

# Controlling Report Content

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## ACD/SpecManager and ACD/ChromManager Version 8.0

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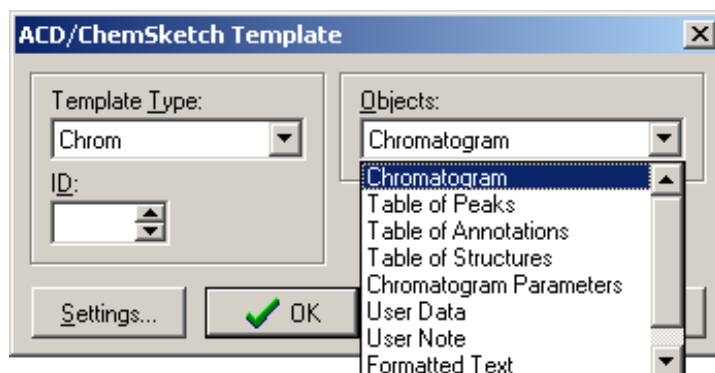
## Introduction

Ensuring that reports are consistent across a group is very important. There are a number of Advanced Chemistry Development, Inc., (ACD/Labs) Technical and Application Notes that detail the ways that report templates can be used to ensure that reports are easy to create, and have a consistent look and feel. The reader is directed to these notes for specific information on how to create effective report templates. This technical note will show how to ensure that report templates are not just consistent, but also complete, by checking to see that certain fields are filled in prior to the creation of the report. In this case, key user data will be missing from the chromatogram. A form will be triggered, asking the chromatographer to fill in this data prior to creating the report. The form will also assist with the fast, accurate input of this data.

**Note** This technical note is for use with the associated example files. The template and macro files should be placed in a single folder to ensure that the macros function correctly.

## Report Templates

Report templates are created within the ChemSketch 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 onscreen. This box can be double-clicked 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 might put a company logo on the top left of the page, formatted text that says: "Product Development Report" on the top center, and a chromatogram in the centre. You could also add in more chromatographic elements such as tables, etc. Any of these components can be configured for style and content by clicking **Settings**. As we have noted in other technical notes, these templates have a great deal of versatility, and you can automatically select between them based on data content. For the purposes of this technical note, only one template will be used. Our macro will examine the data before allowing the report to be created.



**Figure 1:** The report template tool.

Report templates are saved as SK2 files; the templates required to demonstrate the features herein are included for download with this document.

**Note** There are five files included for download with this document:  
 CHROM\_NAME\_FORM.FRM  
 CHROM\_NAME\_FORM\_CB.BAS  
 CHROM\_USERDATACHECK.MCR  
 NO\_ANALYST\_USER\_DATA.ESP  
 USER\_DATA.ESP

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 the creation of report templates, refer to the *ACD/ChromManager User's Guide*.

## SpecManager Macros

[ACD/ChromManager](#) [1] (and [ACD/SpecManager](#) [2]) 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 two new macro buttons in the Processor window. To do this, first open ChromManager and move to the Processor window using the bottom toolbar. Next, open any chromatogram. You can specify 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 COMPLETED\_DATA\_REPORT.MCR.

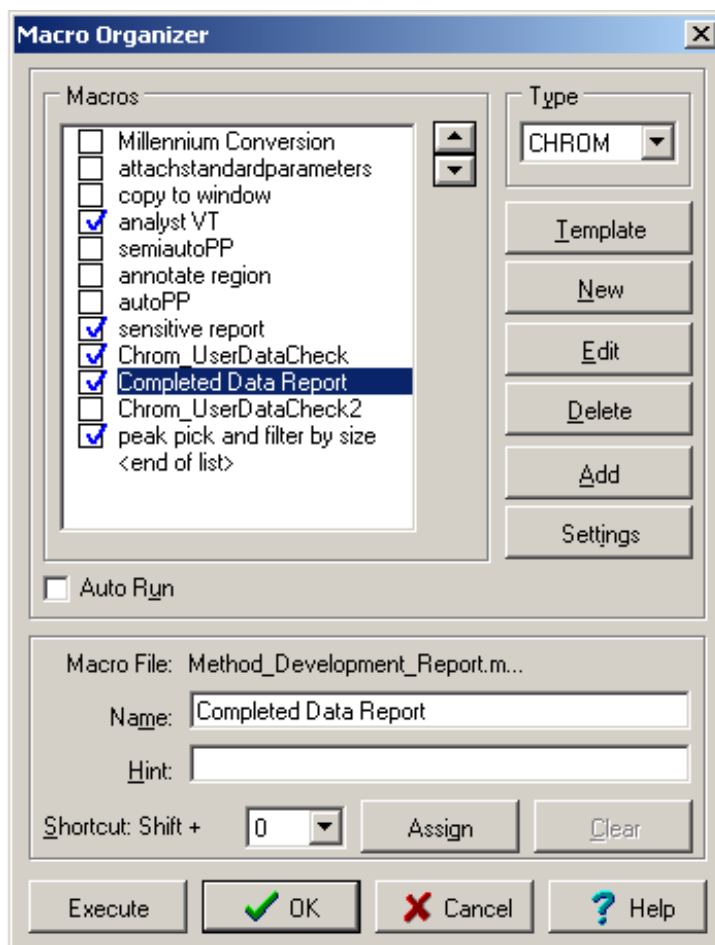


Figure 2: The Macro Organizer.

Select the check box beside the macro and click **OK**. You should now have an extra button at the top of the Processor window: **Completed Data Report**. This button will now 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 used, certain conditions must be met. In this case, the macro will check to make sure that all required user data has been filled in by the chromatographer. If it has not, a form will pop up to allow the user to enter the data easily.

The macro below checks to see if the User Data field **Analyst** is filled in. If the **Analyst** field is filled in, then a report is created. Otherwise the macro will execute an [ACD/ChemBasic \[3\]](#) program where the user must supply the information. Subsequently, the report is generated with all the information in place.

```
; Assign Application value to Variable AnalystVariable
GetSpecData (What = "UserData"; UDName = "Analyst"; Result = AnalystVariable)
SetVariable (Name = OtherVariable1; Value = "0")
;
; If Analyst User Data is blank, pop-up a form
CheckValue (Value = "$(AnalystVariable)"; Pattern = ""; Condition = "Equal"; UseCase = False)
```

```
ExecuteChemBasicApp (Application = "${MACRODIR}\Chrom_Name_Form_CB.bas"; Parameters =
""${MACRODIR}""; Result = "CBRESULT1"; MultiRes = False)
SetUserData (Name = "Analyst"; Value = "${CBRESULT1}"; Type = "Spectrum")
CopyToSketch (ReportType = "Template"; TemplateFile = "${MACRODIR}\Related Substances Template.sk2")
SetVariable (Name = OtherVariable1; Value = "1")
;
; If the Analyst User Data is not empty, create a report
CheckValue (Value = "${OtherVariable1}"; Pattern = "0"; Condition = "Equal"; UseCase = False)
CopyToSketch (ReportType = "Template"; TemplateFile = "${MACRODIR}\Related Substances Template.sk2")
```

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

## ChemBasic Applications

ChemBasic is the programming language for [ACD/ChemSketch](#) [4] and SpecManager. This programming language enables users to write simple applications that can be configured to be chemically-intelligent. In this case, when the current value does not match an item on a pre-specified list, the macro uses ChemBasic to invoke a user data form to prompt the user to input a value for the Optimization Type user data field. Below is the actual ChemBasic code used. To create your ChemBasic program, locate the file CBEDIT.EXE within the ACDLABS folder.

```
function main as string
dim AnalystField, CompName as string
dim Chrom_Name_Form, ps1 as string
dim Frm as object

ps1 = ParamStr(1)           'reads in the macro path, i.e. ${MACRODIR}
Chrom_Name_Form = ps1 + "\chrom_name_form.frm"

Frm=ReadForm(Chrom_Name_Form)
if Frm.ExecForm then CompName = Frm.GetStrValue("Chrom_Name_Userdata")

AnalystField = CompName
main = AnalystField
end function
```

The ChemBasic code is executed from the SpecManager macro. In addition, the macro passes a variable, **MACRODIR** (the directory path to the macro), to the ChemBasic program and is assigned a variable, **ps1**. Hence the form must be in the same location as the macro. The ChemBasic program executes the form, called **Chrom\_Name\_Form**, where you can set the Analyst's name. This value is then assigned as a variable, **CompName**. The variable **CompName** is then passed back to the macro for storage as User Data within the .ESP file.

## 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 and individual chromatograms.

The ChemBasic application included in the first 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 to make it easy to input it. The ChemBasic

application in the second macro is designed simply to communicate an error message to the user before canceling the report operation.

To modify the list of names within the form, open the form and double-click **Analyst**. Click **Edit** followed by **New Value** or **Edit Value**. Finally, save the form.

## A Context-Sensitive Reporting Tool: 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 can require that the field be populated with rigidly-defined values. If the field is not populated with one of these values, the software prompts you to use the drop-down menu to enter the value at that point. In our case, we are simply looking for an entry in each of the required areas.

Open the two example files that accompanied this technical note: NO\_ANALYST\_USER\_DATA.ESP and USER\_DATA.ESP. Our example chromatograms have user data fields associated with them. From the **View** menu, choose **Chromatogram User Data** to see this data. From the Processor window, select the USER\_DATA.ESP file. If we click the **Complete Report macro** button, the data is examined and the report is created according to the template that is specified in the macro. Now move to the ChemSketch window and observe the result. You can now try the NO\_ANALYST\_USER\_DATA.ESP file by returning to the Processor window, selecting this chromatogram, and clicking **Complete Report macro**. This time, a required user data field is missing. The macro triggers a user data form to allow the chromatographer to enter the data. Once the form is completed, the user data fields are filled in, and the report is generated.

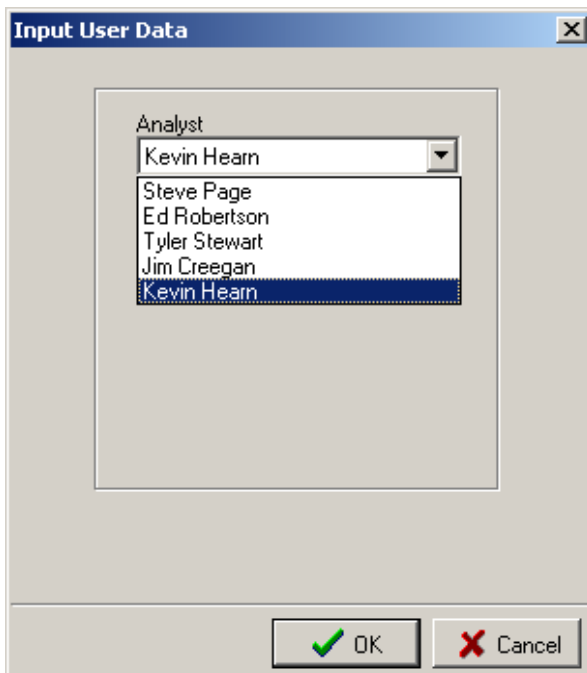


Figure 3: The User Data input form.

All of the tools that we have seen here can be used with other kinds of analytical data, provided that the user has a license for the relevant module. The user must simply specify a report template dedicated to that particular kind of data, and specify the macro type in the same manner.

## Conclusion

With ChromManager 8.0, it is possible to create report templates that not just streamline the production of formatted reports, but also verify that these reports have appropriate content according to the Standard Operating Procedures for the group. The combination of report templates, macros, and ChemBasic applications can help scientists to increase efficiency and consistency within the organization.

## References

1. ACD/ChromManager. <http://www.acdlabs.com/chrommanager/>. January 3, 2005.
2. ACD/SpecManager. <http://www.acdlabs.com/specmanager/>. January 3, 2005.
3. ACD/ChemBasic. <http://www.acdlabs.com/chembasic/>. January 3, 2005.
4. ACD/ChemSketch. <http://www.acdlabs.com/chemsketch/>. January 3, 2005.