

Automated Attachment of Chromatographic Parameters to NetCDF Files

ACD/ChromManager and ACD/ChromProcessor
Version 7.0

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One of the limitations of NetCDF (or AIA) files is the inability to include chromatographic parameters or other associated fields.

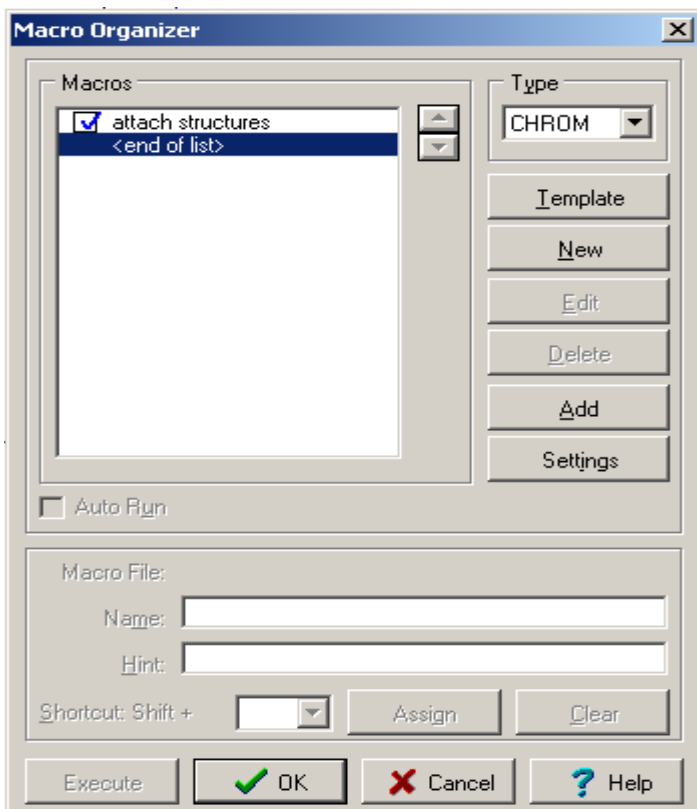
With [ACD/ChromProcessor](#) [1] or [ChromManager 7.0](#) [2], it is possible to attach chromatographic parameters in a few simple steps. This can be done in a semi-automated fashion using a button in the processing window, or automatically as part of group macro processing.

The first step to creating a parameter attachment system is to write a parameters file. If you are performing the same experiment over and over, you may want to create a complete parameter file. If you just have a number of parameters that are always the same, you may create a partial parameters file and manually complete the process.

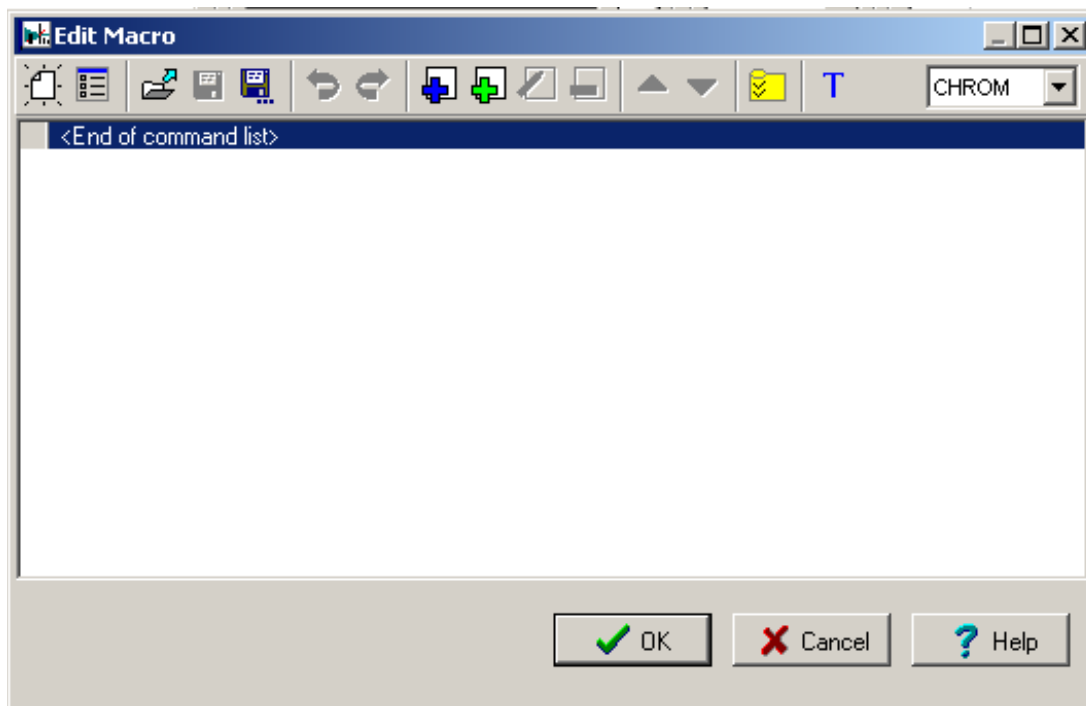
In order to create a parameters file, drop any .CDF file into ChromProcessor. This will enable the chromatographic parameters window. Enter the parameters that you wish to have attached to every chromatogram. Now save the file as a .PA file, such as STANDARDCONDITIONS.PA.

Creating a Parameters Macro Button

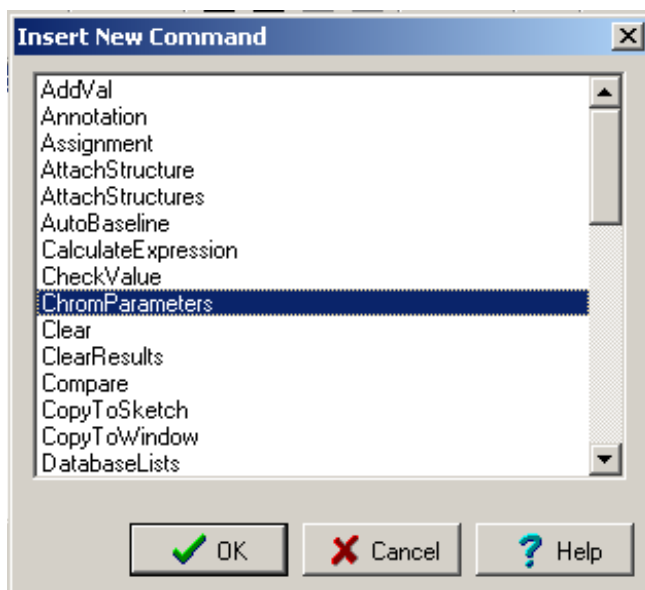
1. In order to create an attach parameters macro, simply choose the macro organizer on top of the chromatogram window.



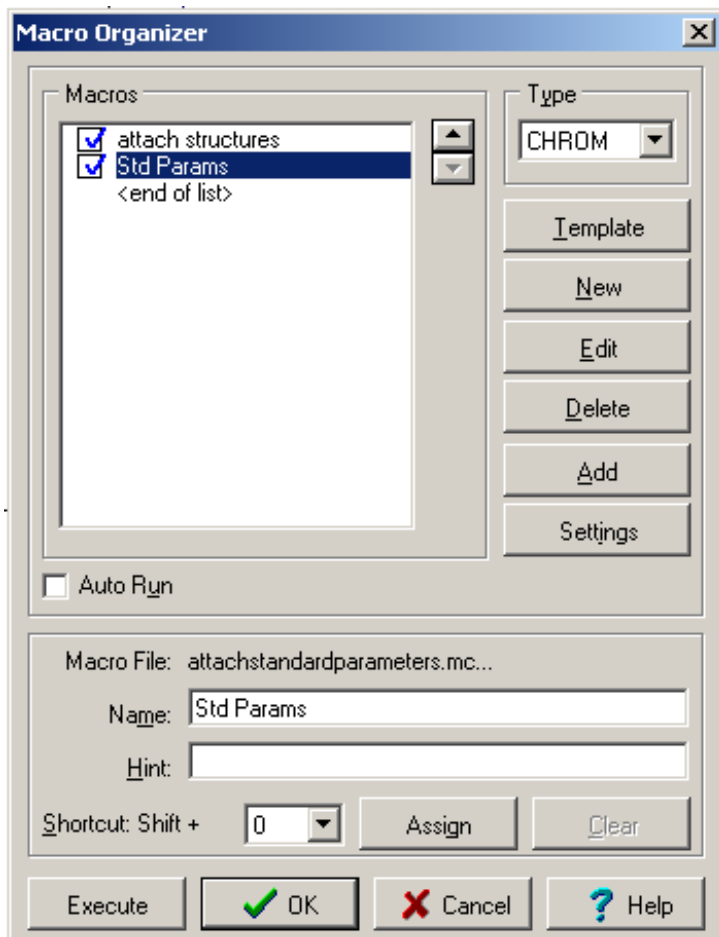
2. Next click **New**.



3. Create a new function by double-clicking on the command line, and choose **ChromParameters**.



- Specify STANDARDCONDITIONS.PA. Save this macro as STANDARDCONDITIONS.MCR. To put a button on the chromatogram window, simply check the box beside this macro in the Macro Organizer dialog box, and then specify a descriptive title.



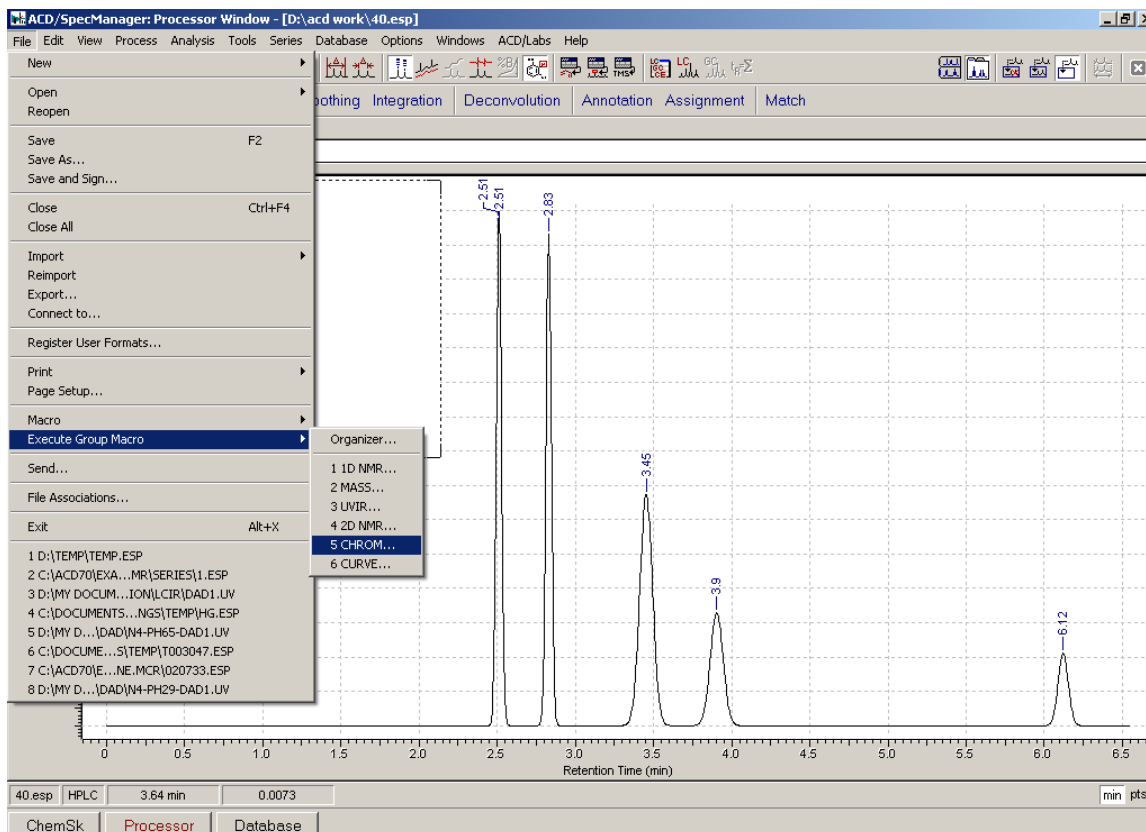
The button is now enabled. If you have a few standard sets of conditions, you may want to create a few more macros, with buttons for each one.

- After you click **OK**, your chromatogram window should have a new button associated with it. Click the button and the parameters that you specified will be attached. To make

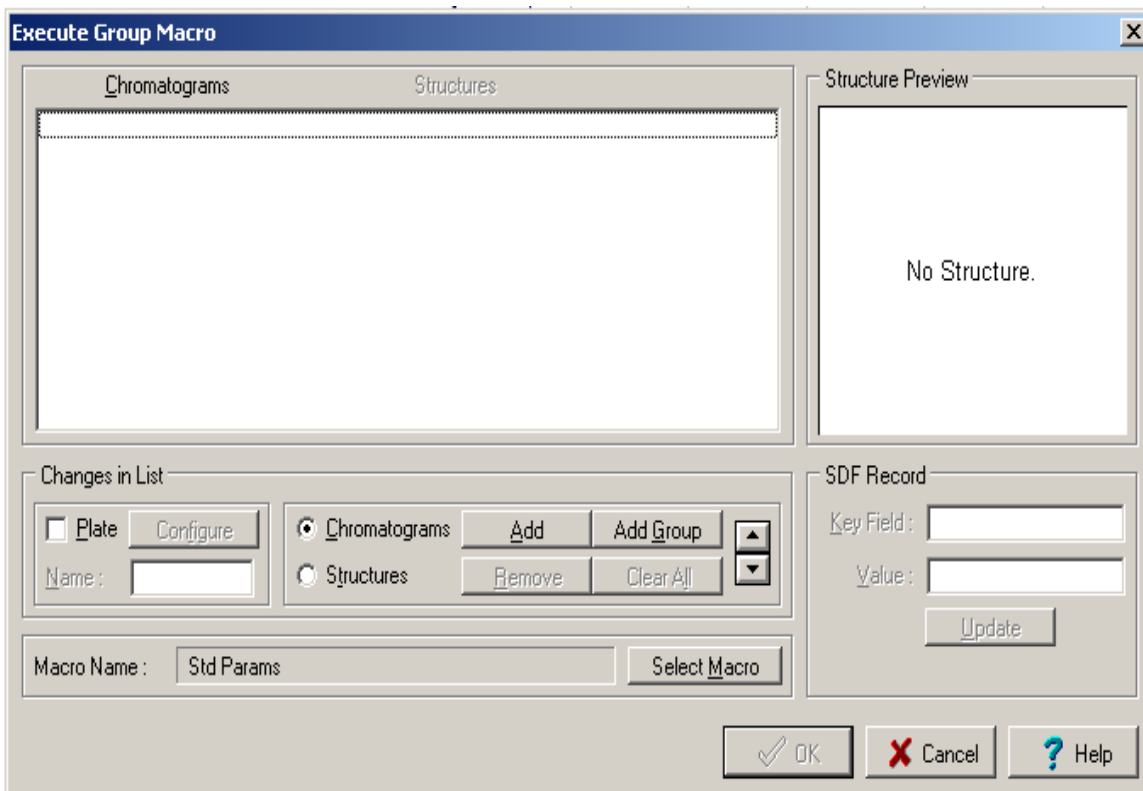
modifications to these parameters, simply click HPLC parameters  and make the inputs.

Attaching Parameters to Multiple CDF Files in One Step

It is very easy to execute group macros in ChromProcessor, where the same operation is performed on many files at the same time. For example, if you wish to open 10 chromatograms and automatically attach chromatographic parameters, you can simply drop the CDF files into the group macro, and specify the ATTACHCONDITIONS.MCR macro that we created in section 2.

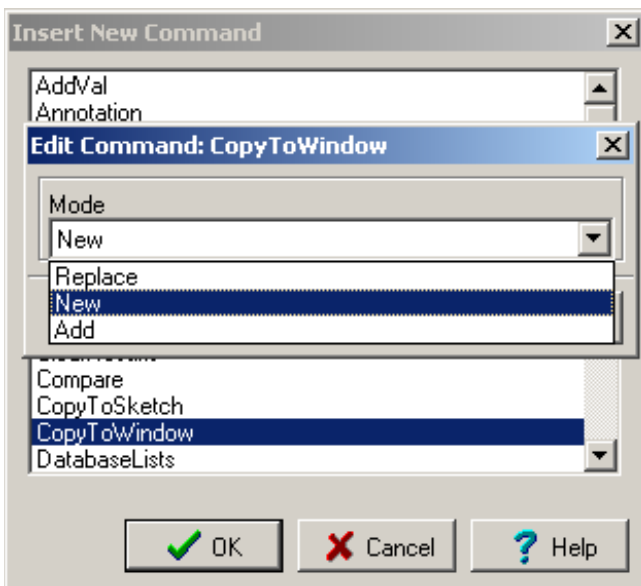


1. In the Chromatogram window, on the **File** menu, point to **Execute Group Macro**, and then choose **Chrom**.
2. In the **Execute Group Macros** dialog box that appears, drop in the files that you wish to process.



You will need to make a slight modification to the macro that we created in section 2. This macro will now need to include the instruction to open or database the chromatograms.

3. Click **Select Macro**, and choose the **Attach Parameters** macro. Edit the macro to include a "CopyToWindow" command prior to the attach parameters command. If you select **New Window**, this will open a new window for each chromatogram, up to about 50 at one time.



4. Save the macro with a new name, like OPENATTACHPARAMS.MCR.
5. Browse to any AIA files that you want to import, and drop them into the group macro window. Clicking **OK** will now open the chromatographic files and attach all parameters. If you want to directly database the files, simply substitute "UpdateDatabase" for "CopytoWindow".

Advanced Work

It is possible to mix and match sets of chromatographic parameters. For example, column, detector, and solvent information can be separated into individual sets of parameters for attachment. This means that individual buttons can be created for different columns and solvent systems if desired. Please see the ACD/ChromManager documentation for more details.

Conclusion

ChromManager is designed to read chromatographic parameters from native data formats. Users that work with standard data formats such as AIA may have issues with the fact that these parameters are not written into their data. Luckily, chromatographers typically work with a limited number of systems. In ACD/ChromManager, with a few minutes' work, it is possible to attach sets of parameters to chromatograms in an automated or semi-automated fashion.

References

1. ACD/ChromProcessor. <http://www.acdlabs.com/chromprocessor/>. January 11, 2005.
2. ACD/ChromManager. <http://www.acdlabs.com/chrommanager/>. January 11, 2005.