

Creating Context-sensitive Report Forms

ACD/ChromManager
Version 8.0

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Introduction

It is very valuable to have consistent reporting within an organization. Reports that are created from an approved template will have data arranged in a consistent manner such that chemists, chromatographers, and managers will all know where to look for a given piece of information. Multiple page templates can be created to contain report summaries and tables of information at the beginning as well as raw data on subsequent pages. However, it can be useful to use different templates depending on certain aspects of the work. For example, preparative scale projects may require different report content than chiral assays. Or metabolism reports may be different from those for method development. In this Technical Note, we will see how to use a macro that invokes a different template depending on the contents of a given field. This note is not intended to give detailed instructions on how to create context-specific report macros, but rather to illustrate the operation and strategies involved.

Note This Technical Note is for use with the associated example files. These files should be placed in a single folder to ensure that the macros function correctly.

Report Templates

Report templates are created within the [ACD/ChemSketch](#) [1] window. Elements of a report can be input in one of three ways. Stagnant components can be input by simply moving to draw mode and placing the material in the appropriate spot on the report. The other two components are inserted using the report template tool. If you select this tool and drag a portion of the page, you will have a box on your screen. You can double-click on the box to change its content. Formatted text (from the common template type) enables the user to put simple text in place. Spectral or chromatographic parameters can be selected by first choosing the technique, and then choosing the element that is desired. To illustrate, you may put a company logo in the top left of the page, formatted text that says: "Chromatographic Report" in the top center, and a chromatogram in the centre of the page. You can also add more chromatographic elements such as tables, etc. Any of these components can be configured for style and content by clicking **Settings**.

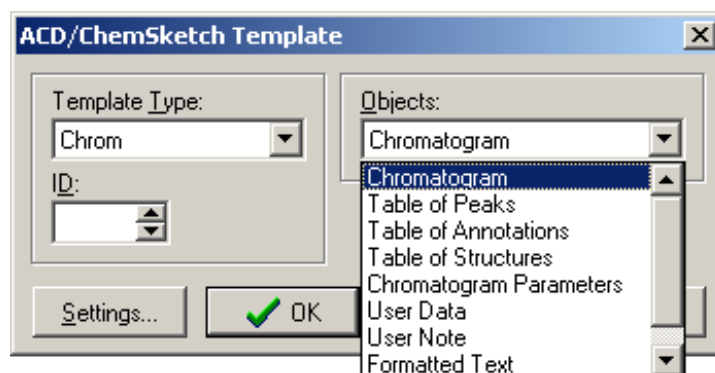



Figure 1: The report template tool.

Report templates are saved as an SK2 file; the templates required to demonstrate the features herein are included for download with this document. For the purposes of this technical note (and compatibility with the associated macro), it is best to store these templates in the directory to which you copied the macro file. For more information on report templates, refer to the *ACD/ChromManager User's Guide*.

SpecManager Macros

[ACD/ChromManager](#) [2] (and [ACD/SpecManager](#) [3]) have a very powerful set of macros that allow the user to automate most processes that can be performed on a given set of analytical data. The first step in trying this reporting style will be to create a new macro button in the processor window. To do this, first open ChromManager and move to the Processor window using the bottom toolbar. Next, open a chromatogram. You can use any of the example chromatograms accompanying this note. Above the chromatogram, you should now see the **Macro Organizer**  button. Open the **Macro Organizer**, click **Add**, and specify **chrom_userdatacheck.mcr**.

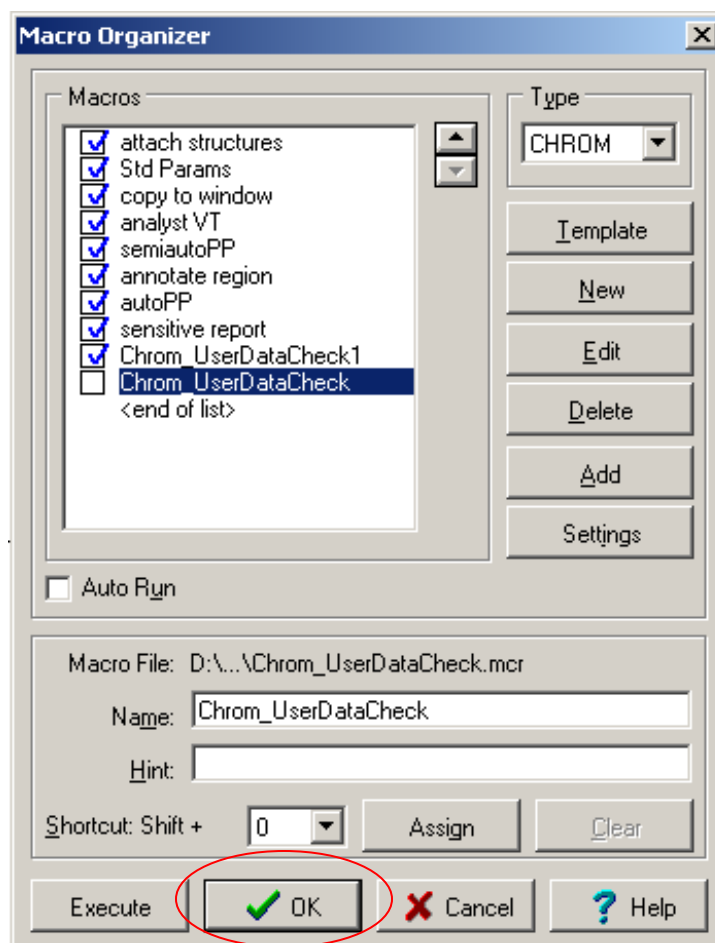


Figure 2: The macro organizer.

Click on the check box beside the macro and click **OK**. You should now have an extra button at the top of the processor window: `Chrom_UserDataCheck`. This button will be available every time you open chromatographic data.

This macro has been created to allow the user to create a template report, but before the template is chosen, certain conditions must be met. In this case, the macro will verify whether the chromatography was performed for an assay procedure, a related substances analysis, or some other purpose.

We'll see the macro in operation shortly; first we'll learn about a few more tools that make this macro more versatile.

ChemBasic Applications

ChemBasic is the programming language for ChemSketch. This programming language enables users to write simple applications that can be configured to be chemically-intelligent. In this case, the macro uses ChemBasic simply to invoke a user data form to prompt you to input a value for the Application user data field, when the current value does not match an item on a pre-specified list.

User Data Forms

User data forms are used in ACD/Labs software to attach additional data to chromatograms and spectra. The use of radio buttons, drop-down menus, and required/optional fields ensures that there is maximum efficiency, accuracy, and consistency in the entries. This is especially useful for database creation, but it can also be used to attach data to reports.

The ChemBasic application included in this macro is designed to invoke a user data form when data is required prior to making a report template decision. This form will communicate to the user what information is required, and can help make it easy to input.

A Context-sensitive Form: Pulling it all Together

The macro that we have created does a bit more than simply choose a report template based on the contents of a user data field. We have created the ability to prompt the user for data if the value is not recognized. This presupposes that the field is meant to be populated with rigidly-defined values. If the field is not populated with one of these values, the software prompts the user to use the drop-down menu to enter the value at that point.

Based on the value contained in the field (in this case, related substances, assay, or other), the appropriate form is invoked. Open any of the example chromatograms that have been provided, and use the report macro. Now move the ChemSketch window and observe the result. The report template has been chosen based on the contents of the application field, and the report has been created in ChemSketch. You can try one of the other report templates by opening other chromatograms and clicking the report macro button. Each time, the template is chosen based on the contents of the "Application" user data field.

But what happens when the field is populated with something other than the values the macro expects?

This macro has been created to preserve any values contained in the user data field. Using any of the chromatograms in the example set, click **Edit**, then **User Data**, and then **Edit**. Change the value for Application to something like "chiral assay". Now try the report macro. The macro prompts you to enter an approved value.

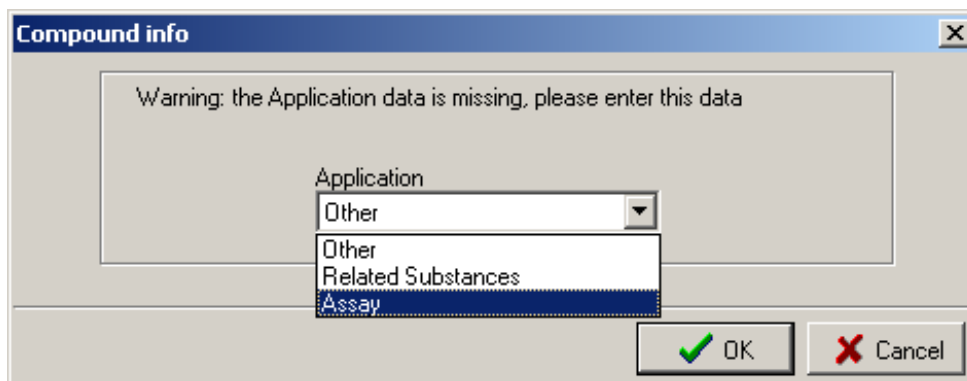


Figure 3: A user data input form.

Scroll down to "assay". The report is created. Now from the **View** menu, choose **Chromatogram User Data**. You will see that the Application field has been filled with the approved value of "assay", but the user input value ("chiral assay" in our case) has been saved to

the Application (original) user data field. In this way, the value specified is not lost. Of course, this is only one way to configure the macro. We could have invoked the user data form and omitted the step of writing the value in the Application field, with subtle changes in the design of the macro.

Conclusion

Context-sensitive reporting can simplify the production of professional, consistent reports a great deal. Organization-approved forms can ensure that data is presented in the same way regardless of the user or even the group which does the work. The fact that given information can be used to automatically select between approved forms can further streamline this process.

References

1. ACD/ChemSketch. <http://www.acdlabs.com/chemsketch/>. December 22, 2004.
2. ACD/ChromManager. <http://www.acdlabs.com/chrommanager/>. December 22, 2004.
3. ACD/SpecManager. <http://www.acdlabs.com/specmanager/>. December 22, 2004.