Using the Formula Editor in QuanLynx and TargetLynx in MassLynx 4.1

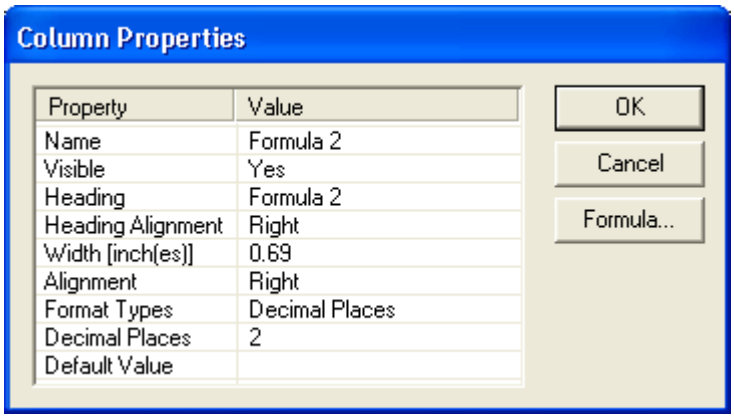
Four new Formula Fields have been added to the Summary Table in QuanLynx and TargetLynx in MassLynx 4.1.These fields allow custom calculations to be carried out in the browser.

Using the Formula Fields

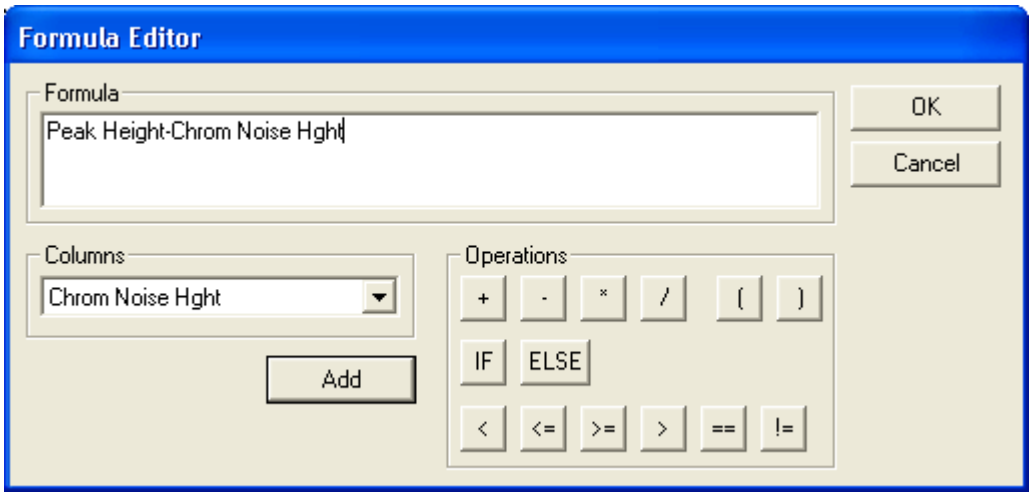
1. In the Summary Table, right-click and choose Change Column Order. Select the required Formula Fields so that they are displayed:

Formula 1	Formula 2	Formula 3	Formula 4
588.25	434.64		
1376.66	1083.34		
1693.60	1346.26		
2442.27	1982.45		
5210.52	4280.44		
14487.26	11900.17		

2. Right-click on one of the fields and select Edit Column Properties. This will result in the display of the Column Properties dialog:



3. Click on the Formula button. The Formula Editor will appear:



4. Set up a user calculation based on the results displayed in different fields in the Browser, then click OK.

5. Once the Formula has been set up, it can be saved as part of the QuanLynx Layout file (.qlt).

Using Logical Calculations in the Formula Editor

The syntax for formulae is similar to the old style of 'C programming' IF-ELSE statements:

<condition> ? <result if true> : <result if false>

The question mark is entered by selecting ‘If’.
The colon is entered by selecting ‘Else’.

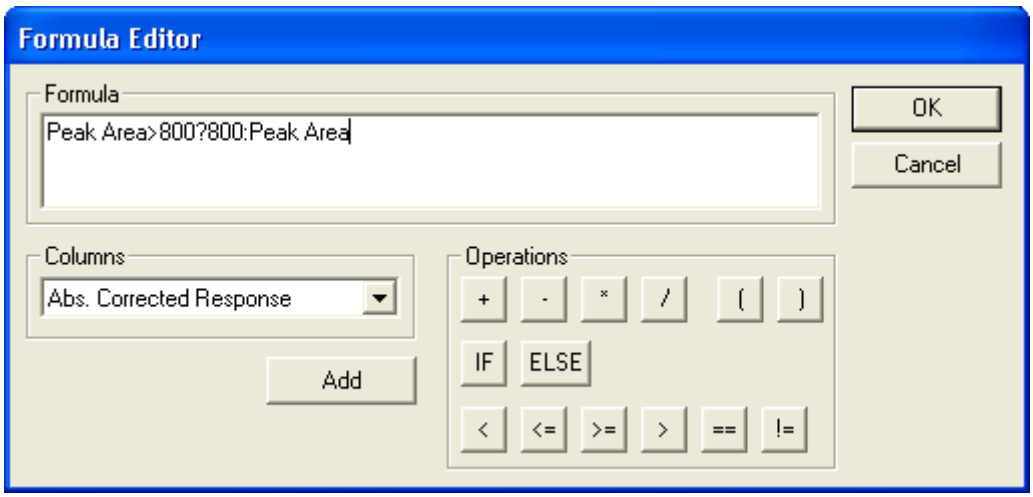
Example 1
To display ‘0’ if the peak area >800, but otherwise display the measured peak area, enter:

Peak Area>800?0:Peak Area

Example 2
To display ‘800’ if the peak area >800, but otherwise display the measured peak area, enter:

Peak Area>800?800:Peak Area

This is shown in the following screendump:



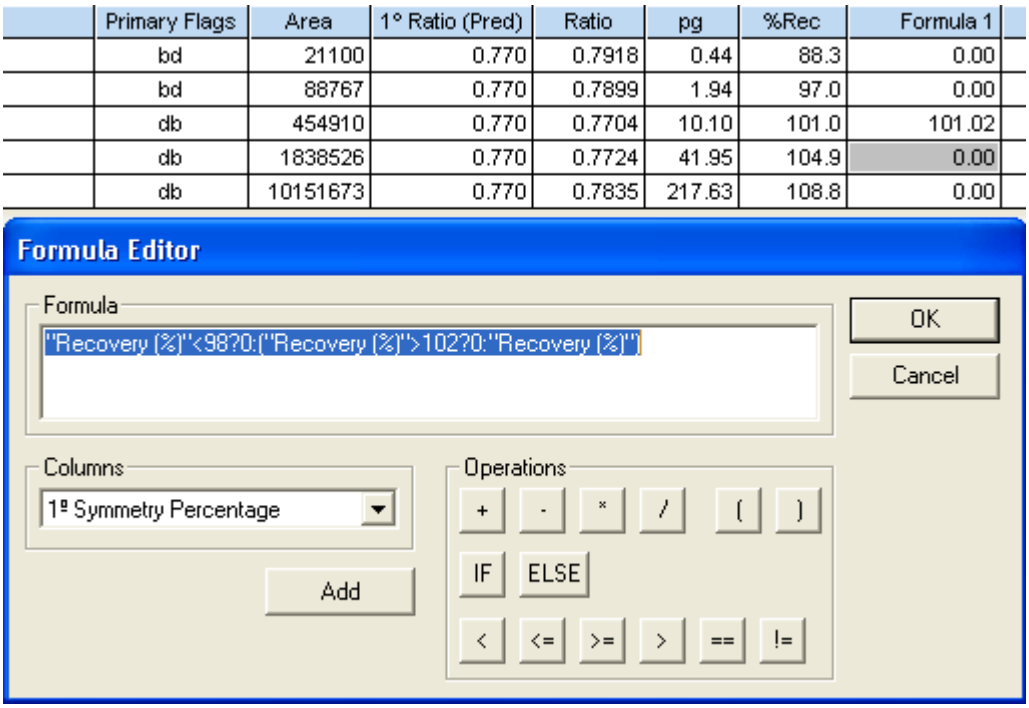
A second condition can be added to the <result if false> eventuality, as follows:

<condition> ? <result if true> : (<condition if false> ? <second result if true> :
< second result if false>)

Example 3
To display 0 if the peak area >500 OR <100, otherwise display peak area, enter:

Peak Area>500 ? 0 : (Peak Area<100 ? 0 : Peak Area).

Example 4
To flag recovery values of <98 and >102 with a '0', use the formula shown in the following screendump:



Note: at present, only numerical values can be used in a formula.

Issues with the Formula Editor

1. If you want to use the Formula field to sum the total peak area (primary area + secondary area (or target area if using TargetLynx), no result will be calculated if the secondary / target peak is not found. This is because, at present, the Formula editor cannot handle zero values.

2. If you want to perform a calculation using the primary / secondary ion ratio (primary / target ratio if using TargetLynx), no result will be calculated if you enter the ion ratio as ion ratio (actual) or ion ratio (pred). This is because the Formula editor does not recognise field names that have brackets.

For example, 1° Ratio (actual) would be read as two different fiields, 1° Ratio and (actual). This does not work, as neither field exists. The workaround for this problem is to use inverted commas when entering ion ratio (actual) or ion ratio (pred). For example, use "1° TargetRatio (actual)".

3. To print the results of Formula calculations, the calculation must be set up in the appropriate Report Format Tab (such as Compound Summary Report Tab). The setup of the Formula for printing is independent of the setup of the Formula to be displayed in the Summary Table.

4. Occasionally the Formula editor may not open properly. When you right-click on the Formula field, and choose 'Edit Column Properties' in the drop down list of options, the Column Properties window does not open. The workaround for this is to close MassLynx, delete the TargetLynx~ql file (or QuanLynx ~ql file) in C: \ MassLynx, then re-start MassLynx.