Instructions for Enabling Compound Math on B.03.0x-B.07.00

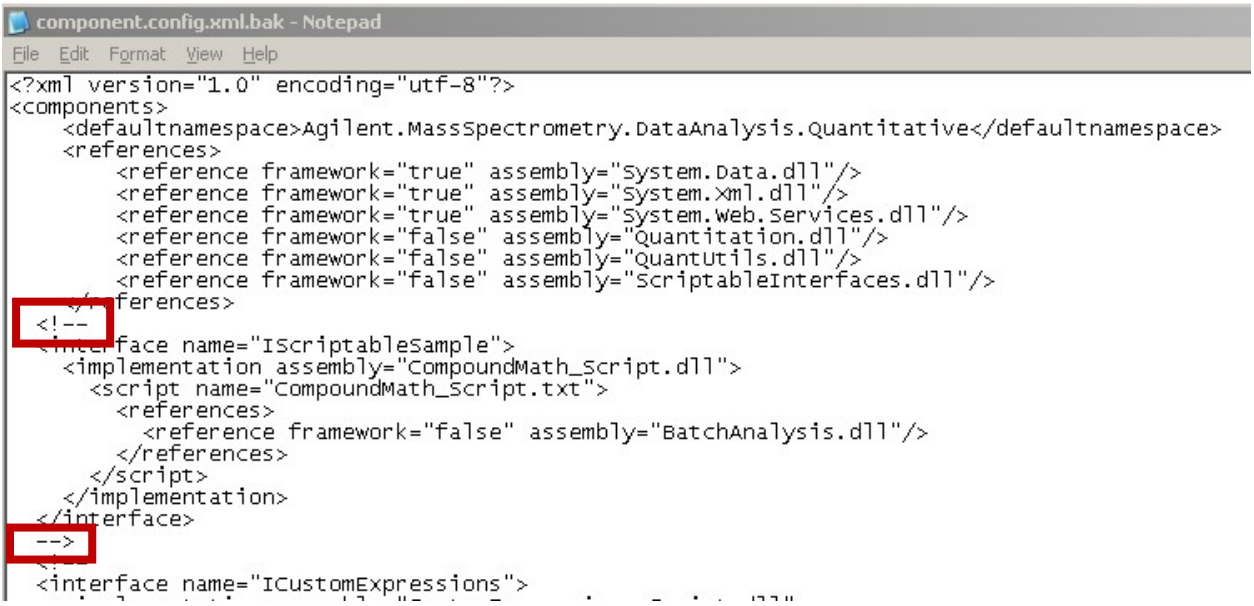
Note: A new concept of Compound Math was introduced with MassHunter Quantitative Analysis B.07.01 making the calculations straightforward. Several new videos are available to introduce and explain the parameter setup.

Navigate to the following directory \Program Files\Agilent\MassHunter\Workstation\Quant\bin

1) Make a backup copy of the following file:

   Component.config.xml

2) Edit the original component.config.xml with Notepad.
3) Uncomment the compound math portion. Before and after images shown below.



Should look as follows:

component.config.xml - Notepad

File Edit Format View Help

```
<?xml version="1.0" encoding="utf-8"?>
<components>
    <defaultnamespace>Agilent.MassSpectrometry.DataAnalysis.Quantitative</defaultnamespace>
    <references>
        <reference framework="true" assembly="System.Data.dll"/>
        <reference framework="true" assembly="System.Xml.dll"/>
        <reference framework="true" assembly="System.Web.Services.dll"/>
        <reference framework="false" assembly="Quantitation.dll"/>
        <reference framework="false" assembly="QuantUtils.dll"/>
        <reference framework="false" assembly="ScriptableInterfaces.dll"/>
    </references>

  <interface name="IScriptableSample">
    <implementation assembly="CompoundMath_Script.dll">
      <script name="CompoundMath_Script.txt">
        <references>
          <reference framework="false" assembly="BatchAnalysis.dll"/>
        </references>
      </script>
    </implementation>
  </interface>

  <!--
  <interface name="ICustomExpressions">
```

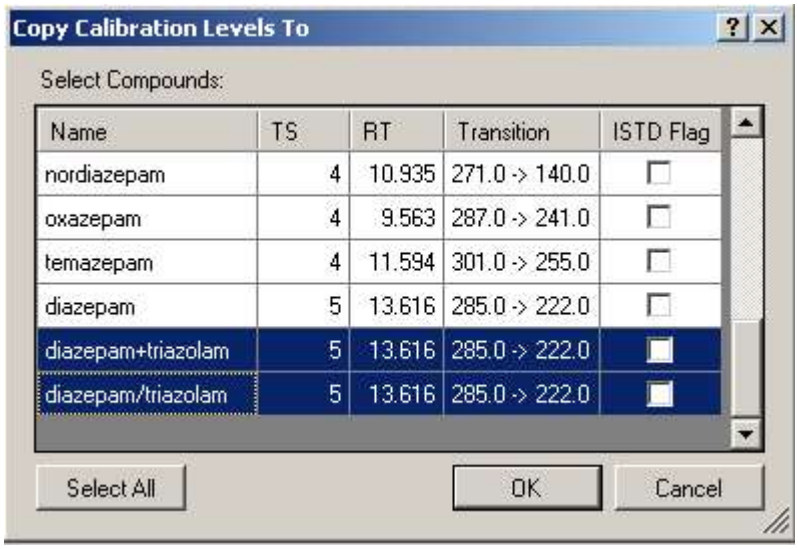
4) Save the file.

Next portion – add a new compound with math as part of the name.

	temazepam	4	301.0 -> 255.0	MRM	Target	301.0	255.0	11.594
	triazolam	4	343.0 -> 308.0	MRM	Target	343.0	308.0	10.521
	diazepam	5	285.0 -> 222.0	MRM	Target	285.0	222.0	13.616
	diazepam+triazolam	5	285.0 -> 222.0	MRM	Target	285.0	222.0	13.616
	diazepam/triazolam	5	285.0 -> 222.0	MRM	Target	285.0	222.0	13.616

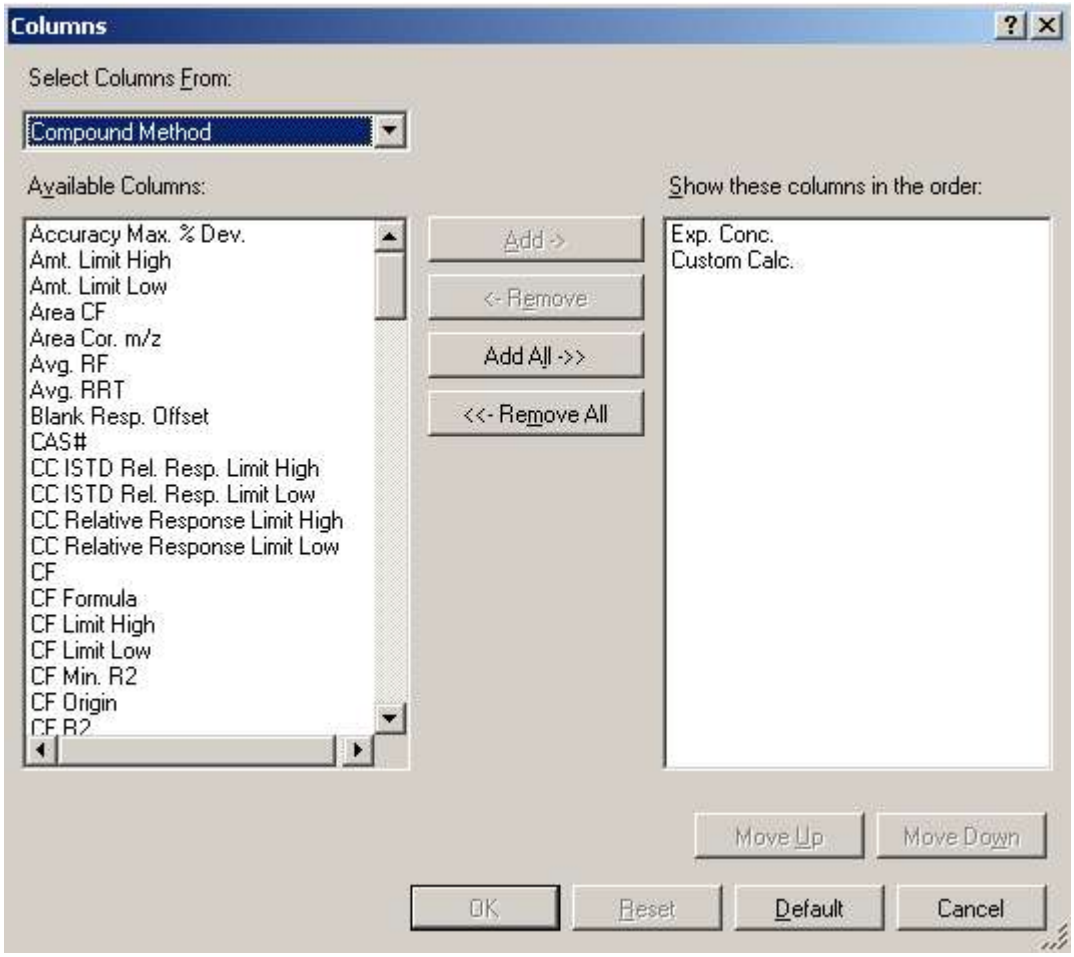
5) In the example above, input diazepam/triazolam. The transition is unimportant as the “math compound” is calculated from the two individual results, but it’s reasonable to put in an actual working value.

6) The “math compound” does require a calibration table. Copy a calibration table from any existing target compound to the “math compound”.



7) Exit and apply the method to the batch.
8) Analyze the batch.

9) Add a column to see the custom calculation results. Note that the custom calculation is displayed in the "Compound Method" and not the "Compound Results".



10) View the results. Notice that for the compound "diazepam/triazolam" the Custom Calc. shows a number close to 1, as would be expected for the calibrators.

5: diazepam/triazolam ISTD:

	diazepam/triazolam Method	
. Date-Time	Exp. Conc.	Custom Calc.
07 1:24 PM		0.6217
07 1:50 PM	10.0000	0.9215
07 2:15 PM	25.0000	1.0475
07 2:41 PM	50.0000	1.0473
07 3:07 PM	125.0000	1.0168
07 3:33 PM	250.0000	0.9893
07 3:59 PM	500.0000	0.9966
07 4:25 PM		0.9617
07 4:50 PM		4.1469