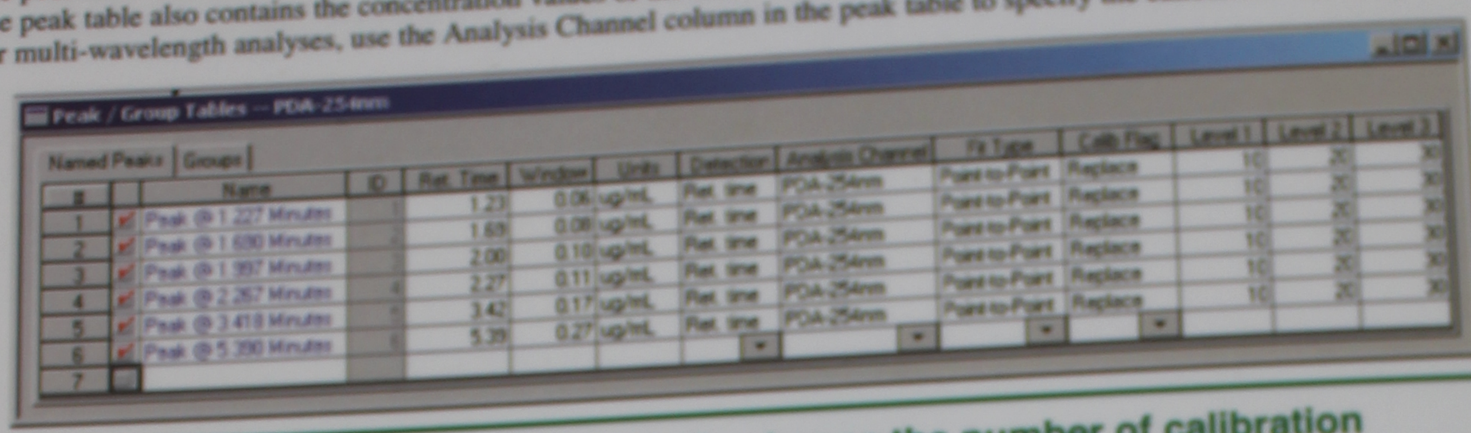
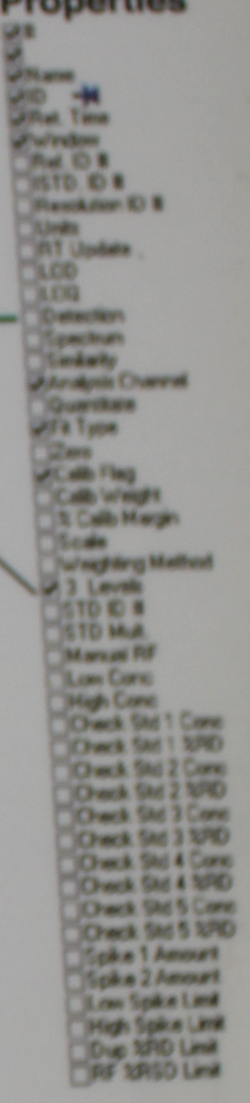
Adding a Peak Table for Identification and Quantitation

The peak table contains the information required to identify the peaks in the chromatogram(s), as well as the information required to build the calibration curve(s). The peak table also contains the concentration values of the check standards and the sample spikes. There is one peak table for each detector in your instrument. For multi-wavelength analyses, use the Analysis Channel column in the peak table to specify the calibration wavelength(s).



By default, the Fit Type is Point-to-Point and the Calib Flag is Replace.

Peak Table Properties



Note. The peak table shown above contains three concentration levels.

To create the Peak table:

1. Open a stored data file.
2. Click anywhere in the Chromatogram window to activate the Integration Events toolbar, and then click on the **Define Peaks button**.
3. Follow the instructions in the status bar.

   After you graphically select your peak range, ChromQuest displays the Define Peaks dialog box.
4. Make the appropriate selections in the Define Peaks dialog box.

✓**Tip** The Minimum Peak Area or Peak Height list box allows you to exclude peaks below the selected value from the Peak table.

5. Click on **OK** to exit the dialog box.
6. Click on the **Peak / Group Tables button** to review the information in the Peak table.

To change the number of calibration levels:

1. Right-click in the Peak Tables window to display the shortcut menu.
2. Click on **Properties** to display the Properties dialog box.
3. In the Properties dialog box, double-click on **Levels** to display the Max # of levels text box. Type a new value into the text box, and then press the <Enter> key.

To quantitate peaks on more than one Analysis Channel:

1. Click on the peak # to highlight the entire row, and then copy the information to a new row.
2. Click on the down arrow in the ***Analysis Channel*** column, and then select the analysis channel from the list of available wavelengths.

Before you run a set of samples...

To automatically inject a set of samples you will need to create a sequence table. To make the task easier, ChromQuest contains a Sequence Wizard. However, the Sequence Wizard does not contain all the available sequence options. You will need to edit the sequence table if you want to add run types that are not available in the Sequence Wizard. After you run your sequence, you might want to modify the method and then reprocess the data. For more information, refer to the following topics:

- Creating a Sequence Table Using the Sequence Wizard
- Editing a Sequence Table
- Starting a Sequence Run
- Reprocessing a Sequence

Creating a Sequence Table Using the Sequence Wizard

The Sequence table contains the information that is required to automatically inject a set of samples or to reprocess a set of stored data files. ChromQuest contains a Sequence Wizard that guides you through the creation of a Sequence table.

To open the Sequence Wizard:

From the menu bar in the Instrument Window, choose **File > Sequence > Sequence Wizard.**

ChromQuest displays the Method page of the Sequence Wizard.

To create an acquisition Sequence:

1. On the Method page, select the For Acquisition option button.
2. Make the appropriate selections and entries in the Method, Unknowns, Autosampler, Calibration, and Reports pages of the Sequence Wizard.
3. After you complete your entries, click on **Finish**.

   The Sequence window opens.
4. Save the Sequence table by choosing **File > Sequence > Save As** from the menu bar.

To create a sequence from existing data files:

1. On the Method page, do the following:

   a. Click on 🗁 and then select a method from a ChromQuest directory.

   b. Select the From Existing Data Files option button, and then click on **Next** to display the Select Files page.
2. Click on 🗁 to display the Open Data Files dialog box, and then open the ChromQuest directory that contains your data files.
3. Click on the last data file that you want to reprocess, hold down the <Shift> key, and then click on the first data file that you want to reprocess.
4. Click on **Open**.

   A list of the selected data files appears in the pane in the order that they will appear in the sequence table.
5. Click on **Finish**.
6. Save the sequence.

✓**Tip**

In the Method page, the values entered in the Amount Values group box affect how ChromQuest reports the concentrations of the quantitated peaks in your unknowns as shown in the following equation.

$$\frac{([Unk]_C \times \text{Multiplier 1} \times \text{Multiplier 2} \times \text{Multiplier 3})}{(\text{Sample Amt} \times \text{Dilutor 1} \times \text{Dilutor 2} \times \text{Dilutor 3})} = [Unk]_R$$

where

$[Unk]_C$ = the concentration of the unknown determined from the calibration curve

$[Unk]_R$ = the concentration of the unknown reported by ChromQuest