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Automatic Dilutions Using Chromeleon AutoDilution and the Partial Loop Injection Capability of the ICS-3000 AS Autosampler

INTRODUCTION

Environmental and wastewater samples often contain compound concentrations that exceed the range defined by a standard curve. In the past, operators would need to identify these outliers, dilute the samples, and often rerun the standards along with the diluted samples. These time consuming steps have now been eliminated with a software enhancement called AutoDilution.

AutoDilution enables the Chromeleon® Chromatography Data System (CDS) software to automatically determine when compound concentrations exceed a set concentration, then dilute the samples, and rerun them along with standards, if needed.

The Chromeleon AutoDilution license is a powerful tool for adding automatic dilutions, using a decision structure, to any Dionex ion chromatography system with the AS Autosampler. If the concentration of a specified compound (target compound) is over a predefined limit (threshold), the Chromeleon software will automatically create a new sequence to adjust the sample concentration and re-run the analysis. (A maximum of 10 target compounds can be selected, each with their own separate threshold level.)

This technical note presents an example of automatic dilutions using the partial loop injection of the AS to automatically run a smaller injection volume of the same sample. Other injection volumes can be selected, as well as multiple conditionals. All dilution runs can be stored in a separate sequence for easy identification of reanalysis results on the same sequence. This dilution sequence is run automatically after the original sequence.

Chromeleon AutoDilution offers a quick, easy, and reliable method to perform automatic dilutions of samples. This tool requires the Chromeleon AutoDilution License P/N 069725.

For automatic dilutions using the vial-to-vial dilution capability of the AS Autosampler with the sample pump option, refer to Technical Note 83.

PROCESS OVERVIEW

The Chromeleon CDS automatically determines if any of the target compounds are above the specified threshold level. Any samples above this level are added to a new dilution sequence. The software then assigns specific sequence parameters and methods using conditionals based on the concentration level or the target compounds or any of many Chromeleon variables. (See Fig. 1).

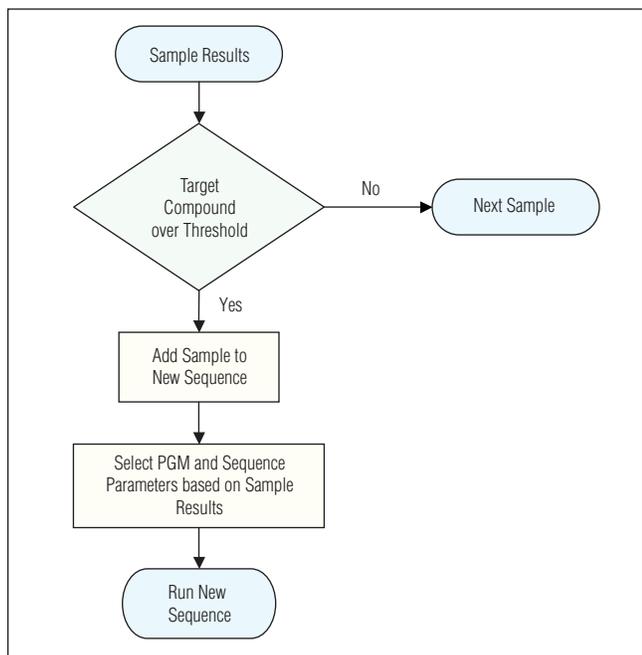


Figure 1. Flow chart.

The dilution of the samples can be from partial loop injections, as in this example, or by calling a PGM file from the conditional program step, which contains a dilution step (vial-to-vial dilution). For this last method, an AS with the sample prep option is needed. See Technical Note 83.

EQUIPMENT

Any Chromeleon-connected Dionex ICS series ion chromatography system
 Chromeleon 6.8 Chromatography Data System software
 AutoDilution License P/N 069725
 AS Autosampler P/N 063102

PREPARATION

Dilutions Using Partial Loop Injections

In this method, the lower injection volumes of samples are achieved with a partial loop injection. The original runs of the samples should be made using the full loop injection method. For example, if a 100 μL full loop is used in the PGM for the original samples, a 1:10 volume injection can be used for any samples run in the lower injection volume sequence, by adding a 10 μL injection volume in the sample properties dialog.

1. The first step is to make a copy of your PGM file. This copy of your PGM file will contain the Post-Acquisition step you will be creating, and will be used with the original run of undiluted samples. The other file (unchanged) will be used for the second run. Re-name this file so you can recognize it as the PGM for the lower injection volume sequence.
2. Add the Post-Acquisition step using the Create Purification Samples Wizard, to the copy of the PGM file you created.
3. Add the appropriate injection volume in the Sample Properties dialog, to achieve the desired dilution ratio.
4. Create your sequence as normal. Any re-runs that are needed will be run from the same vial as the original run.

CREATE PURIFICATION SAMPLES WIZARD

The AutoDilution process is added to a current PGM file by adding a Post-Acquisition step. The Create Purification Samples post-acquisition step is available only if the timebase is connected to the related server, if this server is running, and if an AutoDilution license is installed.

The program for AutoDilution can be created using a built-in Wizard that guides users through the main steps required to create an AutoDilution program. The Wizard automatically shows dialogs needed to create the program. From the PGM, click on the **Post-Acquisition steps icon to add a Post-Acquisition step**. Click on the **Click on this line to add a new step** and select **Create Purification Samples** to start the wizard program.

The dialogs used in the Wizard are listed below:

1. Number of Target Compounds
2. Target Compound X
3. Target Compound X Tests
4. Special Options
5. Conditional Program Selection
6. Sequence Properties
7. Sample Properties
8. Extended Sample Properties

Number of Target Compounds

The first dialog allows you to enter the number of target compounds which will be evaluated in the AutoDilution process. A maximum of 10 target compounds can be selected (Fig. 2), each with their own specific threshold level.

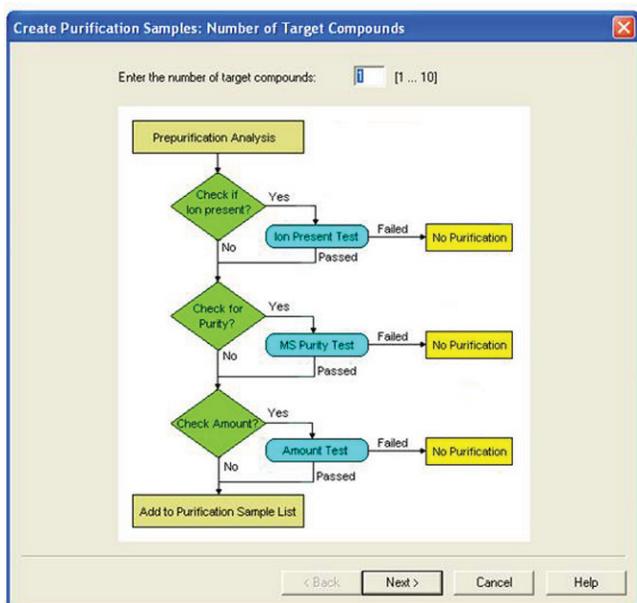


Figure 2. Number of target compounds dialog box.

Target Compound X

The second wizard page, Target Compound X, defines how the target compounds are identified. Any connected detector can be selected from the drop-down list. Peaks may be selected by name (if you have already defined and entered the QNT method in the sample list, the names entered in the QNT method are listed for selection), retention time, greatest height, or greatest area. The Mass Spectrometry Settings are not needed with conductivity detection (Fig. 3). This process is repeated for each target compound.

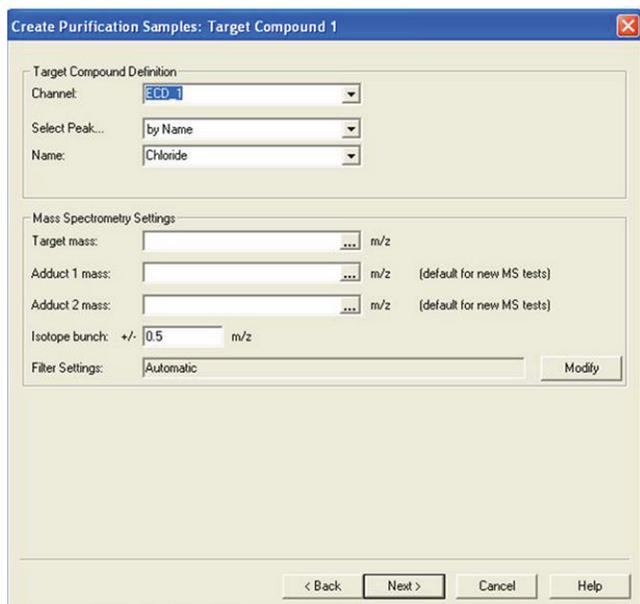


Figure 3. Target Compound X dialog box.

Target Compound X Tests

The Target Compound X Tests dialog defines the test used to determine if the sample is added to the new sequence and re-run (at a dilution). Custom tests can also be created using many of the standard Chromeleon variables, but are not covered by this technical note. For AutoDilution, the Amount Check should be selected. This test checks whether the amount of the target compound is above the threshold amount. Double-clicking on the test name will open the Amount Check Test dialog box. This dialog box allows you to select the channel, from which you want to check the amount of the target compound from a drop-down list. The threshold is the concentration limit for the target compound. Any samples that have a target compound reported result (report units are ignored) above this concentration will be added to the dilution sequence. An amount check test with a specific threshold is defined for each target compound.

If chloride is selected as a target compound, and 10 is selected as the threshold, any samples that have a reported result above 10 (ppm or any concentration units from your QNT file) will fulfill this test and be added to the dilution sequence (Fig. 4).

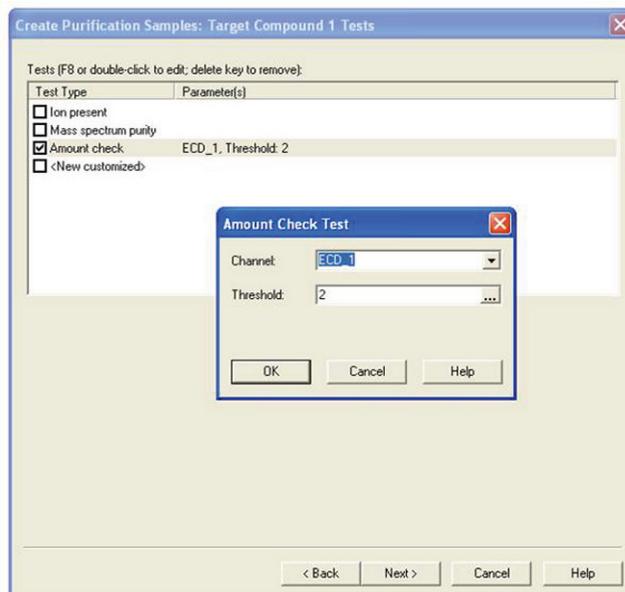


Figure 4. Target Compound X Test dialog box.

Special Options

The use of a conditional program is optional. If multiple dilution levels will be used (each in a separate PGM), they can be specified in the conditional program selection dialog. The use of Conditional Program is not covered in this Technical Note. Refer to Technical Note 83 for the use of conditional programs. If only one partial injection volume will be used for the re-run sample, uncheck both boxes (Fig. 5).

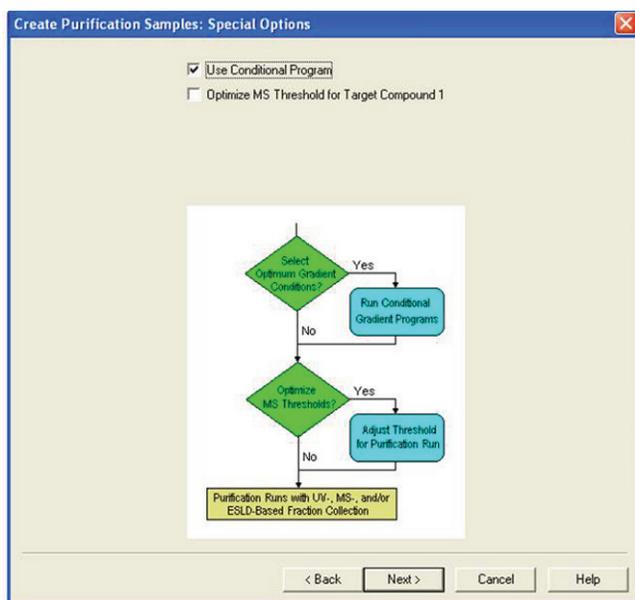


Figure 5. Special Options dialog box.

Conditional Program Selection

This section is only active if the **Use Conditional Programs** box was checked.

Sequence Properties

The Sequence Properties dialog box is where the name of the new dilution sequence is entered. Enter a name that will be readily recognized as containing the diluted samples for your original run. If you use the variable sequence name without an extension, the Chromeleon AutoDilution tool does not create a new sequence. The newly created samples are appended to the existing samples in the current sequence instead.

Use **Sequence Properties** dialog to specify any standards that are needed to run before the dilutions. In Pre-run samples, a previously created sequence containing the needed standards can be selected. The sequence you select will automatically run before the dilution sequence. If desired, standards can be selected to run before or after the diluted samples (Fig. 6).

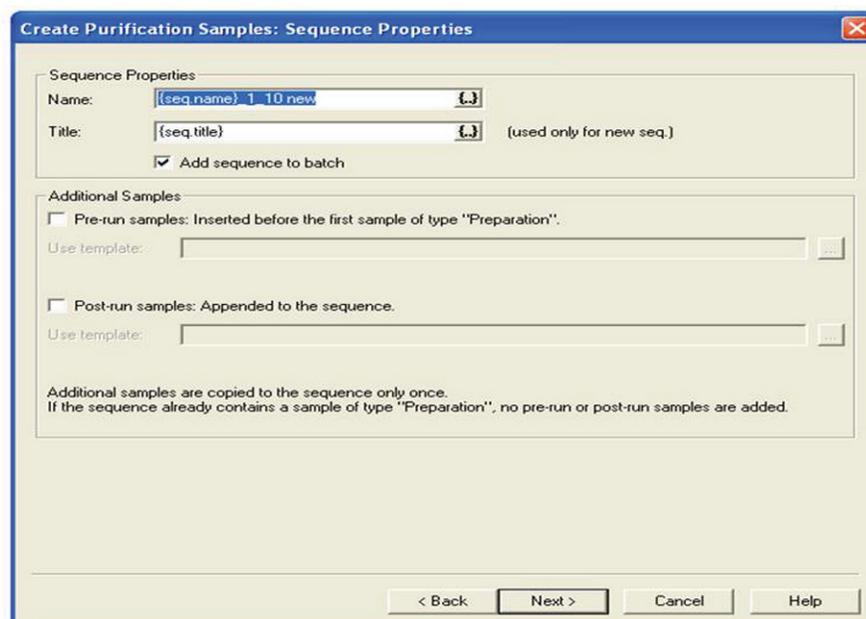


Figure 6. Sequence Properties dialog box.

Sample Properties

In the **Program** box select the PGM file to be used with the re-run samples (without the post-acquisition step). The QNT method can also be entered. This is generally the same QNT method used in the original samples. The sample type and status cannot be edited (Fig. 7).

For the partial loop injection method, the Sample Properties dialog is where the injection volume is entered for all samples run in the dilution sequence. To enter a 1:10 dilution, enter $1/_{10}$ of your full loop volume. As mentioned above, a new sequence can be created for the re-run sampling, or can be appended to the end of the current sequencing.

Extended Sample Properties

The last Wizard dialog box is the **Extended Sample Properties**. In the **Extended Sample Properties** dialog box, you can select the tray and vial locations for the diluted samples (Fig. 8).

For the partial loop method, since the dilution injection are made from the same vial as the undiluted run, select **Use analytic sample tray** and **Same as analytic sample vial**. The number of preparative injection for both methods is one.

The post-acquisition step creation is now complete and ready to run.

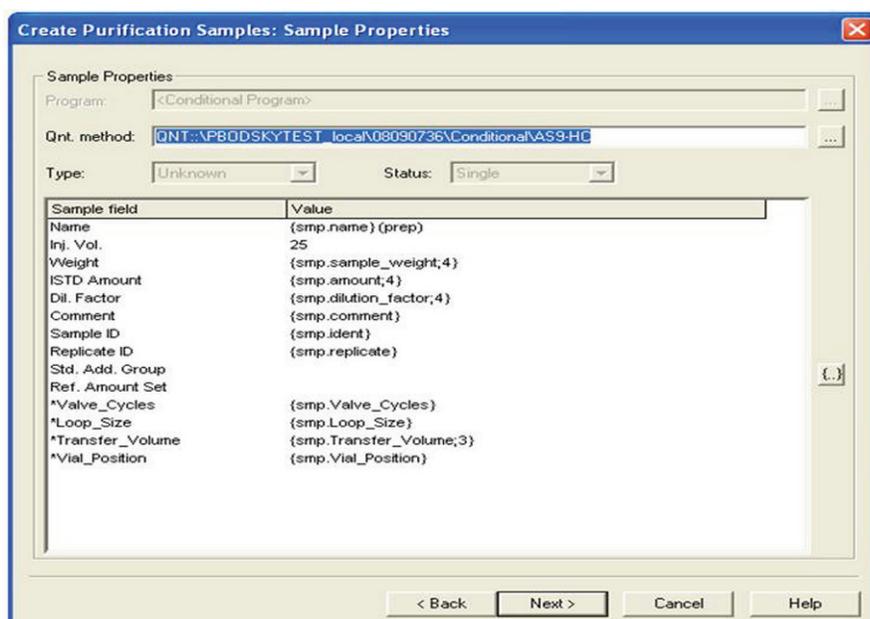


Figure 7. Sample Properties dialog box.

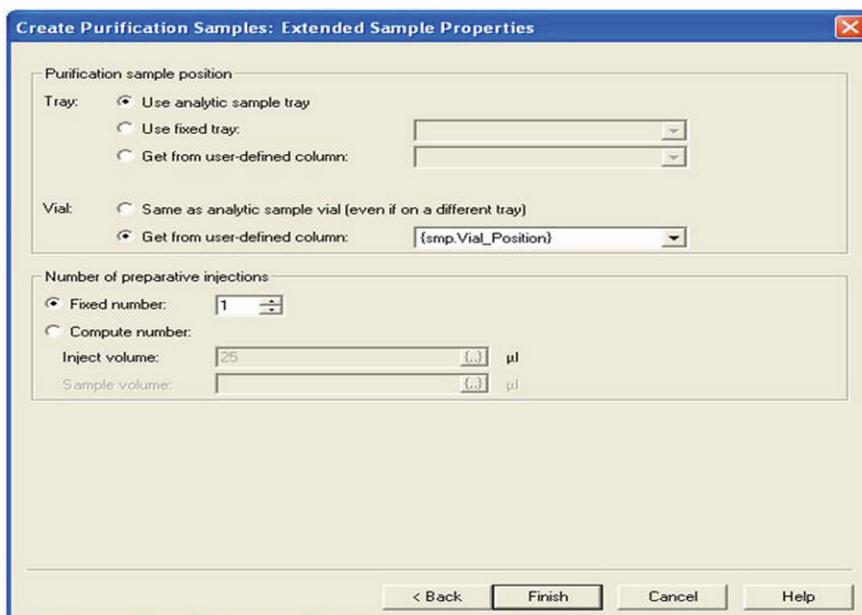


Figure 8. Extended Sample Properties dialog box.

BENEFITS OF CHROMELEON AUTODILUTION

The Chromeleon AutoDilution Tool offers a quick easy and reliable method to perform automatic logical dilutions of samples, saving time and money, and increasing productivity. It offers the following advantages:

- Automated check for samples that exceed threshold.
- Automated re-run of diluted samples if needed.
- All dilutions runs can be stored in a separate sequence for easy identification.
- No additional equipment to install.

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