



Quantitation using MassLynx

3_5_007



Quantitation

- ◆ Determines the concentration of specific analytes within a sample

- ◆ Acquisition Modes:
 - Multiple Reaction Monitoring (MRM)
 - Single Ion Recording (SIR)
 - Full Scan Acquisitions

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QuanLynx Quantification

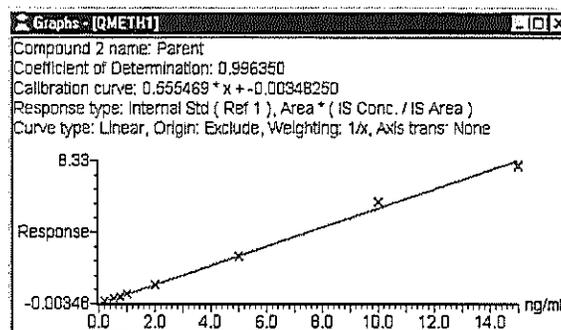
- ◆ QuanLynx with an EPCAS System is Designed to Be a Part of a 21 CFR Part 11 Compliant Environment.
- ◆ QuanLynx Reports are Easy to Customize and Results Can be Easily Stored for Later Viewing.
- ◆ The Numerical Results are the Same with and without QuanLynx.

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How do we quantitate?

- ◆ In addition to unknown samples, run a set of standards to form a calibration curve.
- ◆ MassLynx analyzes the response of unknown samples and compares their response to that indicated by the calibration curve, then calculates the concentrations of the unknowns.



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More on how do we quantitate?

Steps in Creation of a Calibration Curve for Quantitation

- ◆ Integrate peaks in chromatograms
- ◆ In each chromatogram, determine the location of the peak relating to a specific compound
- ◆ Calculate response factor for the located peak
- ◆ Create a Calibration Curve for that compound

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What do I need to do to run Quantify?

- ◆ Standard Sample list plus two additional categories:
 - Sample Type
 - Concentration A (B, C, D....)

	File Name	File Text	MS File	Inlet File	Bottle	Inject Volume	Sample Type	Conc A
1	ASSAY01	plasma blank	DEFAULT	DEFAULT	1	10.000	Blank	0
2	ASSAY02	0.2pg/ml std	DEFAULT	DEFAULT	2	10.000	Standard	0.2
3	ASSAY03	0.5pg/ml std	DEFAULT	DEFAULT	3	10.000	Standard	0.5
4	ASSAY04	0.75pg/ml std	DEFAULT	DEFAULT	4	10.000	Standard	0.75
5	ASSAY05	1pg/ml std	DEFAULT	DEFAULT	5	10.000	Standard	1
6	ASSAY06	2pg/ml std	DEFAULT	DEFAULT	6	10.000	Standard	2
7	ASSAY07	5pg/ml std	DEFAULT	DEFAULT	7	10.000	Standard	5
8	ASSAY08	10pg/ml std	DEFAULT	DEFAULT	8	10.000	Standard	10

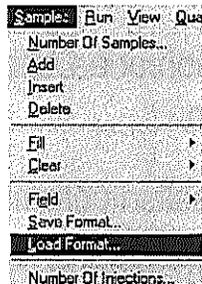
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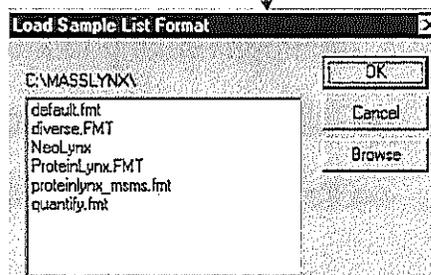
How do I add these?

Two ways to add these fields:

- 1) Use the "**Sample / Load Format**" menu item and load in a format that already has these fields.
- 2) Use the "**Customize Field Display**" button and add the fields.



sample / format / load



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Review of Sample Types

- | | |
|------------|--|
| Blank - | Solvent or matrix, insures that system is clean and/or shows endogenous material in sample. |
| Standard - | Sample of a known concentration, used to form calibration curve. |
| Analyte - | Sample of unknown concentration. |
| QC - | Quality Control - Known concentrations, used to test the validity and accuracy of the calibration curve. |

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Specify Sample Types and Concentrations

- ◆ Pull Down menu within the sample list. Specify whether the sample is a Blank, Standard, Analyte or QC.

Sample Type
Blank
Analyte
Blank
QC
Standard

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Concentration A or (B, C...)

- ◆ The known concentrations of Standards or QC's must be entered into this column.

Conc A
0.2
0.5
0.75
1
2
5
10
15
0.3
2
12



Example Project in MassLynx to Practice On

Project = Quantify.pro

Set of analyses on samples using a MS method that had:

- ◆ MRM of 3 channels

Internal Standard (294.1 > 64.0)

Analyte 1 - Parent Drug (288.1 > 58.0)

Analyte 2 - Metabolite (274.1 > 182.1)

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Internal Standards

- ◆ Used to account for Experimental Drift
- ◆ Can be Added at Various Points in the Analysis
 - In the Original Sample
 - Before Injection by the LC
- ◆ Response of Analyte in a Sample is:

$$\frac{\text{(Peak Area of Analyte)}}{\text{(Peak Area of I.S.) / (Conc of I.S.)}}$$

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Quantification Steps

1. Set up Integration of Chromatogram Peaks.
2. Create Quantification Method.
3. Process Samples.
4. Check Results – Adjust if Needed.
5. Print Out Results – Save Results on Computer.

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1.A Set Up Peak Integration

- ◆ Go to the Sample List and highlight a Standard in the middle of the range.
- ◆ Click on the Chromatogram hot key.

	File Name	File Text	MS File	Inlet File	Bottle	Inj Vol	Sample Type	Conc A
1	ASSAY01	plasma blank	DEFAULT	DEFAULT	1	10	Blank	0
2	ASSAY02	0.2pg/ml std	DEFAULT	DEFAULT	2	10	Standard	0.2
3	ASSAY03	0.5pg/ml std	DEFAULT	DEFAULT	3	10	Standard	0.5
4	ASSAY04	0.75pg/ml std	DEFAULT	DEFAULT	4	10	Standard	0.75
5	ASSAY05	1pg/ml std	DEFAULT	DEFAULT	5	10	Standard	1
6	ASSAY06	2pg/ml std	DEFAULT	DEFAULT	6	10	Standard	2
7	ASSAY07	5pg/ml std	DEFAULT	DEFAULT	7	10	Standard	5
8	ASSAY08	10pg/ml std	DEFAULT	DEFAULT	8	10	Standard	10
9	ASSAY09	15pg/ml std	DEFAULT	DEFAULT	9	10	Standard	15

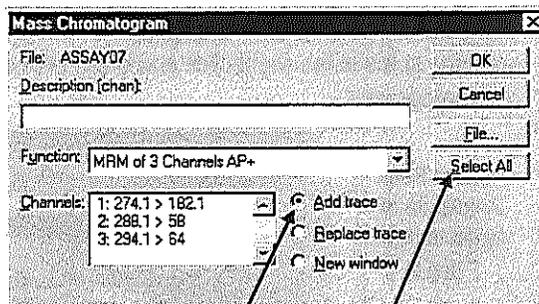
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1.B Peak Integration-Display All Traces

- ◆ The TIC for the highlighted sample will be brought up.
- ◆ Click **Display, Mass** from the top of the chromatogram window.

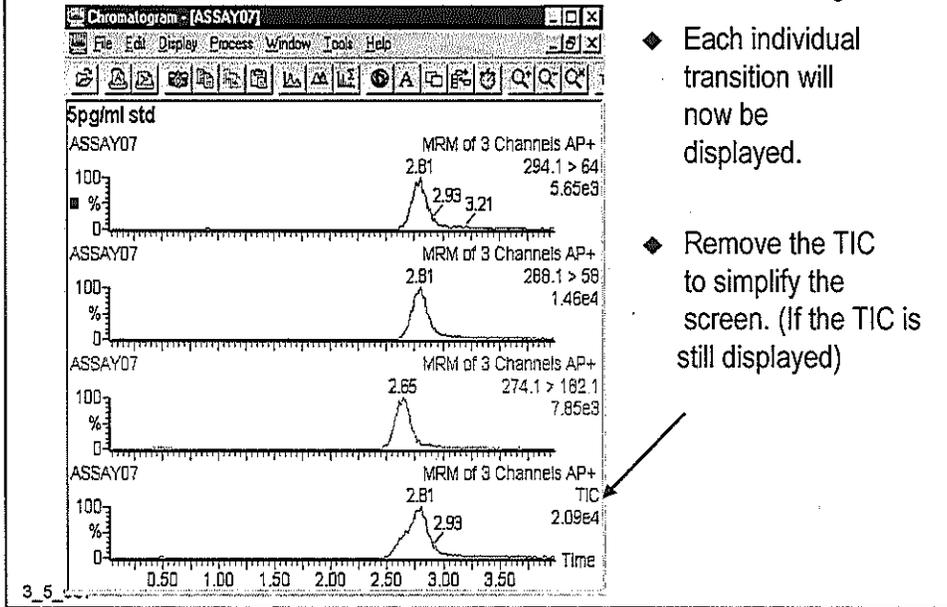
click **Add Trace** and **Select All** to bring up all of the transitions.



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Three Ion Chromatograms Should Now Be Shown

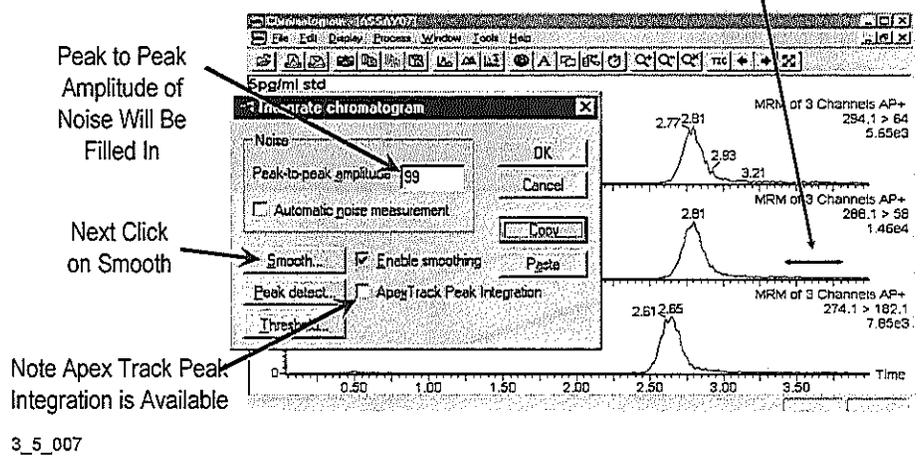


- ◆ Each individual transition will now be displayed.
- ◆ Remove the TIC to simplify the screen. (If the TIC is still displayed)



1.C Setup Peak Integration-Noise

To setup the Integration use the (*Process, Integrate*) menu item to get the 'Integrate Chromatograms' dialog box. First determine the baseline noise by grabbing some noise (right click and drag) over a quieter area of the chromatogram.





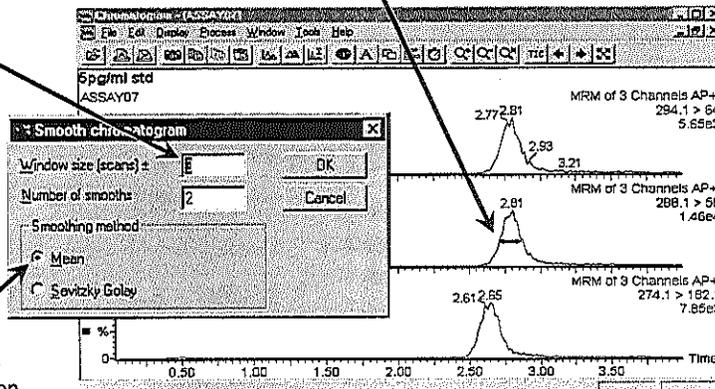
1.D Setup Peak Integration-Smoothing

Continue setting up Integration Process: After Clicking on **Smooth**, Right click and drag over the peak at half height.

Window Size
Will Be
Filled In

Use Mean
Method When
Smoothing
Chromatograms

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1.E Setup Peak Integration – Peak Detect

Integrate chromatogram

Noise
Peak-to-peak amplitude: 1700
 Automatic noise measurement

Smooth... Enable smoothing
Peak detect... ApexTrack Peak
Threshold...

Without Apex Peak
Integration

Setups Baseline

Shoulder

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Peak Detect

Handles Valleys

Baselines

Join valleys if peaks resolved to
30.00 % above baseline

Reduce peak tailing until trailing edge
is no more than
50.00 % wider than leading edge

Raise baseline by no more than
5.00 % of peak height.

Peak separation

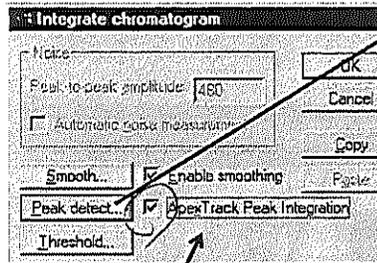
Draw vertical if peaks resolved to
90.00 % above baseline.

Detect Shoulder peaks
if slope is less than
30.00 % of maximum.

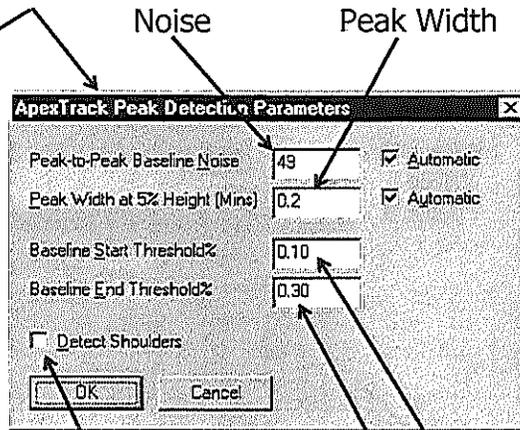
OK Cancel



1.F Setup Peak Integration – Peak Detection with Apex Integration



If Apex Track Peak Integration is selected, noise determination parameters are set up in the peak detect box. Noise and Peak width can be determined automatically.



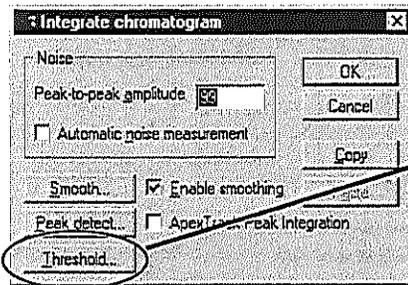
Select if you want Shoulders detected

Set starting and ending Baseline levels

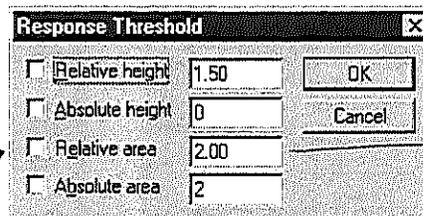
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1.G. Quant Method Editor – Integration Parameters



Peak Threshold parameters can also be adjusted in the Method Editor



Specify Criteria to Discriminate Peaks from Noise. For 'Relative' values, enter the percentage of the largest peak (base peak) a peak must exceed to be integrated.

V 5.00

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1.H Setup Peak Integration Parameters

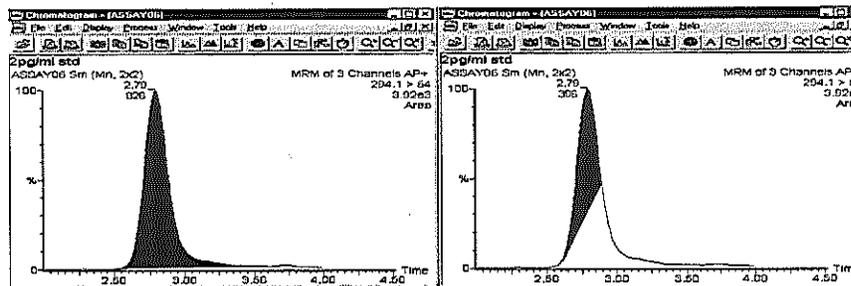
- ◆ After entering Noise and Smoothing parameters, click **Copy** - this will save the integration parameters for this transition to the clipboard.
- ◆ Click **OK**, the peak of interest will be integrated.
- ◆ Review the integration - is it acceptable? If not, repeat the integration with different parameters (noise, peak detect, thresholding) until satisfactory results are obtained.
- ◆ Once an acceptable integration is obtained, you may want to test it on a low range standard and a high range standard to insure that parameters are adequate for the full range of response.

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press 
before integrate
press 



1.I Review Peak Integration



Example of a peak with suitable integration parameters and a poorly integrated peak.

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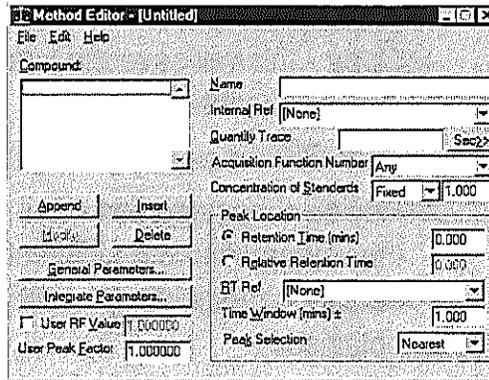
QuantInyx → Edit Method



2. Build Quantitation Method

- ◆ Building the Quantitation Method:
From the 'Quantify' menu,
Choose 'Method'

When the Method Editor dialog appears, choose 'File, New' to get a blank method.



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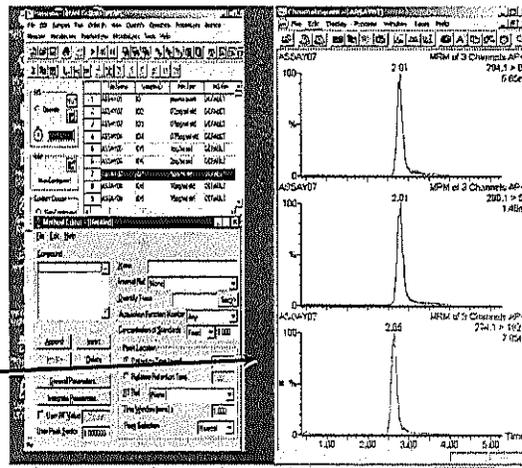
Hint. It will be easier if you:

Reduce the size of the Sample List window so this window along with the Method Editor dialog box occupies half of the screen and the chromatogram window occupies the other half of the screen.

Main MassLynx
Sample List
Window

Method Editor
Dialog Box

Chromatogram
Window



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2.A Quant Method Editor – Name of Substance

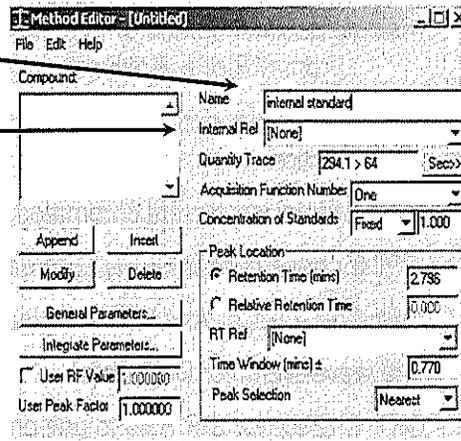
◆ Name

Enter appropriate name

◆ Internal Ref

Use the pull down menu on the right side of the box

- Select Int Std for analytes
- 'None' for Int Std (or if no I.S. is used)



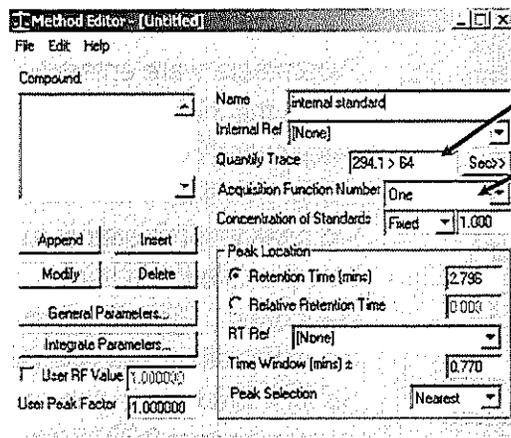
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2.B Quant Method Editor – Trace & Peak Info

◆ Quantify Trace

From the Chromatogram window, 'right click and drag' over the peak of interest and the transition (Quantify Trace) and the Acquisition Function Number will be entered for you.



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The Quantify Trace is the trace descriptor of the chromatogram being used to quantify the compound.

This can be:

- A single decimal number (m/z) for mass chromatograms (from SIR or Full Scan (continuum or centroid))
- Two decimal numbers separated by a ">" for an MRM function e.g. 609.2 > 195.1
- 'TIC' for total ion current chromatograms
- 'BPI' for base peak intensity chromatograms
- An1, An2, An3, or An4 for analog data
- The wavelength for DAD data.
- Ch1, Ch2 etc for SIR data to use one quantify method with multiple SIR functions. Where Ch1 is the first mass in the list, Ch2 is the second etc.

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2.B Quant Method – More on Trace & Peak Info

The screenshot shows a software dialog box with the following fields and values:

- Name: ABC Int Std
- Internal Ref: [None]
- Quantity Trace: 294.1 > 64 (with a 'Sec>' button)
- Acquisition Function Number: One
- Concentration of Standards: Fixed 1.000
- Peak Location section:
 - Retention Time (mins): 2.79
 - Relative Retention Time: 0.000
- RT Ref: [None]
- Time Window (mins) ±: 0.42
- Peak Selection: Largest

Peak Location and Time Window Parameters can be entered from the keyboard if needed. Also to correct the peak retention time you can just 'right click' (no 'drag') on the peak at the correct retention time.

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◆ Peak Location: Retention Time (RT) and Time Window

Parameters were entered during the 'right click and drag' over the peak. 'RT' is center of a time interval that the peak must appear in to be associated with this compound. 'Time Window' is the half width of this interval. So for this example, the peak must appear at 2.79 ± 0.42 min.



2.C Quant Method Editor – Peak Selection

◆ Peak Selection

If more than one peak is detected in the 'Time Window', this designates which peak to choose.

The peak **Nearest** to the entered RT,
the **Largest** peak,
the **First** peak,
the **Last** peak
or **Totals** (sum of all of the peaks).

Method Editor - [Untitled]

File Edit Help

Compound:

Name: internal standard

Internal Ref: [None]

Quantity Trace: 294.1 > 84 Sec>>

Acquisition Function Number: One

Concentration of Standards: Fixed 1.000

Peak Location:

Retention Time (mins): 2.796

Relative Retention Time: 0.000

RT Ref: [None]

Time Window (mins) ±: 0.770

Peak Selection: Nearest

Buttons: Append, Insert, Modify, Delete, General Parameters..., Integrate Parameters..., User RF Value: 1.000000, User Peak Factor: 1.000000

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2.D Quant Method Editor – Add Compound to List & General Parameters

- ◆ Click **Append** to enter into the Compound List (or click on 'Insert' to put a compound in a certain spot in the list).

then

- ◆ Click **General Parameters**. The 'General Method' parameters dialog box should appear.

Method Editor - [Untitled]

File Edit Help

Compound:

Name: internal standard

Internal Ref: [None]

Quantity Trace: 294.1 > 84 Sec>>

Acquisition Function Number: One

Concentration of Standards: Fixed 1.000

Peak Location:

Retention Time (mins): 2.796

Relative Retention Time: 0.000

RT Ref: [None]

Time Window (mins) ±: 0.770

Peak Selection: Nearest

Buttons: Append, Insert, Modify, Delete, General Parameters..., Integrate Parameters..., User RF Value: 1.000000, User Peak Factor: 1.000000

IS → x
Std → choo
IS.c

General Method

Response:

Type: External (absolute)

Areas: External (absolute), Internal (relative)

Concentration:

Units:

Calibration Curves:

Polynomial Type: Linear

Point of Origin: Exclude

Fit Weighing: None

Axis Transformation: None

Buttons: OK, Cancel

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2.E Quant Method Editor – General Parameters

'External' for I.S. (or if no Int Std used)
'Relative' for Analytes with an I.S.

Polynomial Type

For Int. Std. :

Average RF

For Analytes :

Linear or Quadratic

Point of Origin

Typically Exclude

Fit Weighting

Start with 1/X

(none for I.S.)

Axis Transformation

Typically none

◆ **Concentration Units**
Enter Units for X Axis
of calibration curve
(e.g. 'ng/mL')

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IS → External
Std - Interbank

IS → Average
Std → Linear
Exclude
1/X



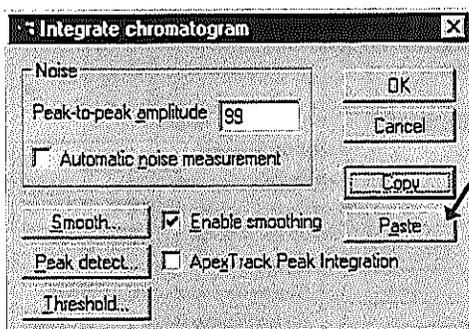
2.F Quant Method Editor – Integration Parameters

Click on 'Integration Parameters' to enter the
integration setup for this method.

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2.F Quant Method Editor – Integration Parameters



◆ Integrate Parameters

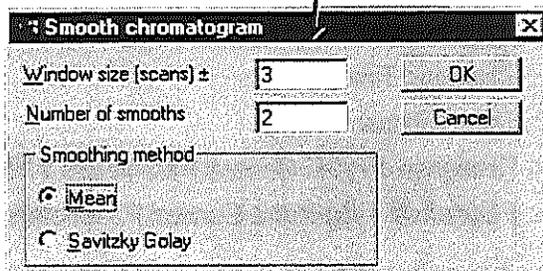
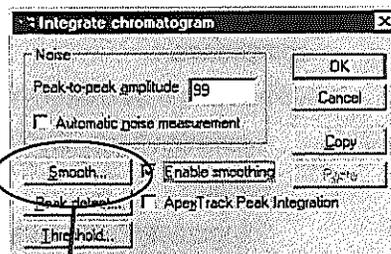
Same window from before appears, click on 'Paste' to input the parameters determined earlier for that transition and 'Copied' from the chromatogram window.

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2.F. Quant Method Editor – Integration Parameters

You can also manually change the Integration Parameters here. Use the same procedures used when integrating peaks in a chromatogram (for example the smoothing parameters can be adjusted).



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2.G Quantification Method Editor

Example of a
Quantification
Method
Filled Out
for the
Internal
Standard

The screenshot shows the 'Method Editor - [Untitled]' window. The 'Compound' dropdown is set to 'Internal standard'. The 'Name' field is 'internal standard'. 'Internal Ref' is '(None)'. 'Quantity Trace' is '294.1 > 64 Sec>>'. 'Acquisition Function Number' is 'One'. 'Concentration of Standards' is 'Fixed' with a value of '1.000'. Under 'Peak Location', 'Retention Time (mins)' is selected with a value of '2.796', and 'Relative Retention Time' is '0.000'. 'RT Ref' is '(None)'. 'Time Window (mins) ±' is '0.770'. 'Peak Selection' is 'Nearest'. At the bottom, 'User RF Value' is '1.000000' and 'User Peak Factor' is '1.000000'. Buttons for 'Append', 'Insert', 'Modify', and 'Delete' are visible, along with 'General Parameters...' and 'Integrate Parameters...'.

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2.H Adding to the Quantify Method

- ◆ This entire process now needs to be repeated for the two other compounds.
- ◆ Things that may differ between compounds:
 - Transition (Quantify Trace)
 - Name
 - Integration Parameters
 - Internal Reference (Select Internal Standard if Used)
 - Concentration of Standards
 - Retention Time
 - Time Window
 - Response Type in General Parameters Window
 - Polynomial Type in the General Parameters Window

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2.I. Quantification Method Editor

Example of Quantification Method Filled Out For All Three Compounds

If you change any of the parameters for a compound (e.g. 'Conc of Stds', R.T., etc.), Click on 'Modify' to save the changes.

Note: Internal Standard Specified For Compound 3.

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2.J. Other Considerations

◆ Propagation

Edit, Propagate

When checked, all values in that category that are entered for any one compound will automatically be assigned and identical for all compounds in that Quantify Method.

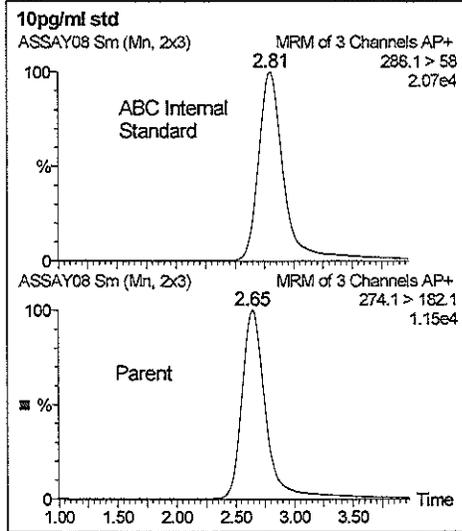
importance

For Example: Since 'Integrate Parameters' is 'checked', all of the compounds will use the same integration parameters (smoothing, etc.) when integrating peaks. You can 'uncheck' this and then enter different integration parameters for each compound if desired.

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2.K. Quantification Method Editor – Relative R.T.



R.T. of Parent Relative to Int. Std.

$$3_5_007 \quad (2.65) / (2.81) = 0.937$$

Method Editor - [Untitled]

Name: metabolite

Internal Ref: 1: internal standard

Quantity Trace: 274.1 > 182.1 Sec>>

Acquisition Function Number: One

Concentration of Standards: Conc. A 1.000

Peak Location:

Retention Time (min): 2.619

Relative Retention Time: 0.937

RT Ref: 1: internal standard

Time Window (min) ±: 0.522

Peak Selection: Nearest

Example of Use of Relative Retention Time



2.L. Quant Method Editor-User RF/Peak

Minor Points About the Method Editor.

User RF Value

If no calibration curve is available, then divide the peak area (response) by this factor to calculate the conc.'s.

User Peak Factor

All concentrations calculated will be multiplied by this factor.

Method Editor - METABOLITE

File Edit Help

Compound:

1: internal standard

2: parent

3: metabolite

Name: metabolite

Internal Ref: 1: internal standard

Quantity Trace: 274.1 > 182.1 Sec>>

Acquisition Function Number: One

Concentration of Standards: Conc. A 1.000

Peak Location:

Retention Time (min): 2.602

Relative Retention Time: 0.000

RT Ref: [None]

Time Window (min) ±: 0.717

Peak Selection: Nearest

Append Insert

Modify Delete

General Parameters...

Integrate Parameters...

User RF Value: 1.000000

User Peak Factor: 1.000000

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2. M. Quant Meth Ed. - Integrate Window

Method Editor - Qmeth1

File Edit Help

Com Delete All Compound:

1.1 User Peak Factor...

2.1 Totals...

3.1

General Parameters...

Integrate Parameters...

Secondary Parameters...

Propagate

Integrate Window...

Mass Chromatograms...

Detection Limit...

Report Settings...

Integration Window

Factor applied to location window to calculate integration window: 2.000

OK

Cancel

Take the 'Peak Location : Time Window' and multiply by it by this factor to get the half width of the 'Integration Window'.

For example if the 'Peak Location': 'RT'=3.0 and the 'Time Window'=0.2 then using the above example, the 'Integration Window' is 0.4. So for a peak to be successfully integrated, its peak top must be in the range of 3.0 ± 0.2 minutes and both its start and endpoints must be in the range of 3.0 ± 0.4 minutes.

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3. Processing Samples

- ◆ Once the entire method is built, it's time to process the samples.
- ◆ Highlight the samples to quantitate. If the entire sample list is to be processed, click on the upper left box to activate the entire sample list
- ◆ Click on *Quantify, Process Samples*.

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3.A. Processing Samples

Run	QuantLynx Method Editor...	File Path	MS File	Inlet File	Ratio	Inject Volume	Sample Type	Conc A
1		ama blank	DEFAULT	DEFAULT	1	10	Blank	0
2	ASSAY02	ID2	0.2pp/ml std	DEFAULT	DEFAULT	2	Standard	0.2
3	ASSAY03	ID3	0.5pp/ml std	DEFAULT	DEFAULT	3	Standard	0.5
4	ASSAY04	ID4	0.75pp/ml std	DEFAULT	DEFAULT	4	Standard	0.75
5	ASSAY05	ID5	1pp/ml std	DEFAULT	DEFAULT	5	Standard	1
6	ASSAY06	ID6	2pp/ml std	DEFAULT	DEFAULT	6	Standard	2
7	ASSAY07	ID7	5pp/ml std	DEFAULT	DEFAULT	7	Standard	5
8	ASSAY08	ID8	10pp/ml std	DEFAULT	DEFAULT	8	Standard	10
9	ASSAY09	ID9	15pp/ml std	DEFAULT	DEFAULT	9	Standard	15
10	ASSAY10	ID10	0.3pp/ml QC	DEFAULT	DEFAULT	10	QC	0.3
11	ASSAY11	ID11	2pp/ml QC	DEFAULT	DEFAULT	11	QC	2
12	ASSAY12	ID12	12pp/ml QC	DEFAULT	DEFAULT	12	QC	12
13	ASSAY13	ID13	Ref sample 01	DEFAULT	DEFAULT	13	Analyte	0
14	ASSAY14	ID14	Ref sample 02	DEFAULT	DEFAULT	14	Analyte	0
15	ASSAY15	ID15	Ref sample 03	DEFAULT	DEFAULT	15	Analyte	0
16	ASSAY16	ID16	Ref sample 04	DEFAULT	DEFAULT	16	Analyte	0
17	ASSAY17	ID17	Ref sample 05	DEFAULT	DEFAULT	17	Analyte	0

Highlight the samples you wish to quantitate and then select 'Process Samples'

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3.B. Processing Samples

This window appears to confirm the specifics prior to processing samples. Double-check that the:

- 1) Designated samples are correct
- 2) That it is using the correct method.

*If use old calibrators
No check*

Quantify Samples

Integrate Samples

Calibrate Standards

Quantify Samples

Print Quantity Reports

Export Results to LIMS

Project: C:\MASSLYNX\QUANTIFY.PRO

Quantify: From Sample: 1 To Sample: 39

Method: Qmeth1 Browse

Curve: QMETH1 Browse

LIMS Export: File: Browse

DK Cancel

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4. Reviewing Results

After samples have been processed, a “**Quantify**” box will appear on the lower tool bar. Double click to bring up the results.

OR

Using the main toolbar, click on the **View Quantify Results** button.

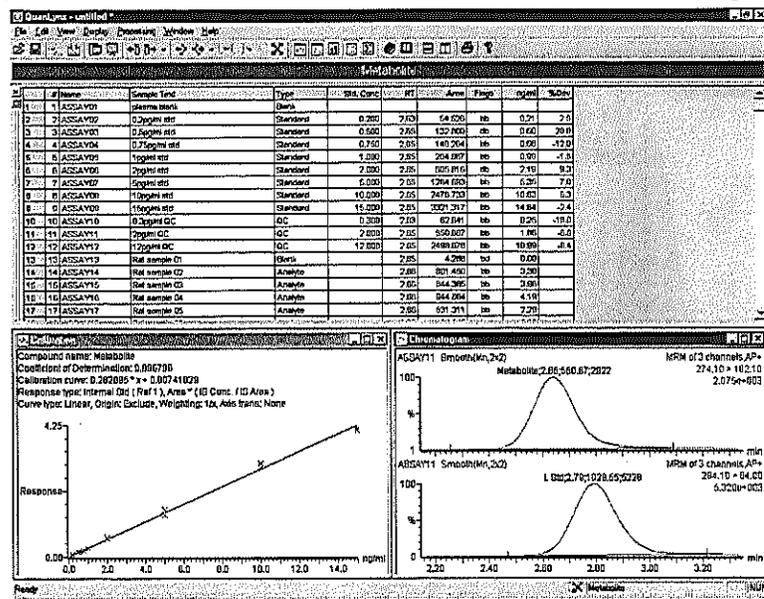
OR

Using the main menu, click on the **Quantify, View Results** menu item.

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4.A. Sample of QuanLynx Quantification Results



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4.B. Some Features of the Menu of the QuanLynx Quantification Results Viewer

Step Through the Different Samples

Step Through the Different Compounds

Turn On or Off the Slide Show

Experimental Record Can Be Displayed Using Menu Item

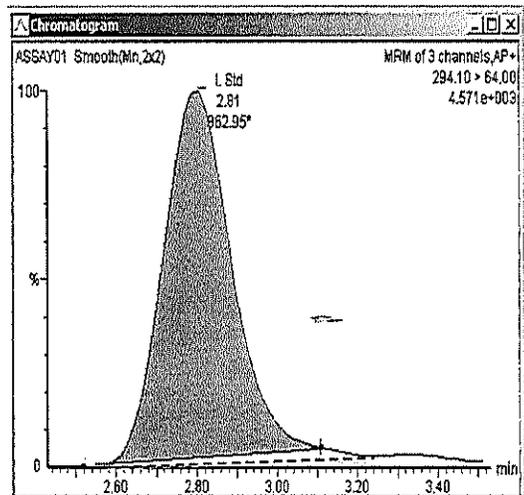
The screenshot shows the 'QuanLynx - untitled' window with a menu bar containing 'File', 'Edit', 'View', 'Display', 'Processing', 'Window', and 'Help'. Below the menu bar is a toolbar with various icons. To the right, the 'Experimental Record: ASSAY14' window is open, displaying the following information:

Experimental Record: ASSAY14	
Reader:	
Acquired File Name:	311C14
Acquired Date:	13-Dec-1994
Acquired Time:	07:54:50
Job code:	
Task code:	
User Name:	User
Laboratory Name:	Lab
Instrument:	Inst
Conditions:	
Submitter:	TD14
SampleID:	
Bottle Num:	
Description:	Rat sample 02
Instrument Calibration:	

3_5_007



4.C. Manually Adjusting Integrations



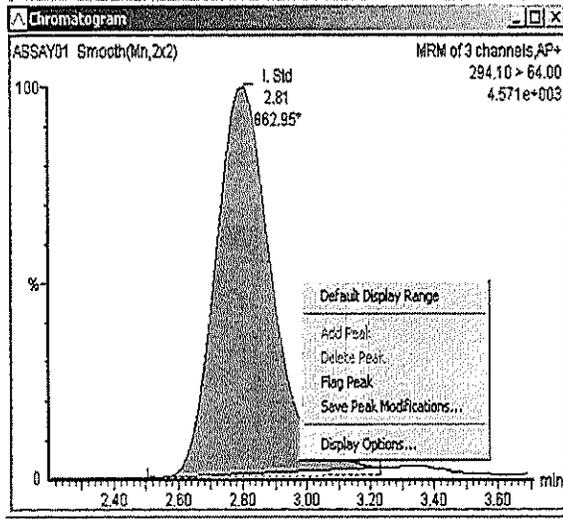
Click on the Baseline, Select the End Point using the Pointer and Left Mouse Button Move the End Point to the desired spot.

A faint line will show the position of the original baseline. Reports will now show that this baseline was manually adjusted.

3_5_007



4.C. Manually Adjusting Integrations



'Right Click' in the window and a menu appears.

Select 'Save Peak Modifications' from this menu to save changes to the baseline.

Go to another chromatogram to keep the original baseline.

3_5_007



4.D. Right Click on the Display and Select 'Display Options' to Customize the Display:

Display → option

For Example the Chromatogram Display Can Be Changed:

Use 'Summary' Page to Control Slide Show

Chromatogram Display Adjustments

Toggle Showing Internal Standard Chromatogram

Y Axis

X Axis

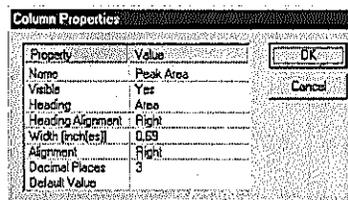
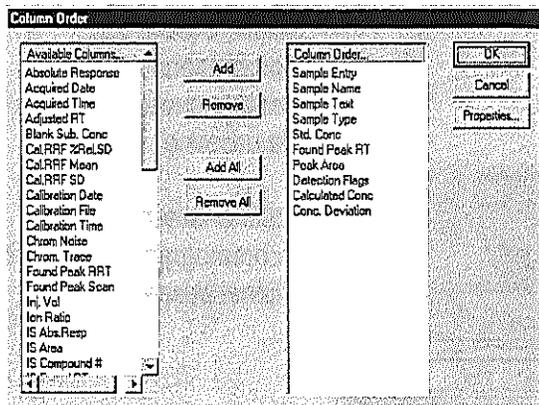
3_5_007



4.E. 'Right Click' On the Summary Table and ...

1) Click on 'Change Column Order' and which columns are displayed in the table can be changed.

2) Click on 'Edit Column Properties' and the properties of this column can be changed.

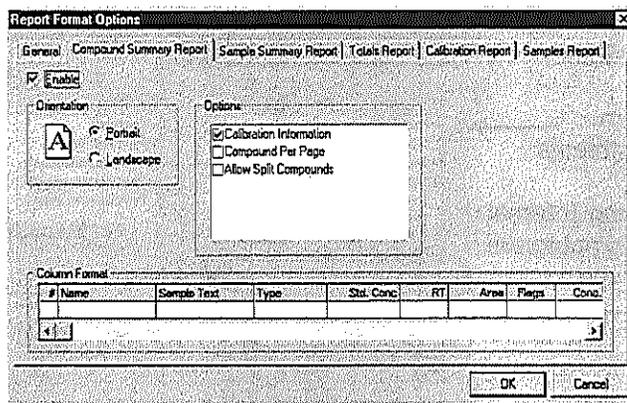


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5.A. Change How the Report Will Be Printed Out

From the 'File' Menu, Select the 'Report Format' Item:

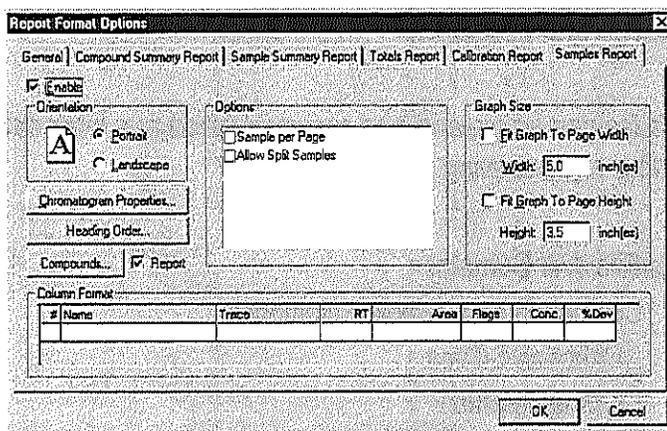


Compound and Sample Summaries Can be Formatted Differently From How They Appear on the Screen

3_5_007



5.B. Chromatogram Print Formats Can Also Be Adjusted



Customized Display and Report Formats Can Be Saved For Later Use

3_5_007



5.C. More on QuanLynx Quantification

- ◆ Printing Reports (**File, Print Report**). Besides a full report, results from a set range of samples can be printed.
- ◆ Screen and Report Format. A customized format can be saved in a *.fmt file for later use.
- ◆ The Quantify Method used with a report can be changed using (**Edit, Quantify Method**)
- ◆ Editing of Calibration Curve (**Edit, Calibration Curve**) allows excluding of specific data points. ('Right Click' on a point in a Calibration Curve and select 'Exclude Point').
- ◆ Reprocessing samples after editing Quantify Method (**Process, Calculate**)

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5.D. When Finished QuanLynx Quantification Results Can Be Saved in a File

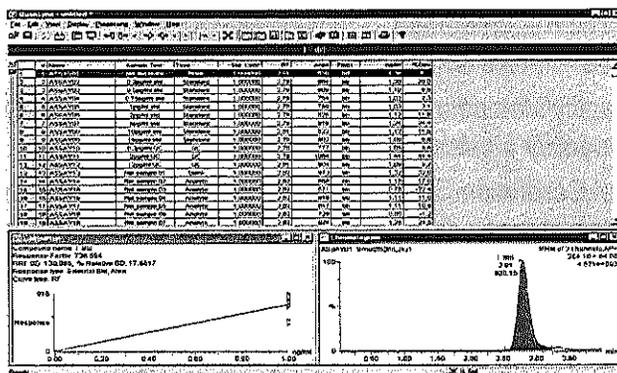
- ◆ Everything is in One File
- ◆ This file can be viewed and reports printed at a later date without reprocessing data
- ◆ This File Will Contain:
 - Compound and Sample Summaries
 - Calibration Curves
 - Chromatograms
 - Experimental Record for Each Analysis Run
 - Quantitation Method

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QuanLynx Report Viewing

The report remains *untitled* until saved. Anytime changes are made and prior to re-saving the file, there will be an asterisk next to the file name.



The information detailed in the Compound Summary is the first compound listed in the Quantitation Method. To see summaries for other compounds, select a molecule button on the tool

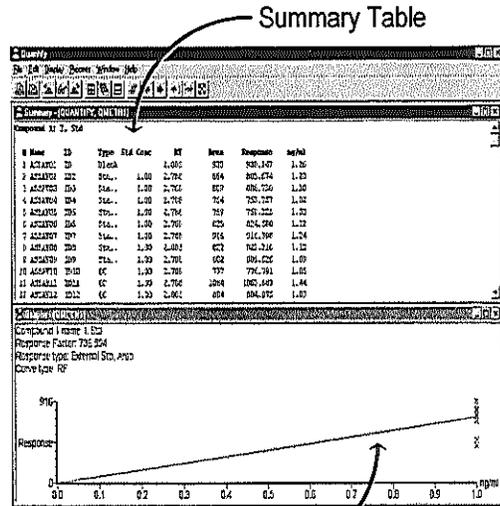
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MassLynx Quantification without QuanLynx: Reviewing Results

After Quantification:

- ◆ You should be able to bring up two separate windows - one with numerical results; the other with the calibration curve.
- ◆ If one or the other fails to appear, use the **'Display, View'** menu item and check the appropriate window to view.



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Reviewing Results (when quantifying using Quantify)

- ◆ Numerical results and the calibration curve will be listed by compound. To review different compounds within the same Quantify Method, use the arrow keys on the toolbar.



- ◆ To view individual peak integrations, highlight a sample and click on the eyeglasses icon. The arrow keys on either side allow scrolling through the sample list.

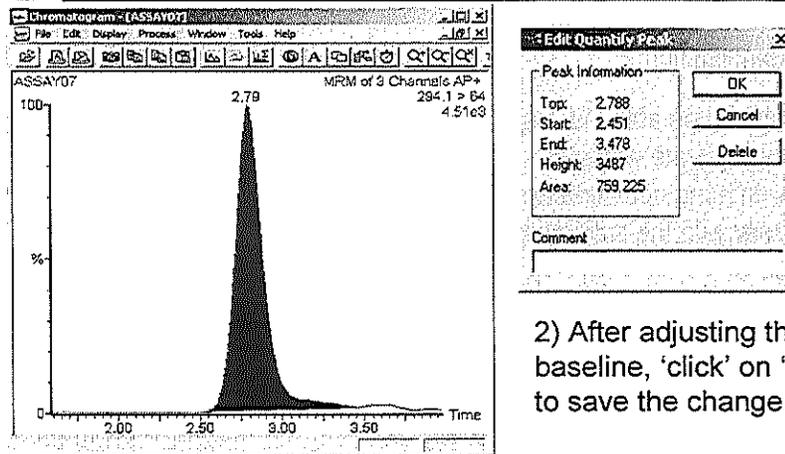


or 'double click' on the desired sample in the summary table and its chromatogram will appear.

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Editing Results (when quantifying using Quantify)



2) After adjusting the baseline, 'click' on 'OK' to save the change.

1) To edit the actual integration, go to the chromatogram window that has been opened and adjust by clicking on the integration endpoints and dragging to the appropriate place.

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Other Options (when quantifying using Quantify).....

Option Available through the 'Quantify' Window Menu Items

- ◆ Printing Reports (*File, Print Report*)
- ◆ Editing the screen format (*Edit, Output Compound Format*) allows addition of fields, editing of fields and editing of numerical format.
- ◆ Editing of printed report format (*Edit, Output Sample Format*)
- ◆ Editing of Quantify Method (*Edit, Quantify Method*)
- ◆ Editing of Calibration Curve (*Edit, Calibration Curve*) allows excluding of specific data points.
- ◆ Reprocessing samples after editing Quantify Method (*Process, Calculate*)

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