SOP 054 - Data Processing - Agilent Chemstation & Thermo Xcalibur Data Reduction

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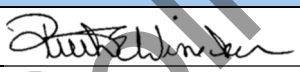
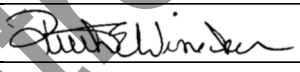
North Carolina Office of the Chief Medical Examiner Toxicology Laboratory	**Revision:**	**Revision Date/Initials:**
Approving Authority Name	**Approving Authority Signature**	**Approval Date**
Ruth E. Winecker, Ph.D.		04/08/2015
Ruth E. Winecker, Ph.D.		06/10/2016
Ruth E. Winecker, Ph.D.		08/29/2017

SOP 054 - Data Processing - Agilent Chemstation & Thermo Xcalibur Data Reduction

1. **Principle**
   1.1. This method is designed to allow a user to process Organic Base Screen, Organic Base Quant, Acid and Neutral Screen, Acid and Neutral Quant, and LC Screen data and create reports from data acquired by an Agilent GC (NPD, FID) and/or, Agilent GC/MS, Thermo GC (NPD, FID), MS, and/or LXQ Ion Trap.
2. **Specimens**
   2.1. N/A

3. **Reagents and Materials**
   3.1. N/A

4. **Instrumentation and Equipment**
   4.1. Agilent GC/MS, Agilent GC (NPD, FID) ,Thermo GC-FID, or Thermo LXQ
   4.2. Agilent Chemstation Software and/or Thermo Xcalibur Software
   4.3. Data reporting system (PC)

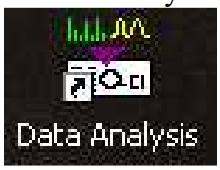
5. **Procedure**

   5.1. Copy the folder containing the acquired data to be processed (instrument PC) located in:
      5.1.1. C:\MSDChem\1\data (Agilent)
      5.1.2. C:\Xcalibur\Data (Thermo)

   5.2. Paste it into:
   S:\toxicology\Instrument Data\gcms\"instrument name" (GC/MS data) – or S:\toxicology\Instrument Data\gclc\"instrument name" (GC-NPD or FID data) - or S:\toxicology\Instrument Data\LC\LXQ (Ion Trap Data)

   5.3. Data Processing - Screen (Agilent GC/MS – Library Report)

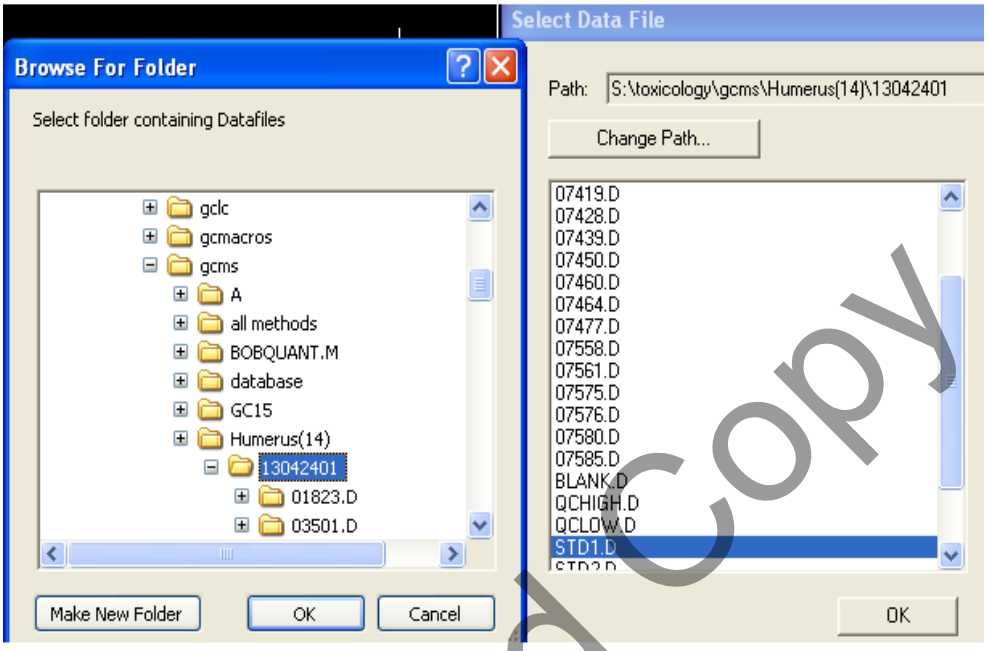
      5.3.1. On a networked PC with Agilent Chemstation Software installed, open the Chemstation software by double-clicking the ICON.

      5.3.1.1.1. 

      5.3.1.2. Open the folder containing data to be reduced by choosing: "File" – "Load Data File".

      5.3.1.3. In "Select Data File" window, select "Change Path"

      5.3.1.4. Select the desired folder – typically located on: S:\toxicology\Instrument Data\gcms\"instrument name"\"Load number".

5.3.1.5. 

5.3.1.6. In "Select Data File" window, choose the desired data file (Typically start with QC LOW). Click "OK".

5.3.1.7. Next, open the processing method to be used for this assay/data type.

5.3.1.7.1. For Organic Bases: SPLITOB.M
5.3.1.7.2. For Acid and Neutrals: ANSCRN1.M
5.3.1.7.3. Or choose appropriate Quantitation method (5.5.1).

5.3.1.7.3.1. From the menu bar select: "Method" – "Load Method..." – (to proceed select "Yes" at the prompt).

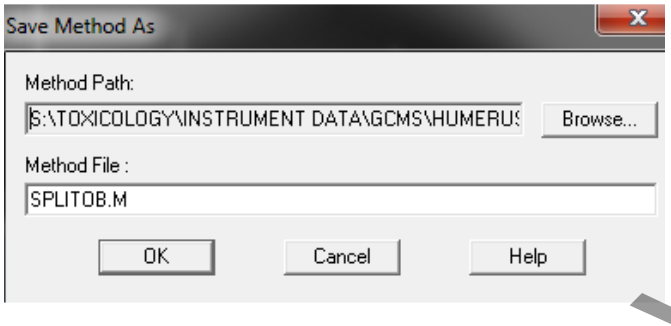
5.3.1.7.3.2. Browse to find desired method. (S:\toxicology\Instrument Methods\GC\Agilent\GCMS) – Click "OK"

5.3.1.8. Save newly loaded method into the current load folder.

5.3.1.8.1. From the menu bar select: "Method" – "Save Method..."

5.3.1.8.2. Click "Browse" and choose the location of the current load folder. Click "OK".

5.3.1.8.2.1.

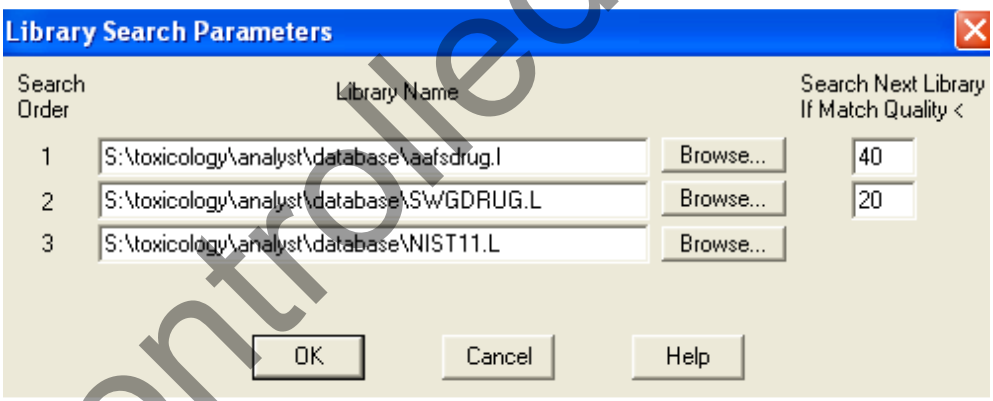


5.3.2. A macro within the software is used to detect each peak (above a specified threshold) and perform a mass spectrum library search on that compound.

5.3.2.1. To select spectral libraries - Select “Spectrum” from the menu bar and choose “Select Library”.

5.3.2.2. Use the “Browse” buttons to select libraries from S:\toxicology\analyst\database. (See Below)

5.3.2.2.1.



5.3.3. Adjust method integration threshold

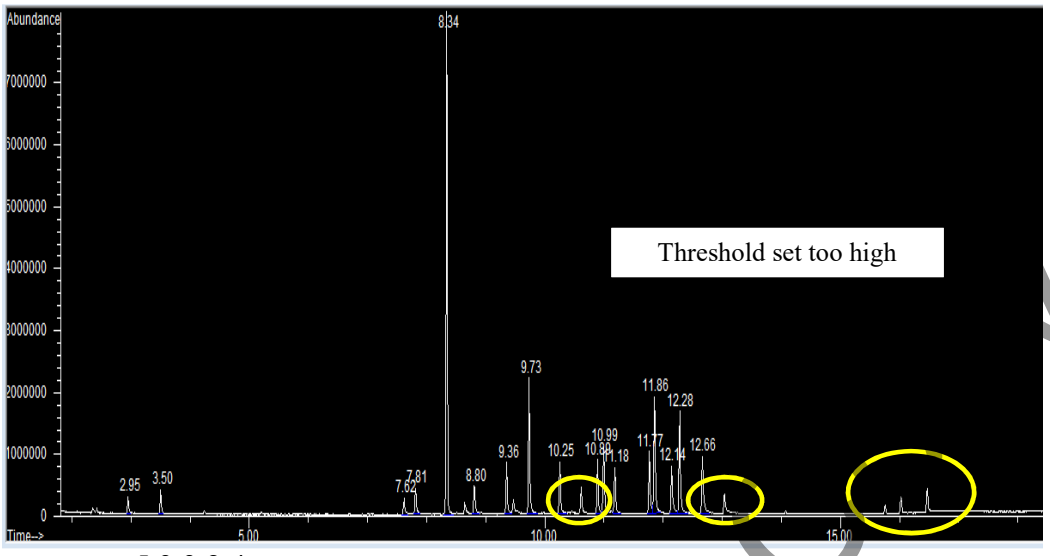
5.3.3.1. Load the “QC LOW” data file.

5.3.3.2. From the menu, select the “Integrate” icon

5.3.3.2.1. 

5.3.3.2.2. Peak integration will be evident by a retention time displayed above each integrated peak.

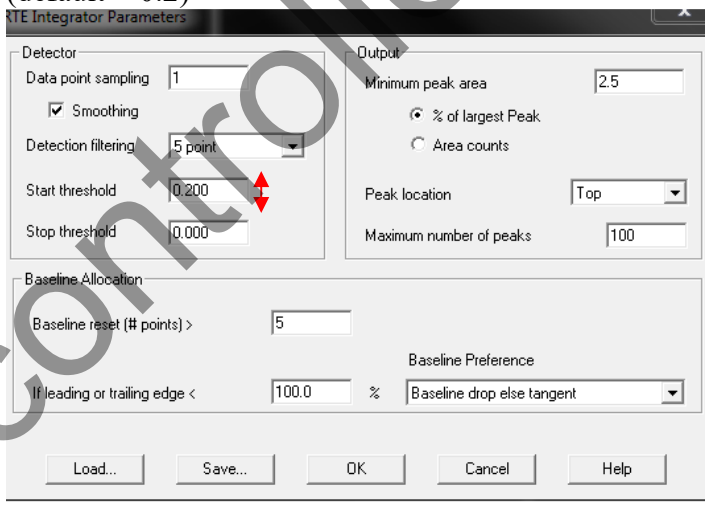
5.3.3.2.3. If all prominent peaks are not integrated (threshold set too high) or baseline noise is being integrated (threshold set too low), the integrated threshold should be adjusted (5.3.3.3).



5.3.3.2.4.

5.3.3.3. From the menu bar, select "Chromatogram – MS Signal Integration Parameters".

5.3.3.4. In the "Start threshold" box, raise or lower the threshold accordingly (default = 0.2)



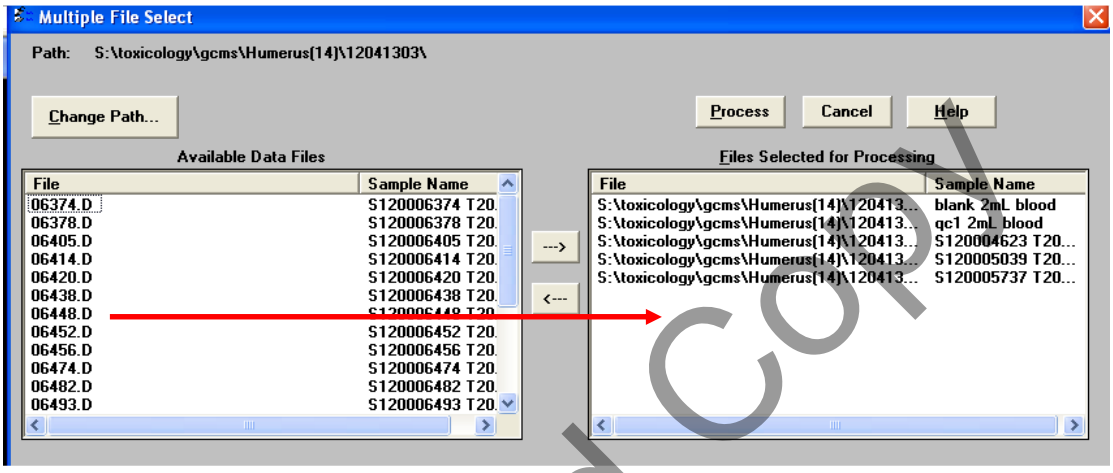
5.3.3.5.

5.3.3.6. Repeat steps from 5.3.3.2 until all prominent peaks are integrated (it is OK if some of the smaller peaks do not integrate (e.g. amphetamine, zolpedem)

5.3.4. To run the Library Match Report, select "Tools" - "DoList" – select "Use Standard DoList Options", click "OK". From the list check the box next to "Detailed Library" and click "OK".

5.3.5. In the "Multiple File Select" Box, double click or highlight and use the arrows to select files for processing (files for processing will be displayed in the box on the right). Click "Process".

5.3.5.1.



5.3.5.2. As a rule, the Blank, QC Low, and all of the cases are to be processed in this manner.

5.3.6. The requested reports will be transferred to the printer.

5.3.7. After organizing the printed reports, open each data file in turn.

5.3.8. Starting with the blank, use the detailed library reports to identify each peak based on retention time and mass spectral match.

5.3.9. For peaks with areas below the integration threshold, the library match must be performed manually.

5.3.9.1. To zoom in on a peak, hold down left mouse button and drag diagonally to form a rectangle around the area to be expanded (zoomed).

5.3.9.2. To zoom back out, double click left mouse button over chromatogram.

5.3.9.3. To view mass spectrum of a peak, double right click on the chromatogram at the retention time of the apex of the peak of interest. The mass spectrum should appear in the bottom window.

5.3.9.3.1. To search the MS library, double right click in the lower window containing the spectrum of interest.

5.3.9.3.2. In the library search window, choose the chemical name that provides the best spectral match and click "print".

5.3.9.3.3. Label the corresponding peak on the printed chromatogram with the name of the compound with the best spectral match.

5.3.9.3.3.1. **Note: For Guidelines for MS Peak Identification See Chromatographic And Mass Spectral Quality Control Section of the QA/QC Manual.**

5.3.9.3.4. Repeat for all other non-integrated peaks

5.3.10. There are often extraction artifact peaks that will be present in all chromatograms. On the blank blood chromatogram, mark these un-identified peaks with an "Ø" (not). Also, make a note on the chromatogram identifying what the not symbol represents. "Ø = Extraction Artifact".

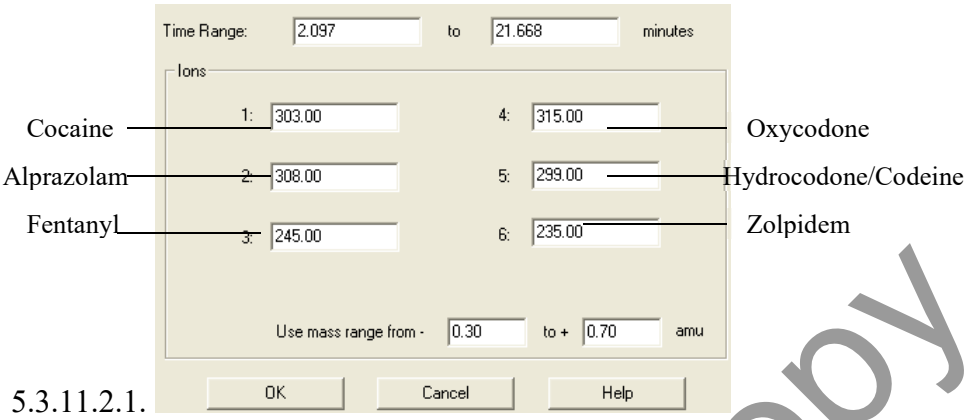
5.3.10.1. On all subsequent chromatograms peaks matching the "Ø" labeled peaks on the blank blood chromatogram can be labeled with a "Ø" symbol – all other peaks must be identified or labeled as "NI" (Not Identified).

5.3.11. Once all peaks are labeled, an Extracted Ion Chromatogram (EIC) shall be displayed

5.3.11.1. From the menu bar select: "Chromatogram" – "Extracted Ion Chromatograms..." The Extracted Ion Chromatograms window appears.

5.3.11.2. In the six "Ions" fields, enter the following ions: 303, 308, 245, 315, 299, 235. Click "OK" (see below).

5.3.11.2.1.



5.3.11.2.1.1. Note: Other ions may be substituted as needed on a case to case basis.

5.3.11.3. To display the individual EICs in merged format, select "Chromatogram" – "Display Ion Chromatograms in Merged Format".

5.3.11.4. Using the EIC, repeat steps outlined in 5.3.9.

5.4. Data Processing - Screen (Agilent GC-NPD and/or FID)

5.4.1. To Start, follow steps outlined in 5.3.1 (Processing method can be found in: S:\toxicology\Instrument Methods\GC\Agilent\NPD or FID.

5.4.2. With "STD1" loaded, Select: "Chromatogram" – "Integrate". All target peaks should be integrated with retention times displayed at their apex.

5.4.3. Select: "File" – "Print". Under "Enter window # to print" enter "2" and click "OK".

5.4.4. Repeat steps above for all calibration levels. – Collect chromatograms from printer.

5.4.5. Update retention times (RT)

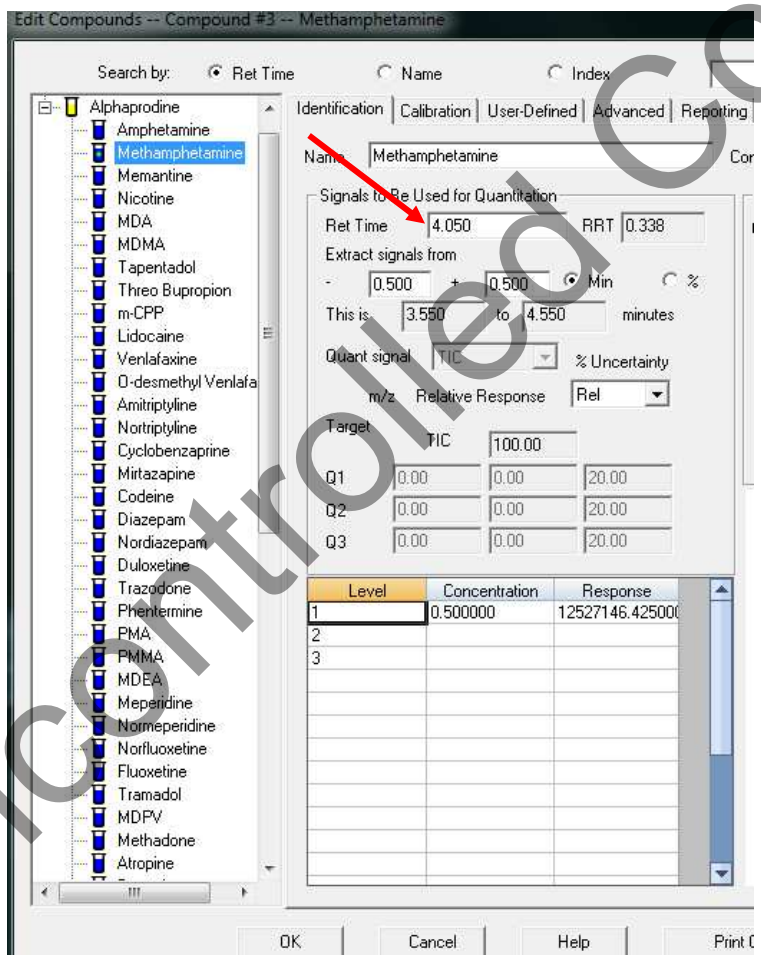
5.4.5.1. With STD1 loaded, select "Calibrate" – "Edit Compounds"

5.4.5.2. In the navigation pane, maximize the internal standard to reveal its associated analytes.

5.4.5.3. Using printed STD1 chromatogram as a reference, update the RTs for each analyte by entering the RT of the corresponding peak into the "Ret Time" field.

5.4.5.4. *Note that though the Internal Standard is listed first, it does not have the earliest retention time. Check the blank for RT of the IS.*

5.4.5.4.1. Hint: Use the Standard and Control Worksheet and GC/MS data as a reference for elution order and contents of each standard.



5.4.5.4.2.

5.4.5.5. Repeat steps outlined in 5.4.5 for all calibrators.

5.4.6. Update Calibration Levels

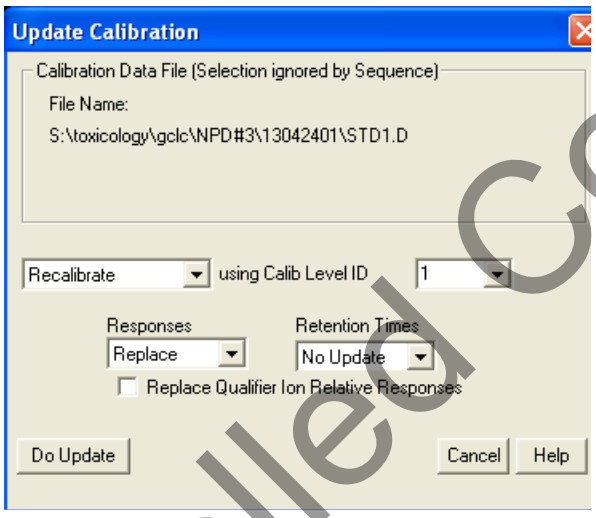
5.4.6.1. Select "Calibrate" – "Update" – "Update One Level" – click "OK".

5.4.6.2. Select "Yes" to Quantitate/Requantitate.

5.4.6.3. In “Update Calibration” window, select from the dropdown menus: “Recalibrate”, Level ID*: “1”, Responses: “Replace”, retention Times: “No Update”. (See Below)

5.4.6.3.1. *Use the following Level IDs:Std1 Level ID = 1, Std2 Level ID = 2, Std3 Level ID = 3 (Organic Bases Only)

5.4.6.3.2.



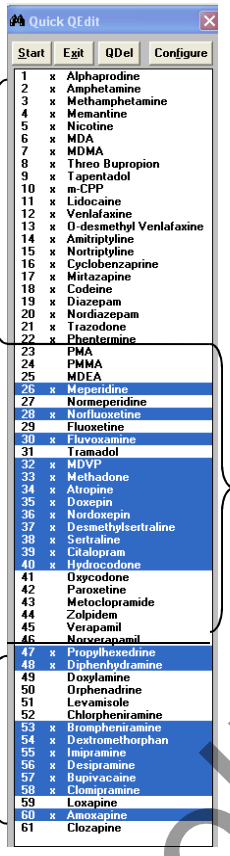
5.4.6.4. Click “Do Update”

5.4.6.5. From the menu bar, select: “Quantitate” – “Calculate”.

5.4.6.6. Select: “View”, “QEdit Quant Result”.

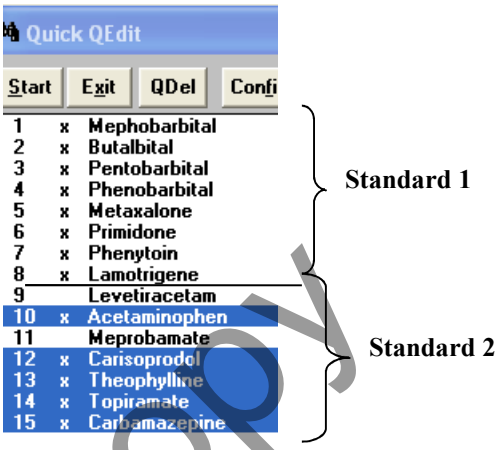
5.4.6.7. In the Quick QEdit window, while holding the Ctrl key, click on (to highlight) all detected analytes (x) that are not present in the current specimen. (Be sure not to highlight the Internal Standard (IS)).

OB Screen



5.4.6.7.1.

A/N Screen



5.4.6.7.2.

5.4.6.8. Click “QDel”. Click “Exit”

5.4.6.9. When prompted, click “Yes” to save changes made to quantitation results (Click “No” to discard changes).

5.4.6.10. Repeat steps outlined in 5.4.6 for Std2 and Std3 (if applicable).

5.4.6.10.1. For multipoint curves, print calibration plot for each analyte (follow steps outlined in 5.5.5)

5.4.6.11. Print method parameters – **Note: To print GC method data, a GC/MS data file must first be opened (any GC/MS data file).**

5.4.6.11.1. Select “File – Print – Method”.

5.4.7. Calculate and Generate Reports

5.4.7.1. Open desired data file

5.4.7.2. Select “File” – “Edit File Info...”

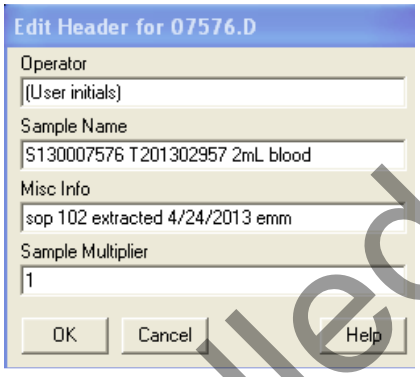
5.4.7.2.1. Operator: “User Initials”

5.4.7.2.2. Sample Name: (Sample ID + aliquot volume) e.g. “std1 2mL blood” or “S130007576 T201302957 2mL blood”

5.4.7.2.3. Misc info: (SOP# -extraction date – extractor initials) e.g. “sop 102 extracted 4/24/2013 emm

5.4.7.2.4. Sample Multiplier: Dilution factor (1 is default).

5.4.7.2.5.



5.4.7.3. Click “OK”

5.4.7.4. From the menu bar, select: “Quantitate” – “Calculate”.

5.4.7.5. Select: “View”, “QEdit Quant Result”.

5.4.7.6. In the Quick QEdit window, while holding the Ctrl key, click on (to highlight) all detected analytes (x) that are not present in the current specimen. (Be sure not to highlight the IS).

5.4.7.6.1. Us the GC/MS data generated earlier to determine which analytes are actually present in the specimen.

5.4.7.7. Click “QDel”. Click “Exit”

5.4.7.8. When prompted, click “Yes” to save changes made to quantitation results (Click “No” to discard changes).

5.4.7.9. Select “Quantitate” – “Generate Report”

5.4.7.10. Style: “Summary”, Destination: “Printer”

5.4.7.11. Click “OK”. – A report will be generated

5.4.7.12. Compare GC/MS Data to GC-NPD or FID data.

5.4.7.12.1. Hand-label any non-target analyte peaks on the GC chromatogram that have a corresponding GC/MS peak with the same relative retention time.

5.4.7.12.2. Any peaks without a GC/MS match will be labeled "NI".

5.4.7.13. Repeat steps outlined in 5.4.7 for all data files.

5.4.8. Reporting Results

5.4.8.1. Screen - Only compounds detected on both the GC/MS and GC-NPD/FID will be considered confirmed and therefore reported.

5.5. Data Processing - Quantitation (Agilent GC/MS, NPD, FID)

5.5.1. To Start, follow steps outlined in 5.3.1

5.5.2. Clear any previous calibration results:

5.5.2.1. Select "Calibrate – Clear", choose "Clear Compound Responses" and "OK".

5.5.3. Verify calibration levels match Standard and Control Worksheet.

5.5.3.1. Select "Calibrate – Edit Compounds".

5.5.3.2. The Identification Tab displays retention time, target and qualifying ions (if applicable), concentration units, and other quantitation and calibration parameters.

5.5.3.2.1. Edit these parameters as needed – see a senior chemist with any questions.

5.5.3.2.2. Navigate between compounds using the navigation pane on the left side of the screen

5.5.3.2.2.1. **Note: Target analytes can be found by maximizing (+) its associated Internal Standard.**

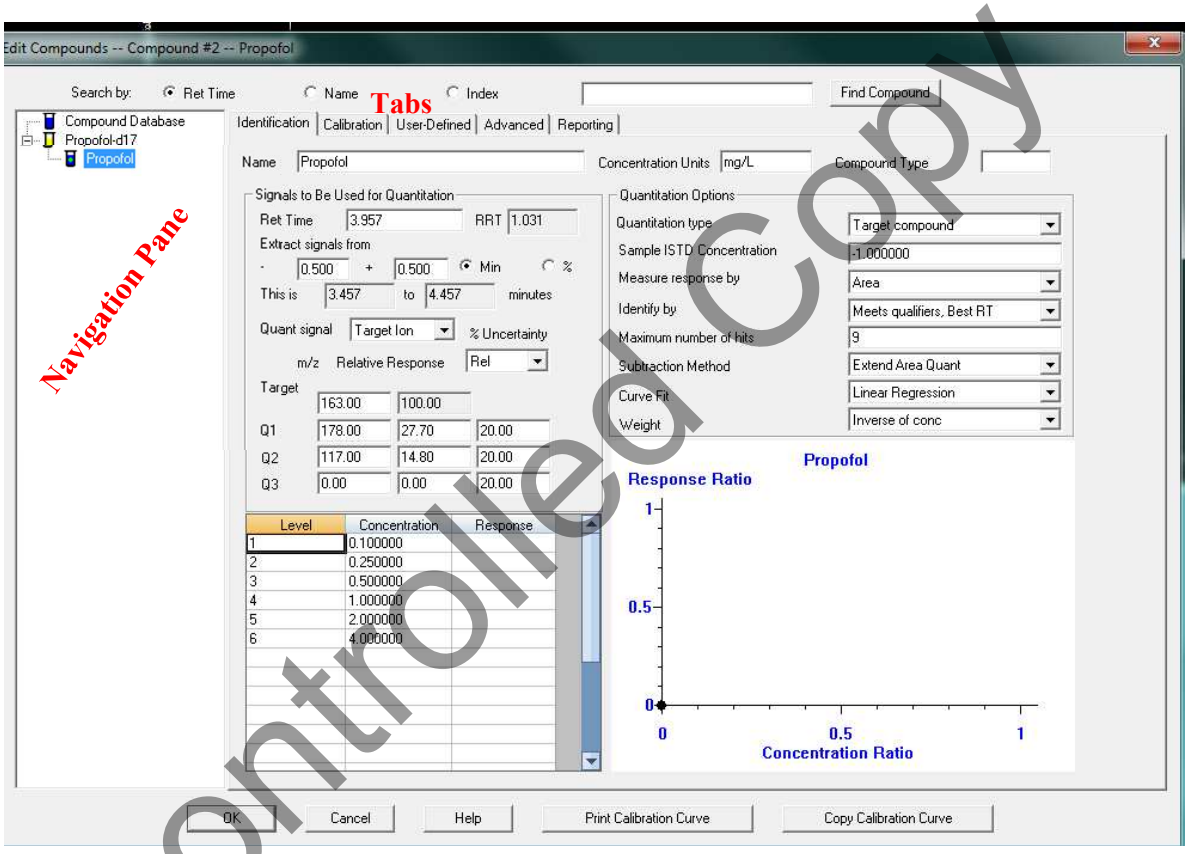
5.5.3.3. Click on the "Calibration" tab

5.5.3.3.1. Verify the levels and concentrations correspond to the Standard and Control Worksheet.

5.5.3.3.2. Navigate between compounds by selecting them on navigation pane.

5.5.3.4. Select “Exit” on Edit Compounds window and save changes when prompted

5.5.3.5.



5.5.4. Update Calibration Levels

5.5.4.1. Open datafile for the calibration level to be updated (Start with Standard 1).

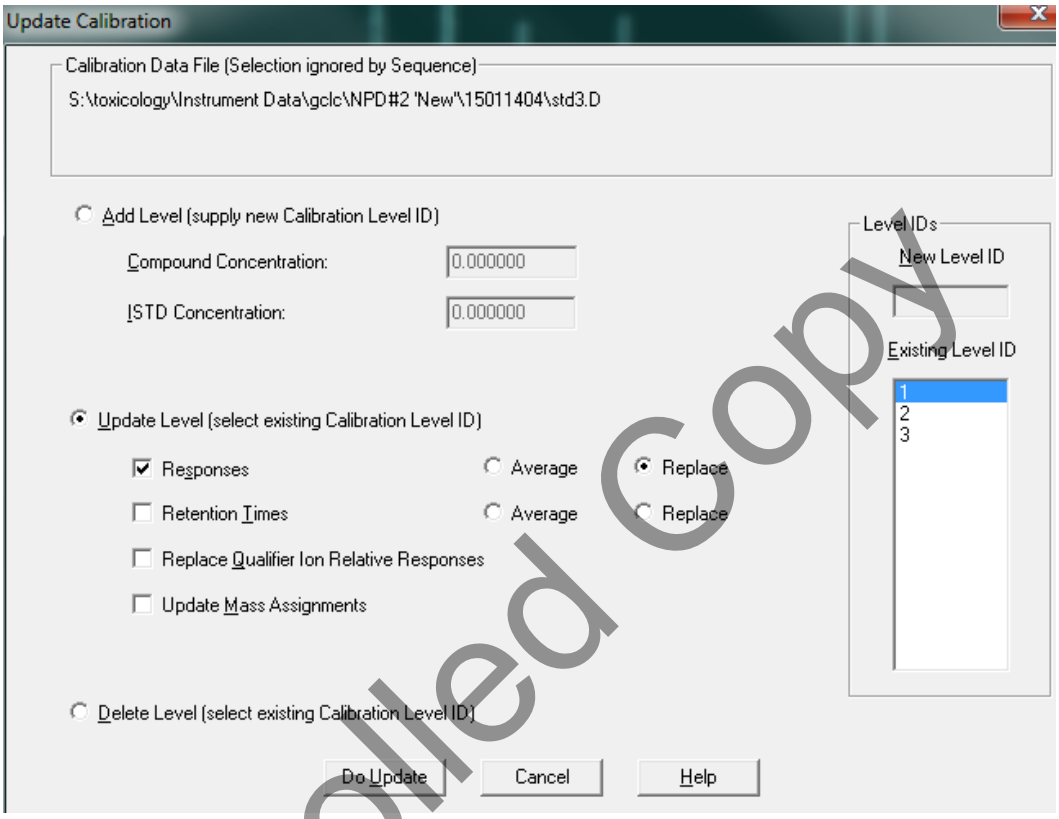
5.5.4.2. Select “Calibrate” – “Update” – “Update One Level” – click “OK”.

5.5.4.3. Select “Yes” to Quantitate/Requantitate.

5.5.4.4. Select which level to update in the “Existing Level ID” box.

5.5.4.5. Using the radio and check boxes, select to “Update Level (select existing Calibration Level ID)”, Check box next to “Responses”, and “Replace” (See Below).

5.5.4.5.1.



5.5.4.6. Click “Do Update”

5.5.4.7. Repeat steps 5.5.4.1 through 5.5.4.6 for all calibration levels.

5.5.4.8. Reload data file - Std 1

5.5.4.9. From the menu bar, select: “Quantitate” – “Calculate”.

5.5.4.10. Select: “View”, “QEdit Quant Result”.

5.5.4.11. In the Quick QEdit window, while holding the Ctrl key, click on (to highlight) all detected analytes (x) that are not actually present in the current specimen. (Be sure not to highlight the Internal Standard (IS)).

5.5.4.12. Click “QDel”. Click “Exit”

5.5.4.13. When prompted, click “Yes” to save changes made to quantitation results (Click “No” to discard changes)

5.5.5. Check Calibration Curve:

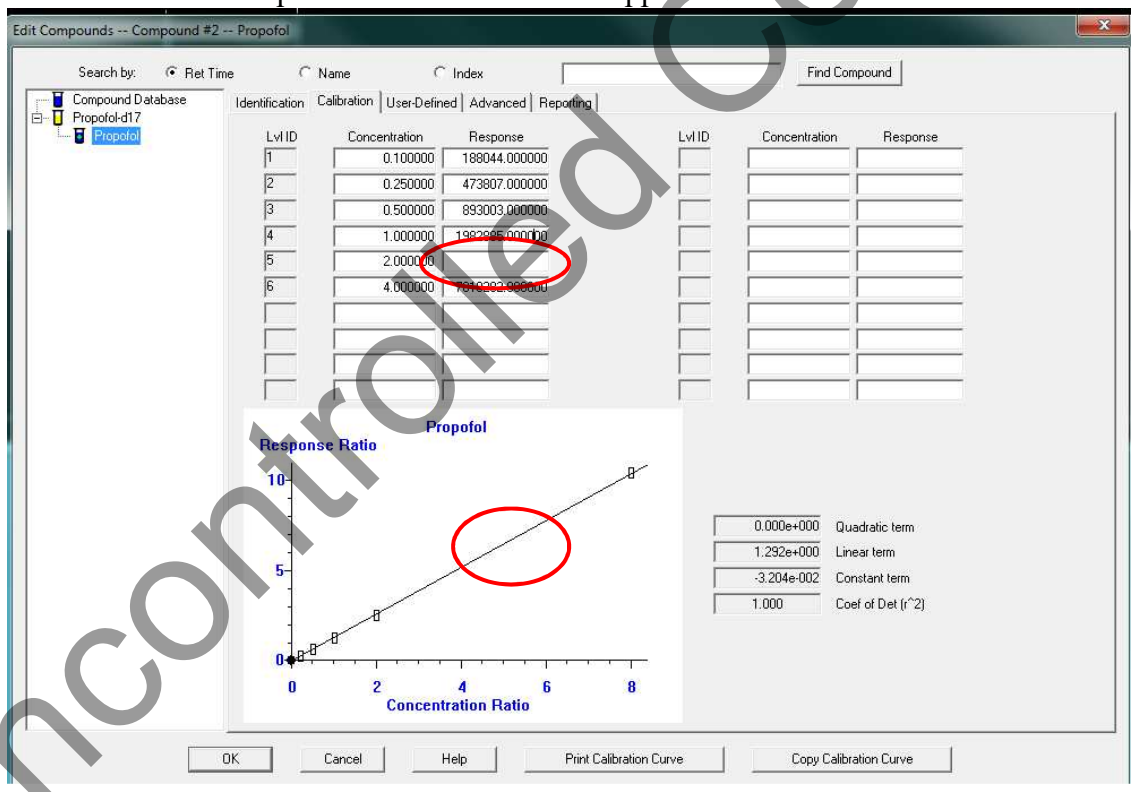
5.5.5.1. Select “Calibrate – Edit Compounds”

5.5.5.2. Choose target analyte from the navigation pane.

5.5.5.3. Open the “Calibration” Tab to view calibration curve parameters.

5.5.5.4. Check the curve parameters to see that SOP acceptance criteria is met.

5.5.5.4.1. If a calibration level must be removed in order for the curve to pass calibration criteria, delete the area response that corresponds to the level to be dropped.



5.5.5.4.2.

5.5.5.5. Select “Print Calibration Curve”.

5.5.5.6. Repeat steps outlined in 5.5.5 for all target analytes.

5.5.5.7. Select “OK”, “OK.”

5.5.6. Save Method

5.5.6.1. Select “Method – Save Method”.

5.5.6.2. "Browse" to select the current load folder, and choose "OK".

5.5.7. Print Method Parameters

5.5.7.1. Select "File – Print – Method".

5.5.8. Calculate and Generate Reports

5.5.8.1. Open desired data file (Start with Std1)

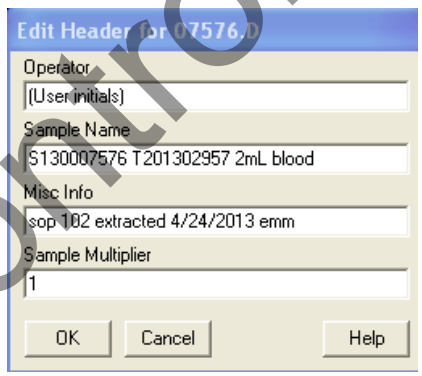
5.5.8.2. Select "File" – "Edit File Info..."

5.5.8.2.1. Operator: "User Initials"

5.5.8.2.2. Sample Name: (Sample ID + aliquot volume) e.g. "std1 1mL blood" or "S130007576 T201302957 1mL blood"

5.5.8.2.3. Misc info: (SOP# -extraction date – extractor initials) e.g. "sop 102 extracted 4/24/2013 emm

5.5.8.2.4. Sample Multiplier: Dilution factor (1 is default).

5.5.8.2.5. 

5.5.8.3. Click "OK"

5.5.8.4. From the menu bar, select: "Quantitate" – "Calculate".

5.5.8.5. Select: "View", "QEdit Quant Result".

5.5.8.6. In the Quick QEdit window, while holding the Ctrl key, click on (to highlight) all detected analytes (x) that are not actually present in the current specimen. (Be sure not to highlight the Internal Standard (IS)).

5.5.8.7. Click “QDel”. Click “Exit”

5.5.8.8. Double click on remaining detected analytes to verify peak shape and retention time.

5.5.8.8.1. QDel any analytical peak that does not meet chromatographic acceptance criteria.

5.5.8.9. When prompted, click “Yes” to save changes made to quantitation results (Click “No” to discard changes).

5.5.8.10. Select “Quantitate” – “Generate Report”

5.5.8.11. Style: “Detailed”, Destination: “Printer”

5.5.8.12. Click “OK”. – A report will be generated

5.5.8.13. Repeat steps outlined in 5.5.8 for all calibrators, specimens, and QC data.

5.6. Data Processing (Thermo GC/MS)

5.6.1. On the PC attached to the instrument that acquired the data to be processed, open Xcalibur by double-clicking the ICON.

5.6.1.1. 

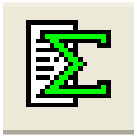
5.6.2. At the welcome screen, click on “Sequence Setup”.

5.6.3. Open the sequence that was used to acquire the data to be processed (See SOP 053).

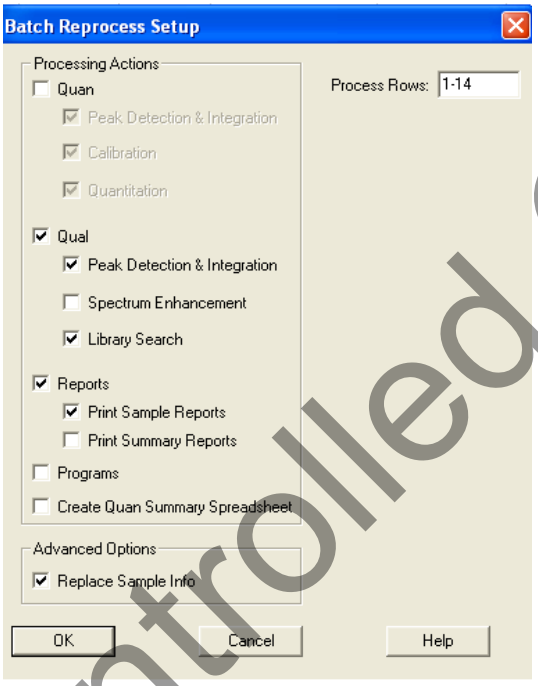
5.6.4. Double left click in the 1st row of the “Proc Method” Column, navigate to C:\Xcalibur\methods and select the appropriate processing method – the processing method will automatically fill down through the rest of the sequence.

5.6.5. Save the sequence.

5.6.6. Process the sequence by clicking on the “Batch Reprocess” icon

5.6.6.1. 

5.6.7. In the Batch Processing Setup window, select **Qual**, **Peak** Detection & Integration, and **Library Search**. Also Select Reports and Print Sample Report (see below).

5.6.7.1. 

5.6.8. Click "OK" - the software will process the data and print reports.

5.6.9. Manually label the peaks on each chromatogram using the information found in the library search report associated with each data file.

5.6.10. Click the "Roadmap" icon.

5.6.11. Choose Qual Browser.

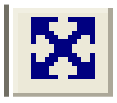
5.6.12. Open a raw file to be reduced from the load file found in C:\Xcalibur\Data

5.6.13. For all peaks of interest that were not integrated by the processing method, a library search must be done.

5.6.13.1. Click the "Pin" icon in the upper right corner of the window displaying the chromatogram – the pin should turn yellow.

5.6.13.2. Zoom in on peaks of interest by holding down the left mouse button and dragging over a section of the chromatogram.

5.6.13.3. Zoom out using the "Reset Display" icon on the menu bar.

5.6.13.3.1. 

5.6.13.4. Once the peak of interest is displayed as desired, click the "Pin" in the upper right corner of the Spectra Window.

5.6.13.5. Left click the pointer at the apex of the peak of interest, or drag it across the peak at half its height. The Spectra will be displayed in the pinned window.

5.6.13.6. Right click in the window displaying the Mass Spectra and choose "Library – Search".

5.6.13.7. A library search window will open. Adjust the window panes so the information is displayed as desired and print using the printer icon (select "All Cells in the selected window" and "One Page" in the dialog box).

5.6.13.8. Close the library report window to go back to the chromatogram display.

5.6.13.9. Repeat steps outlined in 5.6.13 for all data files in load.

5.7. Data Processing (Thermo GC- FID)

5.7.1. On the PC attached to the instrument that acquired the data to be processed, open Xcalibur by double-clicking the ICON.

5.7.1.1. 

5.7.2. At the welcome screen, click on "Sequence Setup".

5.7.3. Open the sequence that was used to acquire the data to be processed.

5.7.4. Double left click in the 1st row of the "Proc Method" Column, navigate to C:\Xcalibur\methods and select the appropriate processing method – the processing method will automatically fill down through the rest of the sequence.

5.7.5. Save the sequence.

5.7.6. Go back to the “Roadmap” page and select “Processing setup”.

5.7.7. Open the processing method located in C:\Xcalibur\Methods.

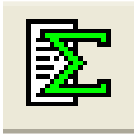
5.7.8. Choose “File – Open Raw File”. Browse to the load folder and select the data file associated with Std1.

5.7.9. In the Identification Tab, using the chromatogram display at the bottom of the screen and the MS data as a reference of retention order, update the retention times for each of the analytes in Std1.

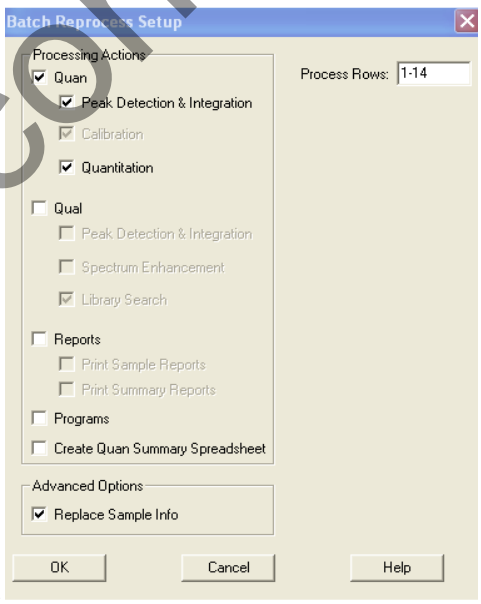
5.7.10. Repeat steps 5.7.8– 5.7.9 for Std2.

5.7.11. Save and close the Processing Method.

5.7.12. Process the sequence by clicking on the “Batch Reprocess” icon.

5.7.12.1. 

5.7.13. In the Batch Processing Setup window, select **Quan**, **Peak Detection & Integration,** and **Quantitation (**see below).

5.7.13.1. 

5.7.14. Click “OK” – the software will process the data. (Listen for the beep upon completion).

5.7.15. Go back to the “Roadmap” page and select Quan Browser.

5.7.16. Select the “All” tab to display all of the data.

5.7.17. Click on the first data file in the sequence (you can skip methanol blanks) and then click on the first analyte in the right hand column.

5.7.18. Arrow down the analyte list, fixing any poor integrations and deleting any non-peak integrations (right click on chromatogram and select “Set Peak to Not Found Status”.

5.7.19. Once all data files and analytes have been reviewed, Print reports:

5.7.19.1. Select “File – Print – Reports Dialog”.

5.7.19.2. In both the Sample Reports and Summary Reports sections, click on the first two rows in the ”Enabled” column and check the check boxes

5.7.19.3. In both the Sample Reports and Summary Reports sections, click on the second rows in the ”Save As” column and select “PDF” from the drop down box.

5.7.19.4. Select the “Select Samples...” button and, using the buttons, move the data files to be printed from the left window to the right window and select “Print Reports”.

6. Data Processing (Thermo LXQ LC/MS)

6.1.1. On the PC attached to the instrument that acquired the data to be processed, open Xcalibur by double-clicking the ICON.

6.1.1.1. 

6.1.2. In the “Roadmap View”, click on “Sequence Setup”.

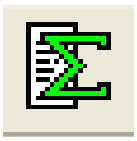
6.1.3. Open the sequence that was used to acquire the data to be processed.

6.1.4. If the processing method is not already selected, double left click in the 1st row of the “Proc Method” Column, navigate to

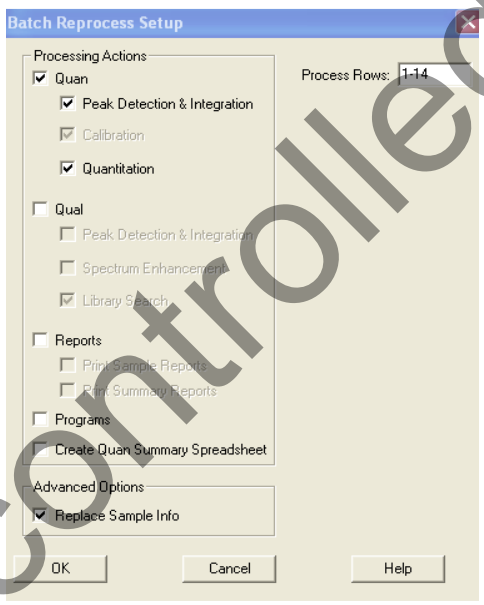
C:\Xcalibur\methods\LCMS Screen and select either the "LCMS Screen – Blood Urine" or "LCMS Screen – Liver", depending on the specimen type – the processing method will automatically fill down through the rest of the sequence.

6.1.5. Save the sequence.

6.1.6. Process the sequence by clicking on the "Batch Reprocess" icon.

6.1.6.1. 

6.1.7. In the Batch Processing Setup window, select **Quan**, **Peak Detection & Integration,** and **Quantitation (**see below).

6.1.7.1. 

6.1.8. Click "OK" – the software will process the data. (Listen for the beep upon completion).

6.1.9. Go back to the "Roadmap View" page and select Quan Browser.

6.1.10. Select the "All" tab to display all of the data.

6.1.11. Click on the first data file in the sequence (you can skip methanol blanks) and then click on the first analyte in the right hand column.

6.1.12. Review every analyte of each sample.

6.1.12.1. Delete any non-analyte integrations by right-clicking on the chromatogram and select “Set Peak to Not Found Status.”

6.1.12.2. To manually add a peak right-click on the chromatogram and select “Manually Add Peak”

6.1.12.3. To change an integration parameter, right-click in the chromatogram and select “User Peak Detection Settings” and adjust parameters under the “Identification” tab.

6.1.12.3.1. Click “OK” to apply to only that sample, or

6.1.12.3.2. Click “Apply to All” to apply settings to all samples.

6.1.12.4. After all integrations have been checked and/or changed, select File-Save All.
NOTE: Failure to do so will result in the changes not being reflected in the Sequence Summary report.

6.1.13. Once all data files and analytes have been reviewed, Print reports:

6.1.13.1. Select “File – Print – Reports Dialog”.

6.1.13.2. In both the Sample Reports and Summary Reports sections, click on the first two rows in the ”Enabled” column and check the check boxes

6.1.13.3. In both the Sample Reports and Summary Reports sections, click on the second rows in the ”Save As” column and select “PDF” from the drop down box.

6.1.13.4. If needed, select a report template by navigating to C:\Xcalibur\templates\LCMS Screen and select either “LCMS Screen – Sample Report” or “LCMS Screen – Summary Report” for the sample and summary reports, respectively.

6.1.13.5. Select the “Select Samples...” button and, using the buttons, move the data files to be printed from the left window to the right window, or click “Add All”, click “OK”, then select “Print Reports”.

7. **References**

7.1. Hewlett Packard Corp. Understanding Your Chemstation. 1994. User Manual. Waldbronn, Germany.

7.2. Thermo Scientific. *Thermo Xcalibur Acquisition and Processing User Guide*. Sept. 2010. User Manual. USA.