) data collection end time. This change does not alter the Scion SQ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

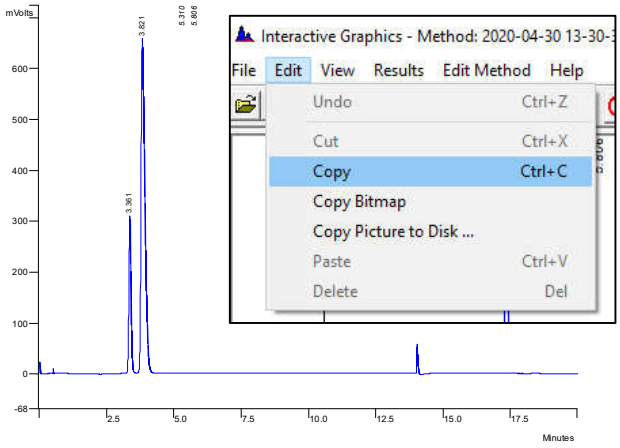


121. **Hide Keypad** – to set chromatogram display for full screen.



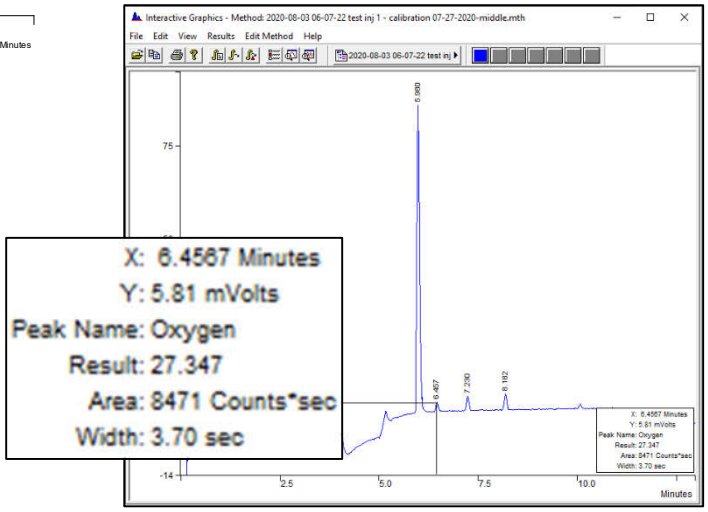
122. **Add/remove extra notations** on displayed chromatogram in Interactive Graphics.



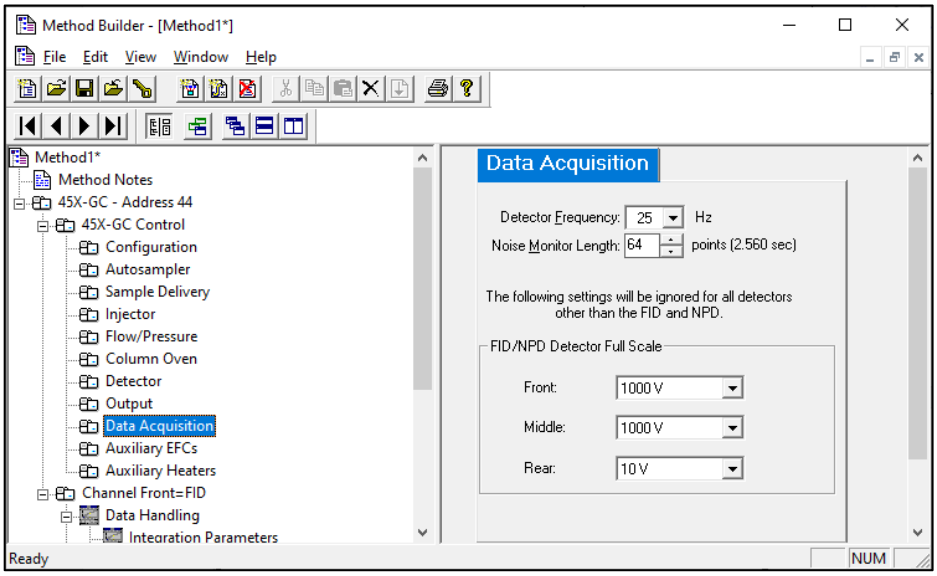


123. **To display a chromatogram in external documents**, such as Word, "copy" from Interactive Graphics to Clipboard and then "paste" into the Word.docx. This action allows the chromatogram labels to be edited and comments added.

124. **Interactive Graphic display of retention time** to 0.0001 minutes.



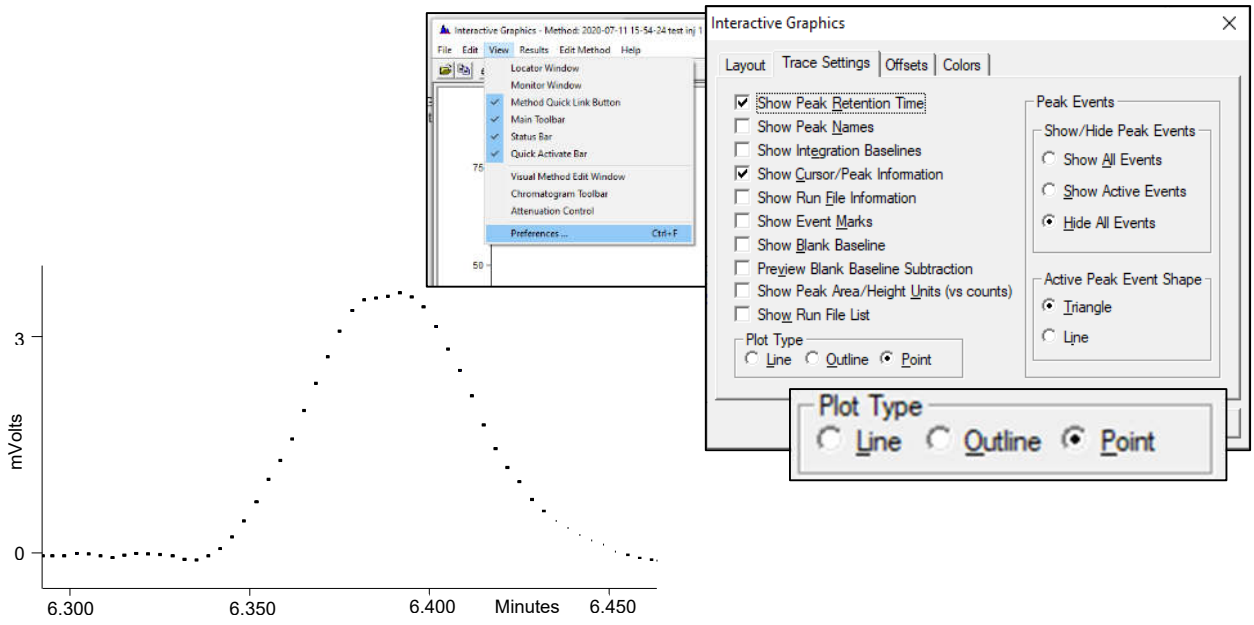
125. **Detector frequency** - This parameter impacts data collection with number of data points used to define the peak combined with monitored noise level.



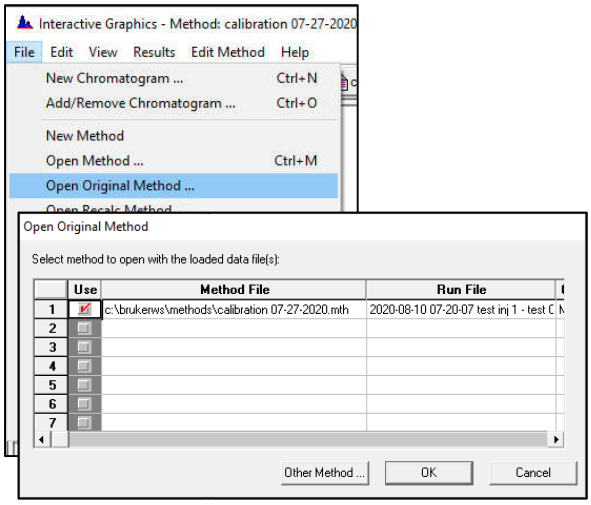
126. **Single method possesses:**
    - Full set of parameters for control of GC
    - Full set of parameters for computation of results
    - Complete calibration data
        - Raw data points
        - Last computed results
        - Copy of last method used
        - Link to original method
        - 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

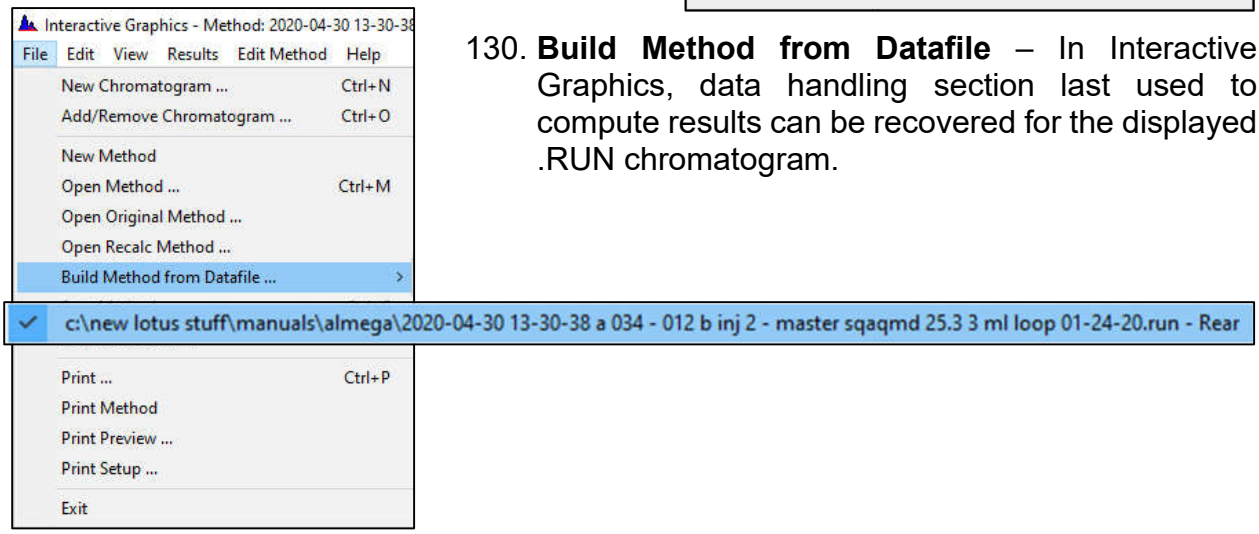
128. **Display of data points** - provides visualization of proper definition of peak shape. Data interval is set by detector frequency and expected peak width. Optimum settings should yeild 10 data points across top of peak.



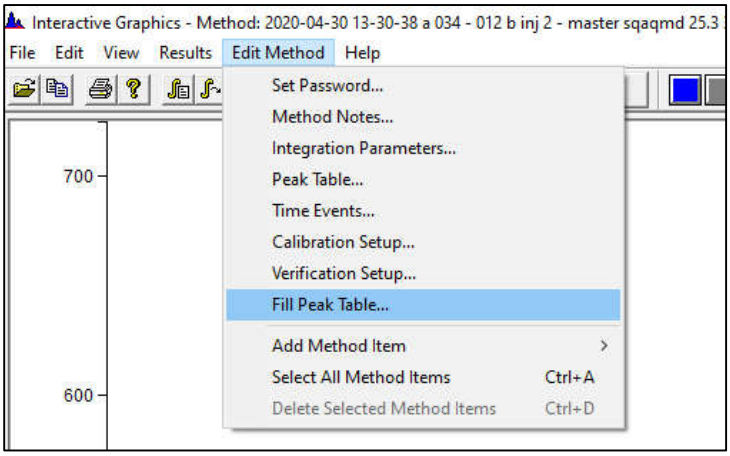
129. **Open Original Method** - .RUN files possess a link to the original method used to collect the data.

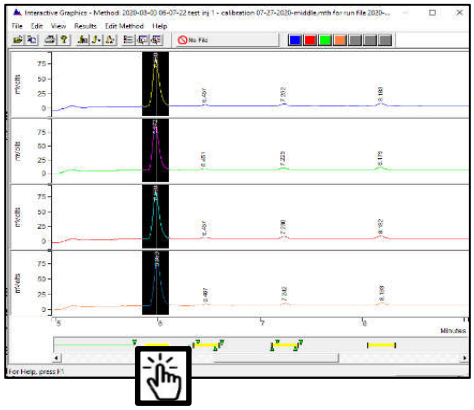


130. **Build Method from Datafile** – In Interactive Graphics, data handling section last used to compute results can be recovered for the displayed .RUN chromatogram.



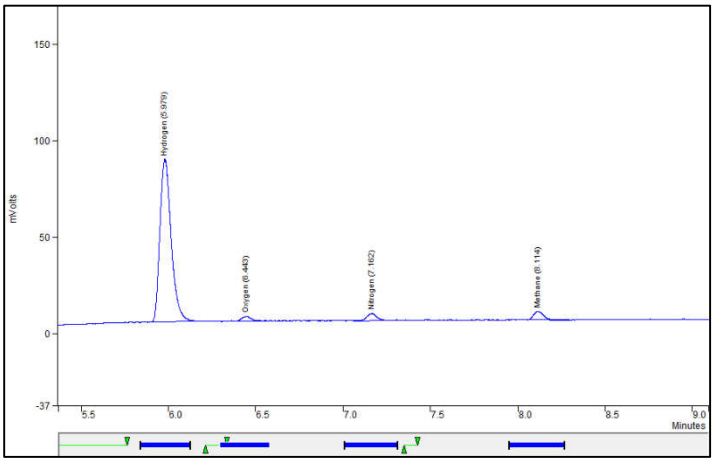
131. **Fill Peak Table** - is accessible through Interactive Graphics. Clicking on peaks in the displayed chromatogram will add these peaks to Peak Table of active method.

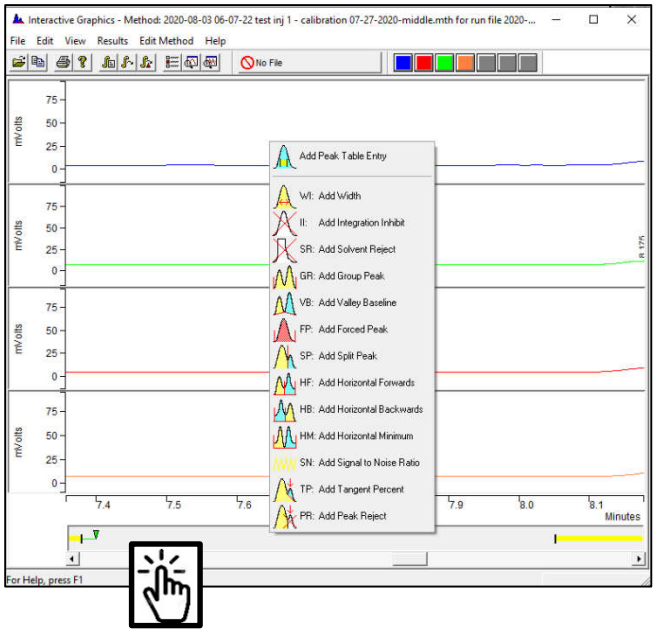




132. **Graphically relocate retention times in Peak Table** - by right-clicking on yellow window under peak and move to adjust.

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

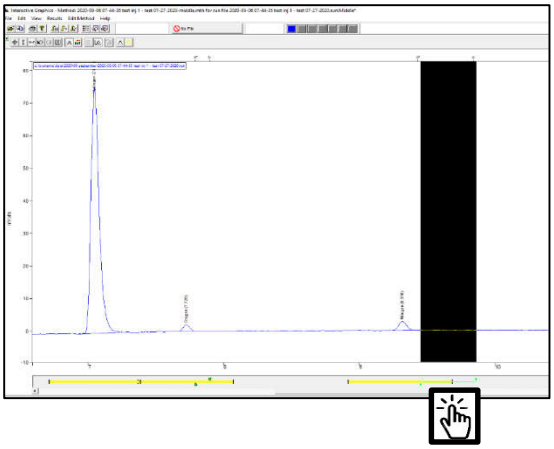




134. **Add peak table entry**- by right-clicking in window below the chromatogram.

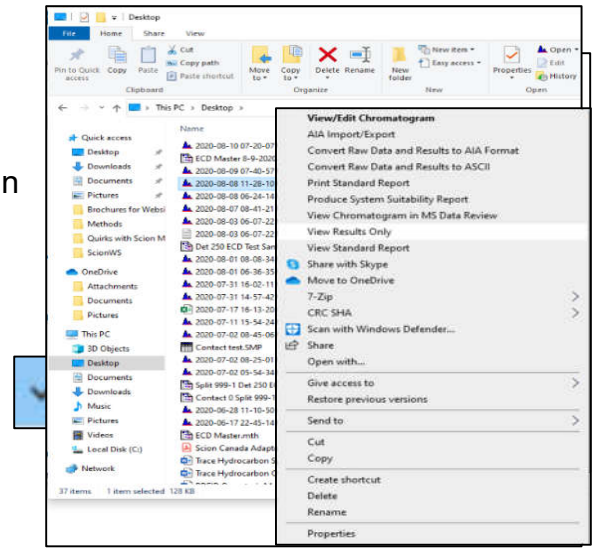
135. **Add timed events** - by right-clicking in window below the chromatogram.

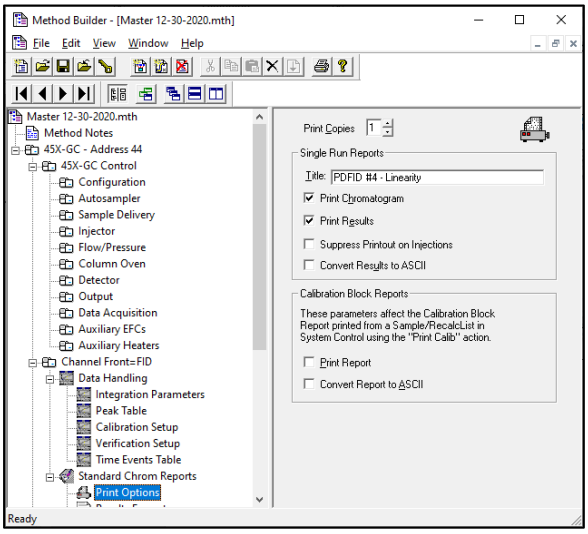
136. **Graphically relocate time events** with mouse.



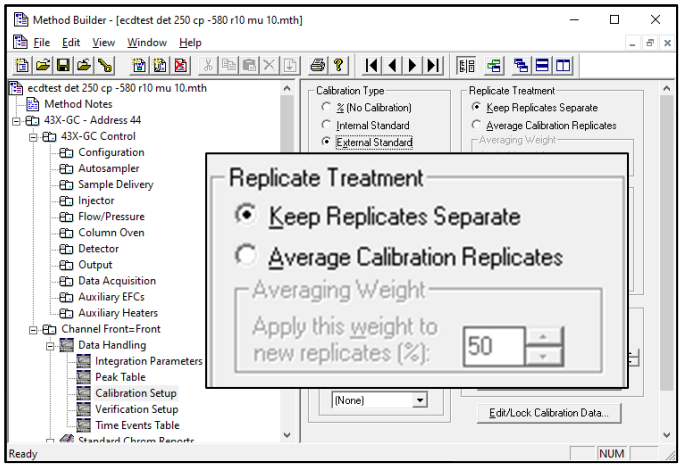
137. **Reporting and Printing of Results**:

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

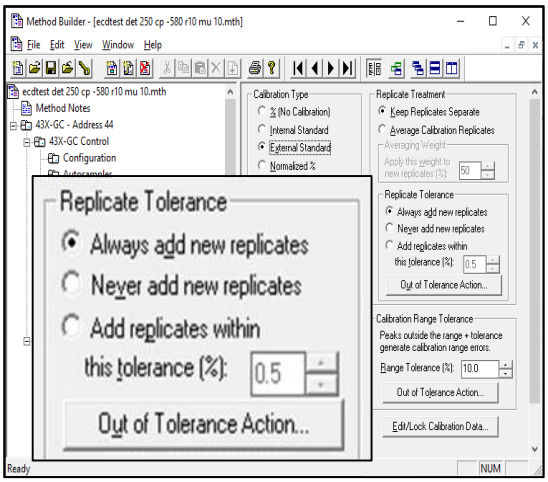




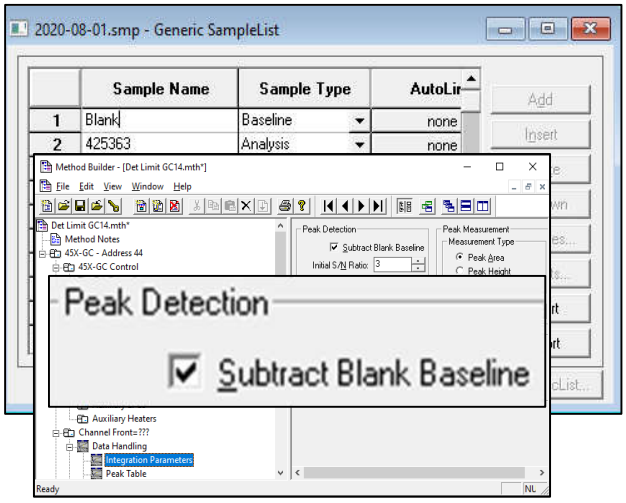
- **Chose printing parameters in method.** Printouts on injection can be suppressed to prevent operations to be locked up if printer jams.



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”.

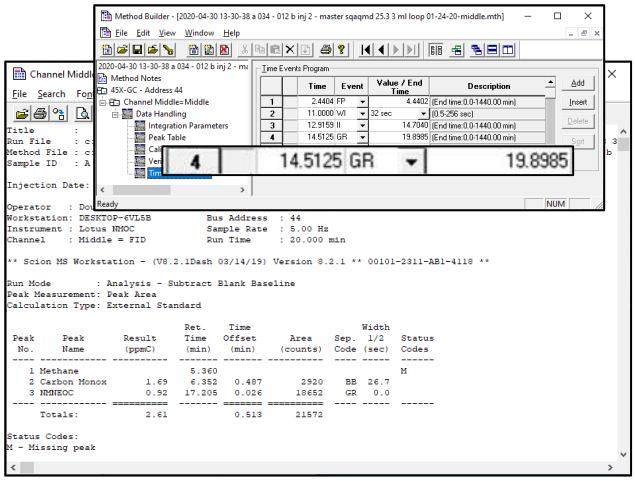


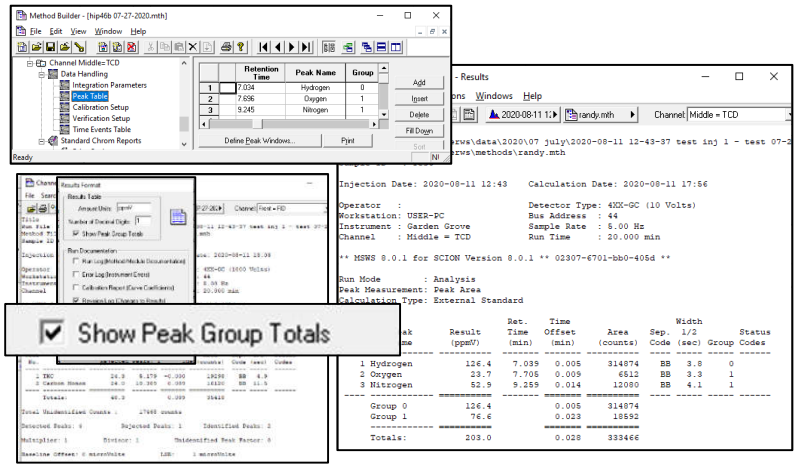
139. **Replicate Tolerance in Method Builder** - Preset value is set to add replicates within a tight tolerance of 0.5%. Better choice is either to widen the tolerance or “Always add new replicates”.



140. **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”.

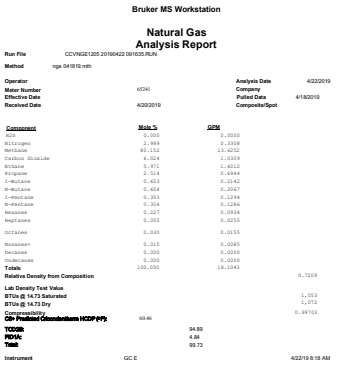
141. **Grouping by time interval** – detector response can be grouped over a user-selectable time interval. This process is often used for grouping non-methane hydrocarbons in EPA Method 25, and for summing up all hydrocarbons in natural gas for Hexane+. Assigned retention time for the group is the midpoint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

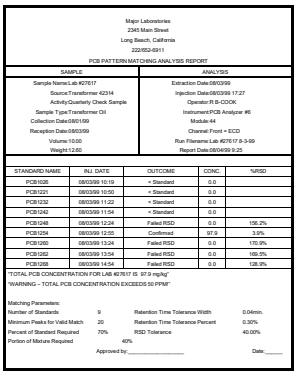




142. **Grouping by peak label** – After computations are perfomed for peak concentrations, selected peaks can be grouped by peak name. Examples include summing up separate peaks in measurement of polychlorinated biphenyls, toxaphenes, and aromatic hydrocarbons.

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.

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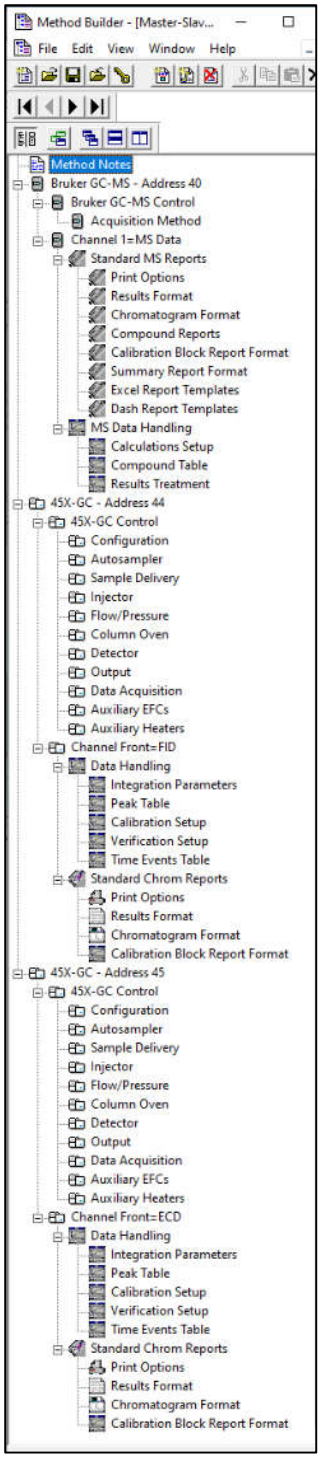
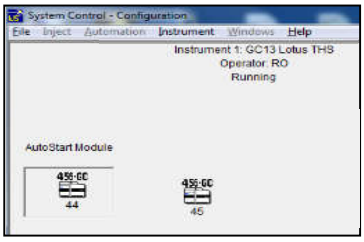
[3] Gas Processor Association, 6525 East 60th Street, Tulsa, Oklahoma 74145, http://ihsmarkit.com/products/gpa-standards.html



145. **Master/Slave Gas Chromatographs** - Some applications require more hardware capabilities than are available in one instrument. By combining two gas chromatographs 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. The configuration allows a single method to fully control two separate temperature-programmable 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 vehicle exhaust (http://lotusinstruments.com/wp/wp-content/uploads/Quantitation-of-Hydrocarbons-in-Vehicle-Exhaust-and-Ambient-Air.pdf) and measurement of trace impurities in hydrogen fuel (http://lotusinstruments.com/applications/hydrogenfuel/#hfa).



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