

## Setting Up and Using ChroTool

This procedure describes how to set up and use the ChroTool function in the MassLynx software. ChroTool allows you to open and view a pre-set selection of chromatograms easily. A ChroTool method is used to set up the types of chromatogram to be displayed.


**NOTE:** *This procedure covers all instruments using the MassLynx software. The example uses the data acquired from the ACQUITY UPLC with LCT Premier/XE system performance tests.*

### Procedure

The procedure to set up and use ChroTool consists of two sections:

1. Setting up the ChroTool parameters
2. Using the ChroTool method

### Setting up the ChroTool parameters

1. Open a data file in the Chromatogram window.
2. In the Chromatogram window, click Display > ChroTool, or click the ChroTool toolbar  button to open the ChroTool window.
3. If this button is not visible, add it to the toolbar using the Display/Customise toolbar.

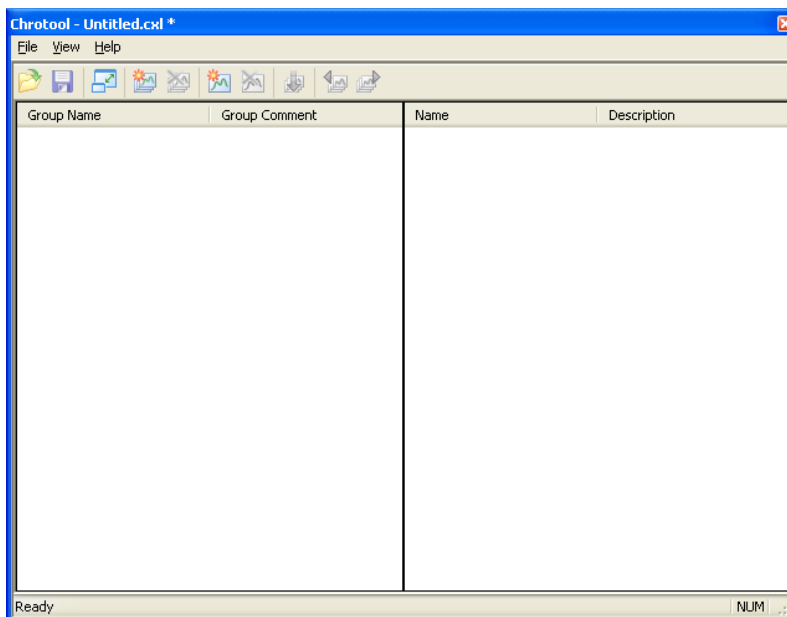



Figure 1 - ChroTool main window

4. In the ChroTool window, click File > New to set up a new Method file.
5. Click the Add Group  button and add a name for the group, e.g. System Performance Test (Figure 2).
6. In the Range parameter field, select Use current, and then click OK.

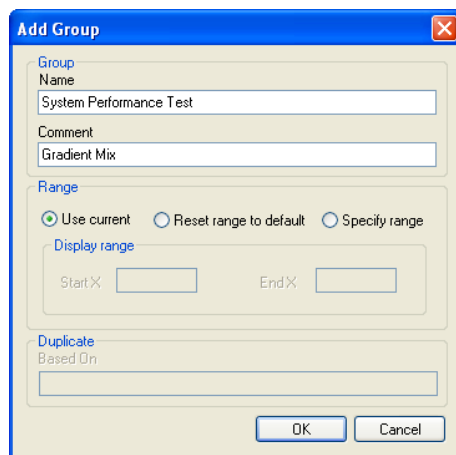



Figure 2 - Add Group window

7. Click the Add Chromatogram  button to display the Chromatogram Details window.
8. Complete the Chromatogram Details window, and then click OK. See Figure 3 as an example.
  - a. Type the name of the chromatogram to be displayed.
  - b. Select the type of chromatogram, e.g. mass/channel for an extracted mass chromatogram.
  - c. Select the TIC function number, e.g. 1 for analyte data on a LockSpray system.
  - d. For a mass chromatogram, input the m/z value into the description field.

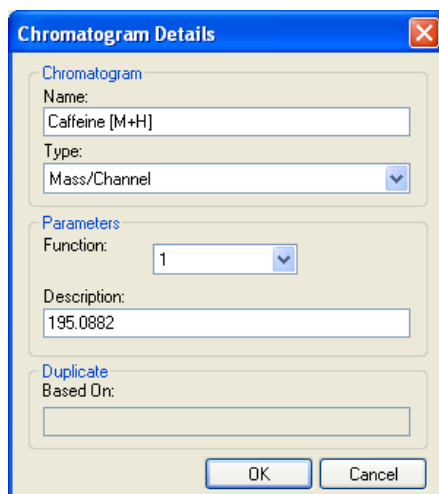


Figure 3 - Chromatogram Details window

- Repeat step 8 for any other masses to be extracted.
- Click File > Save As and save the Method file under an appropriate filename, e.g. System\_Test.cxl.

**NOTE:** *Figure 4 shows an example of the ChroTool window with a number of masses added.*

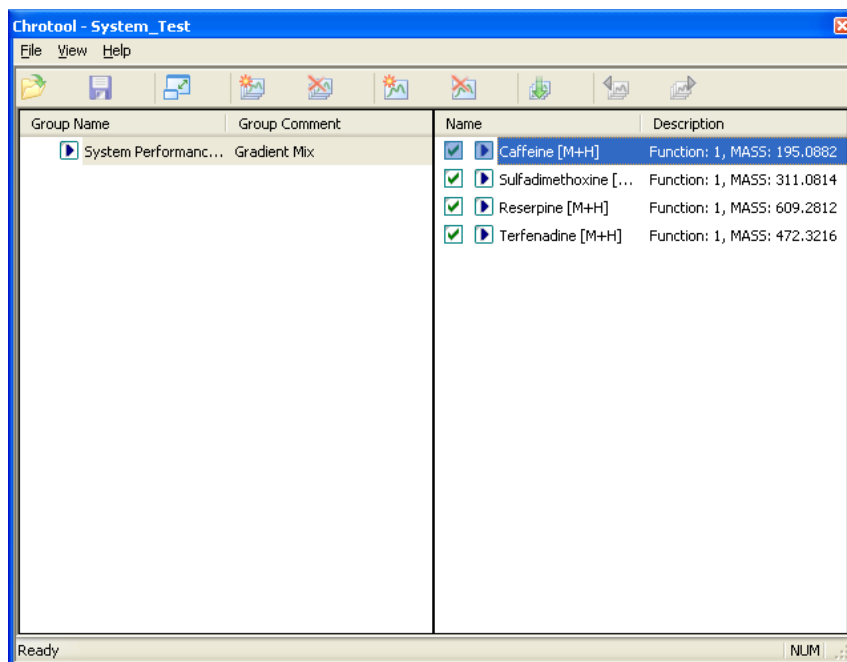





Figure 4 - ChroTool window with entries

**NOTE:** *It is possible to add several groups for a single \*.cxl method file. For example, a positive and negative set of m/z values.*

## Using the ChroTool method

- Open the data file in the Chromatogram window.
- Open the ChroTool window, and click  to reduce the size of the window.
- To extract the chromatogram, click the  symbol of an individual chromatogram entry, or to extract all the listed chromatograms, click the  symbol next to the group name as shown in Figure 5.

**NOTE:** *The extracted chromatograms should be displayed in the Chromatogram window, as shown in Figure 6.*

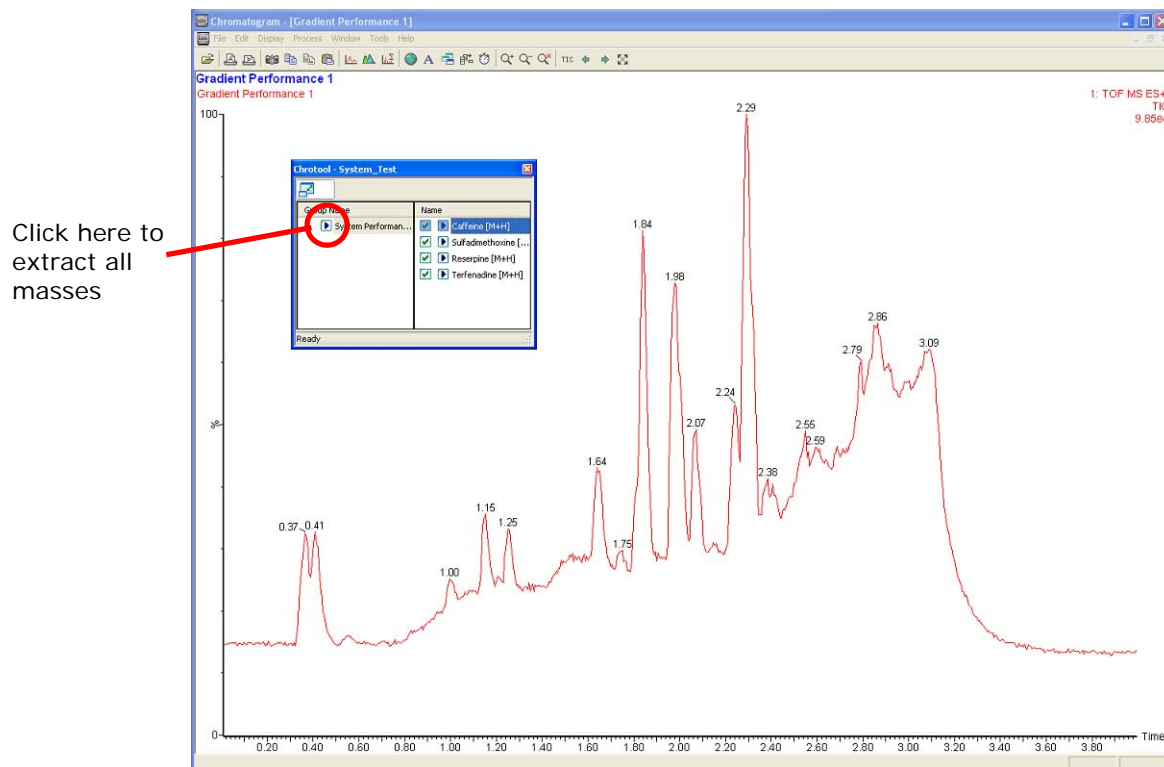


Figure 5 - Using ChroTool to extract the chromatograms

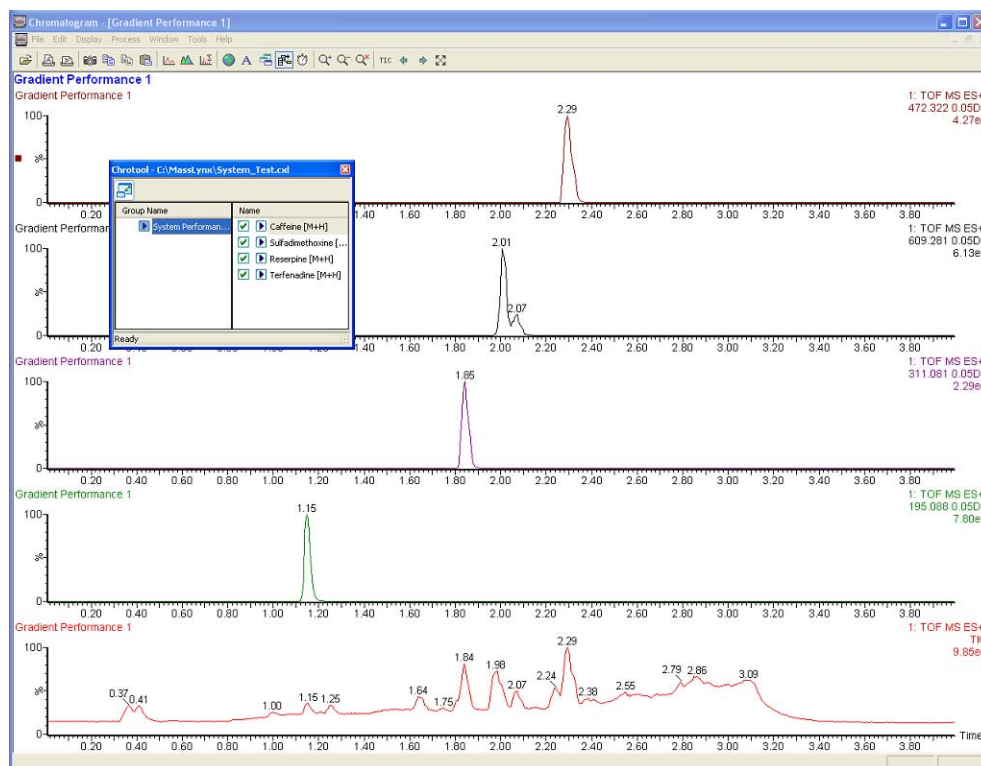



Figure 6 - Extracted mass chromatograms

## Additional information

### Using ChroTool to display a composite chromatogram

Perform the following procedure to prepare a single chromatographic trace (the sum of a number of specified mass chromatograms).

1. In the ChroTool window, click the Add Chromatogram  button.
2. Add the mass values for the extracted mass chromatograms, and specify a "+" sign between each mass (Figure 7).
3. Click OK.

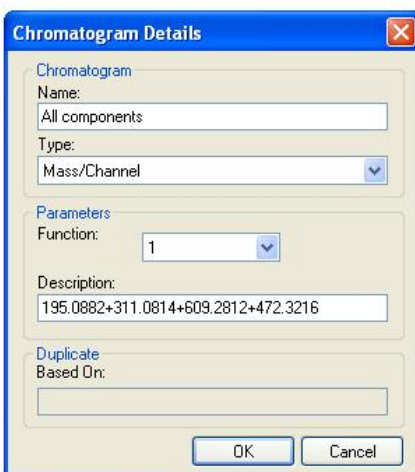


Figure 7 - Specifying multiple masses

**NOTE:** The resulting ChroTool method now has a single chromatogram entry (Figure 8).

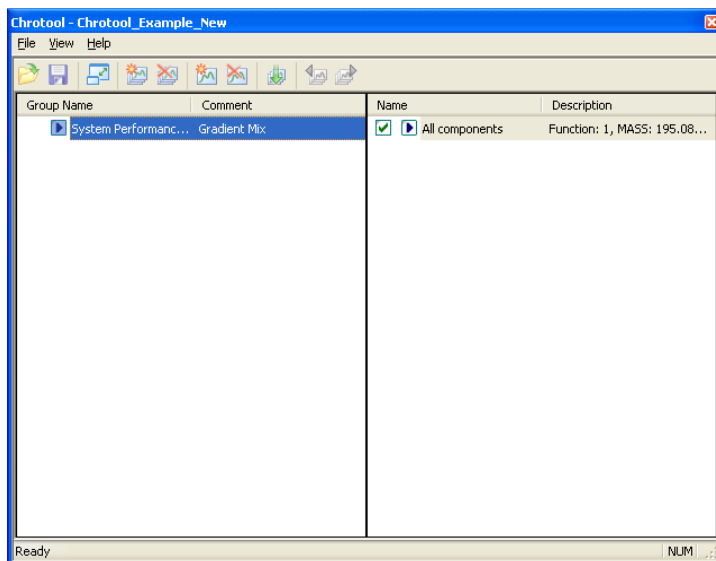


Figure 8 - ChroTool method for preparing a composite MS trace

**NOTE:** When extracted, the entry produces a single MS trace made of the sum of the individual masses (Figure 9).

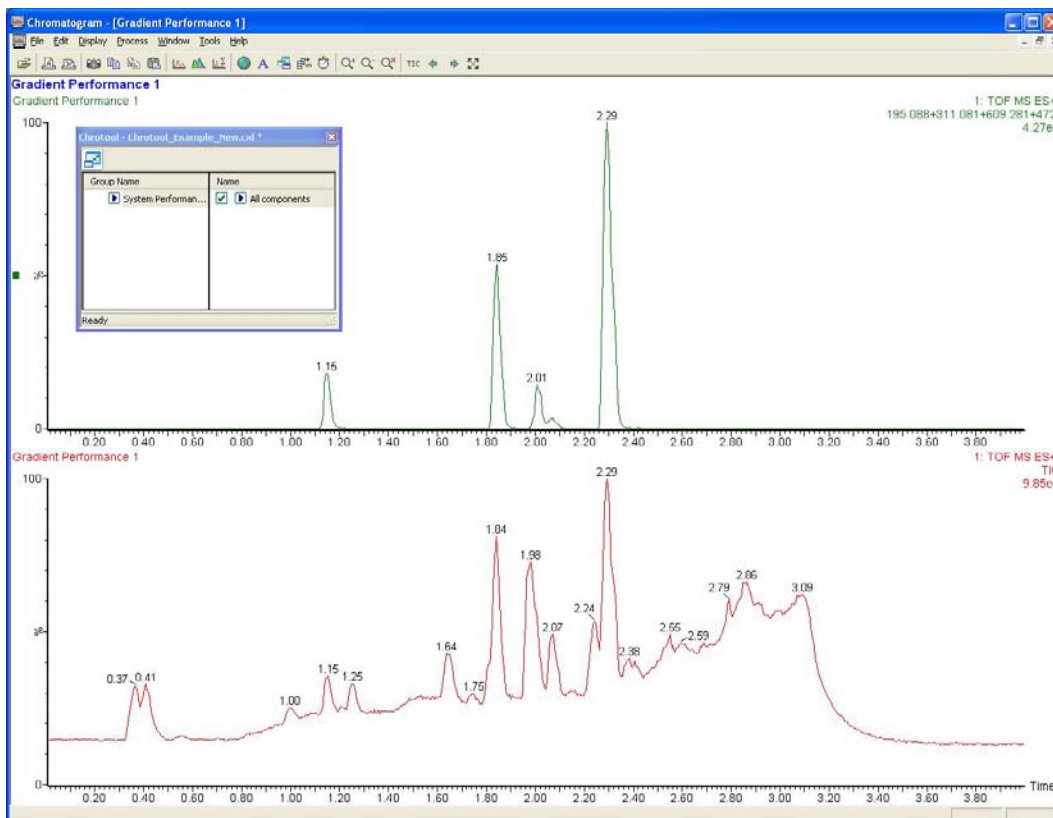


Figure 9 - Example of composite MS trace