

Checking a Signature and Reporting a Chromatogram

ACD/ChromManager, version 9

Arvin Moser
Advanced Chemistry Development, Inc.
Toronto, ON, Canada
www.acdlabs.com

Introduction

With [ACD/SpecManager v.9.09¹](#), it is possible to execute a macro that will check a dataset to ascertain that it has been signed and then report the information. The purpose of signing a dataset is to indicate to future viewers that the dataset has undergone a strict inspection and has been approved.

This capability impacts a range of products including [ACD/ChromProcessor²](#), [ACD/Curve Processor³](#), [ACD/MS Processor⁴](#), [ACD/1D NMR Processor⁵](#), [ACD/2D NMR Processor⁶](#), and [ACD/UV-IR Processor⁷](#).

The power of a macro is to execute multiple tasks with the push of a single button. This Technical Note describes how to build and execute a macro to check for a signature and then report the results. The results of this report can be stored with the data, or used to enable a decision-making system, potentially involving some separate application.

Applying a Signature to a Dataset

Once a spectrum has been processed in the Processor, including assigning a structure(s), the next stage is to add a signature.

1. From the **File** menu, choose **Save and Sign**.

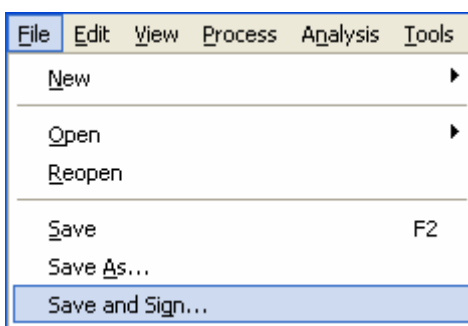


Figure 1: Saving the chromatogram with a Signature.

The **Sign File/Record** dialog box appears which requests a **User Password** and **Domain**. Any pertinent information can be stored in the **Comment** field.



Figure 2: Signing a dataset through a login.

2. Click **OK** to set the chromatogram as signed.

To manually check signed data, from the **View** menu, choose **Signatures**. Comments can also be appended where applicable.

Preparing the Macro

The macro can be built in the Processor.

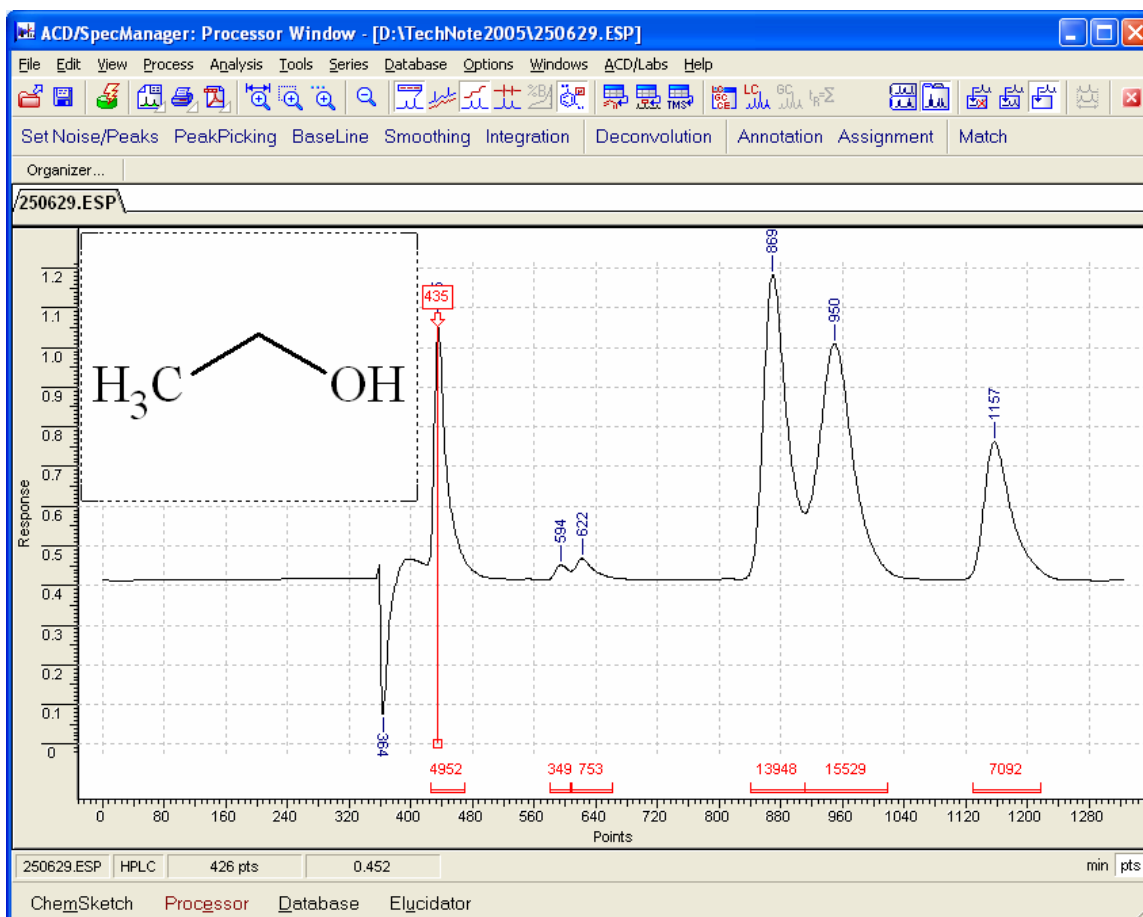


Figure 3: The processed chromatogram complete with integration, peak picking, and peaks assigned to a structure.

1. On the **File** menu, point to **Macro**, and then choose **Organizer**.

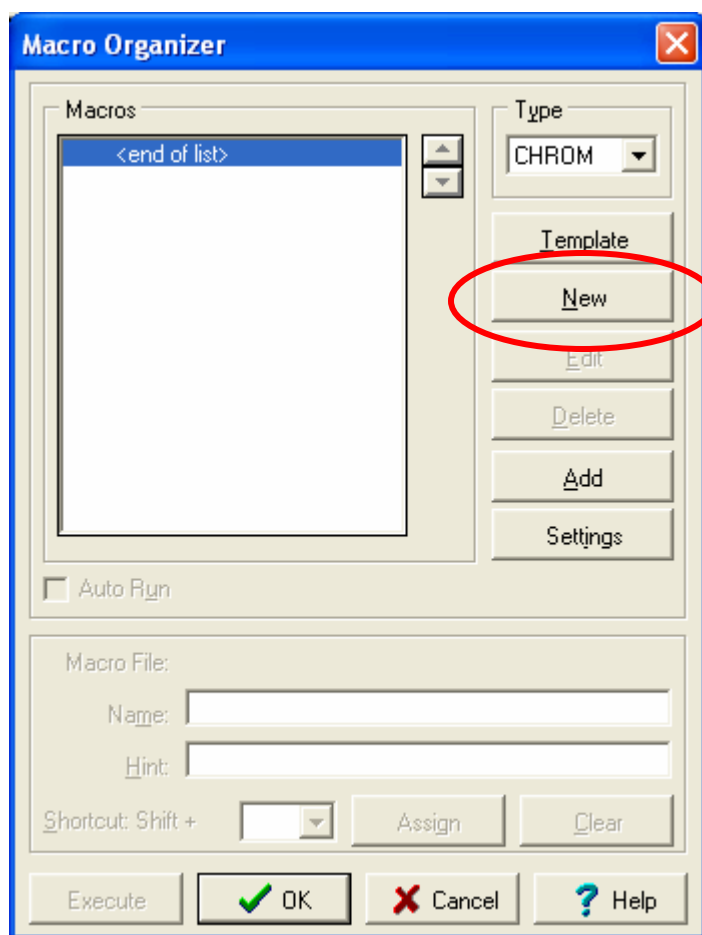


Figure 4: The blank Macro Organizer.

2. Click **New** to create a new macro.

- Click **Insert Macro Command** (shown in Figure 5) and start building the macro as described in Figure 6.

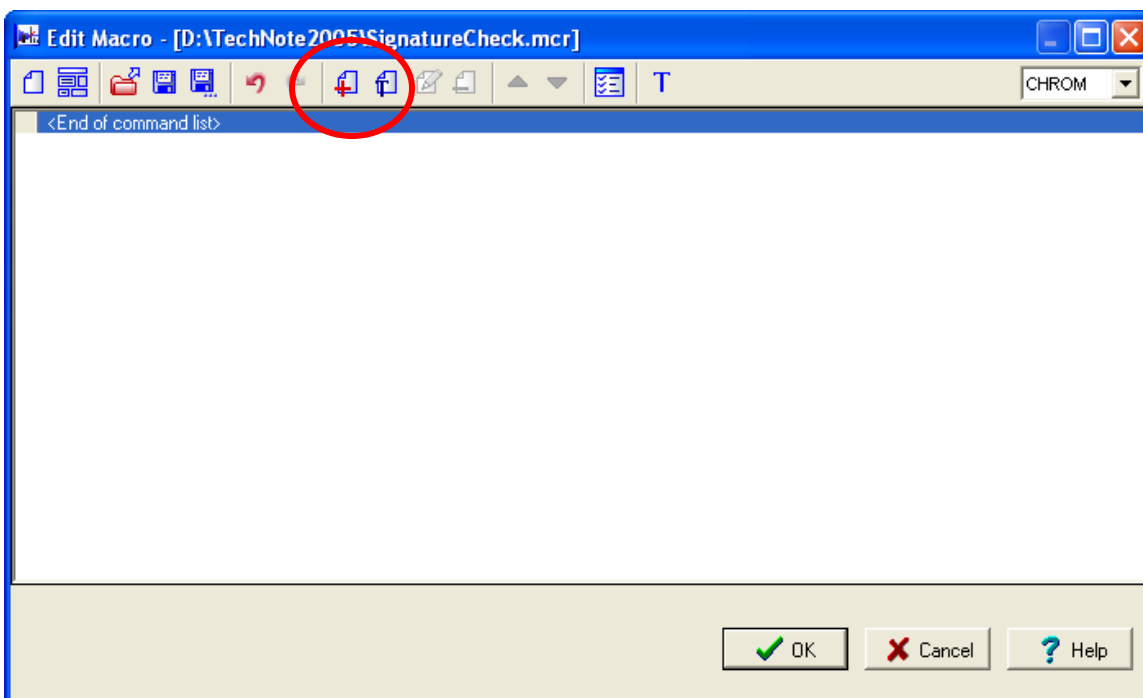


Figure 5: The blank Macro editor.

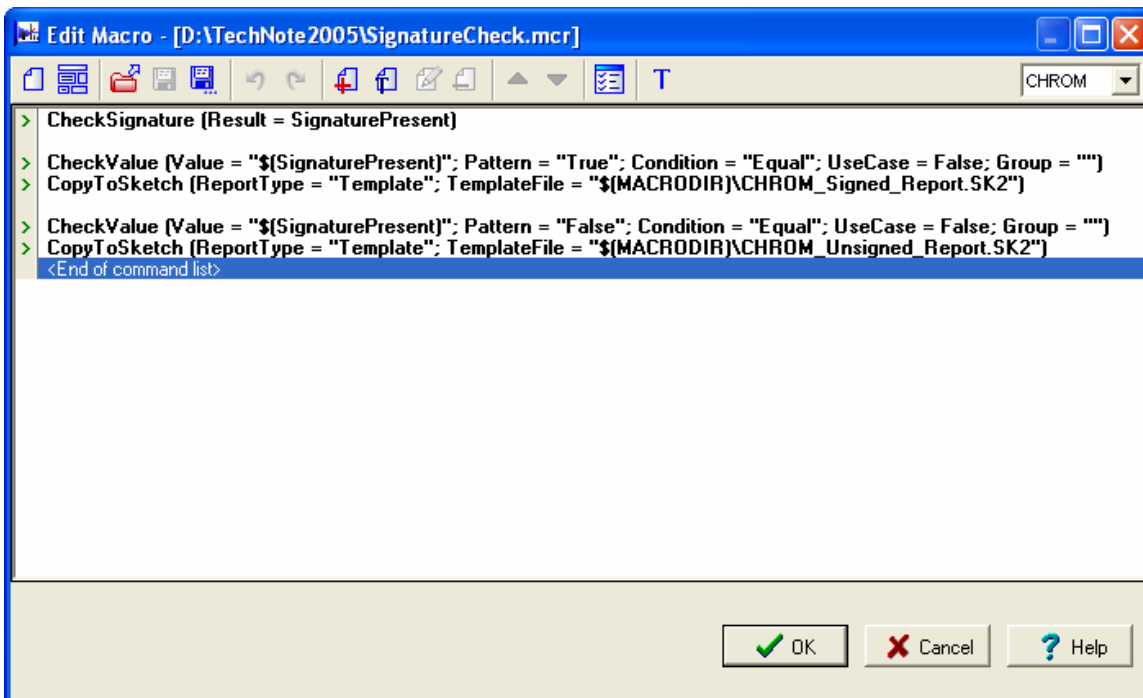


Figure 6: The completed macro showing macro commands in black.

Each macro command is built using the dialog boxes shown in Figures 7 to 11.

Figure 7 shows the dialog box to store the result of CheckSignature. The result is a True or False statement and is stored in the variable \$(SignaturePresent).

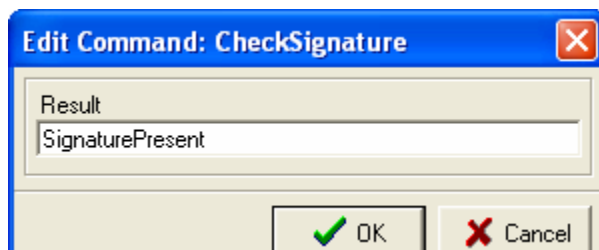


Figure 7: The CheckSignature macro command stores a value in the variable SignaturePresent.

Figure 8 shows the dialog box to check whether the variable \$(SignaturePresent) is equal to True. If \$(SignaturePresent) equals True, then execute the next command until another CheckValue has been reached.

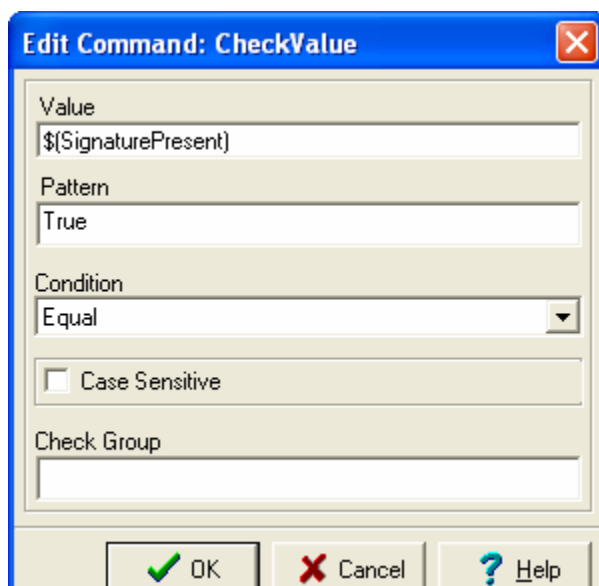


Figure 8: Checks whether \$(SignaturePresent) equals True.

Figure 9 shows the dialog box to create a report based on the template CHROM_Signed_Report.sk2. If the condition from the CheckValue has been met, a signed report is created.

A report is created and saved using ACD/ChemSketch set in Draw mode.

The report path is defined by the macro variable \$(MACRODIR). If the SK2 report file is placed in the same folder as the macro file, then this variable can be used. Otherwise the path should be explicitly shown.

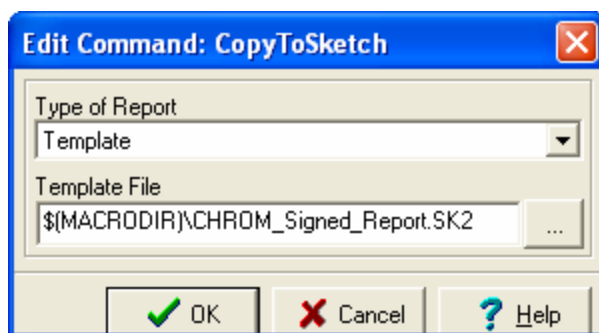


Figure 9: UpdateCurrentDatabase command is for a local SpecDB database.

Figure 10 shows the dialog box to check whether the variable \$(SignaturePresent) is equal to False. If \$(SignaturePresent) equals False, then execute the next command until another CheckValue has been reached or the macro has reached the <End of command list>.

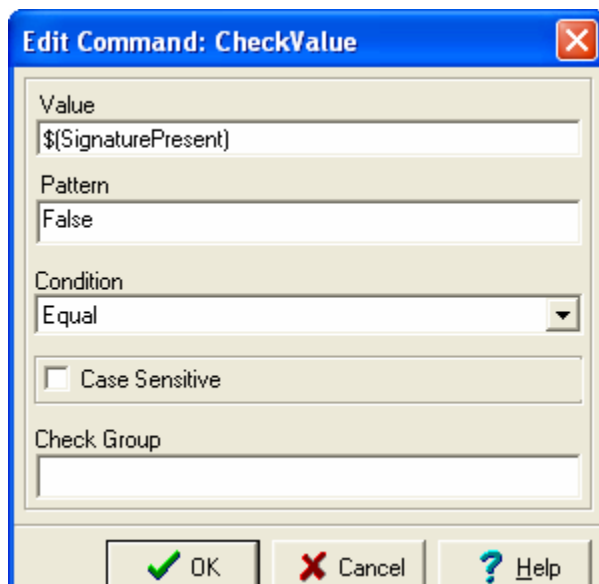


Figure 10: Checks whether \$(SignaturePresent) equals False.

Figure 11 shows the dialog box to create a report based on the template CHROM_Unsigned_Report.sk2. If the condition from CheckValue has been met, a signed report is created.

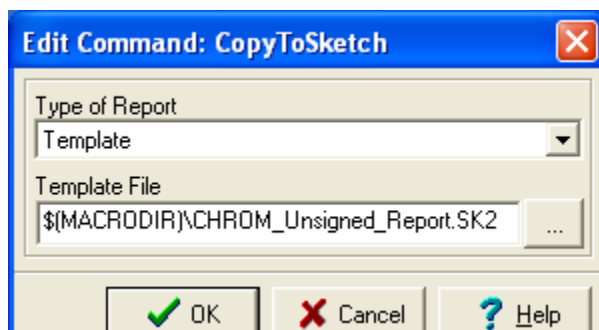


Figure 11: SetUserData command is for HNMR DB.10

When the macro is complete, click **OK**. Save the macro as SignatureCheck.mcr. Finally, select the macro in the **Macro Organizer** so that a blue arrow appears, as shown in Figure 12.

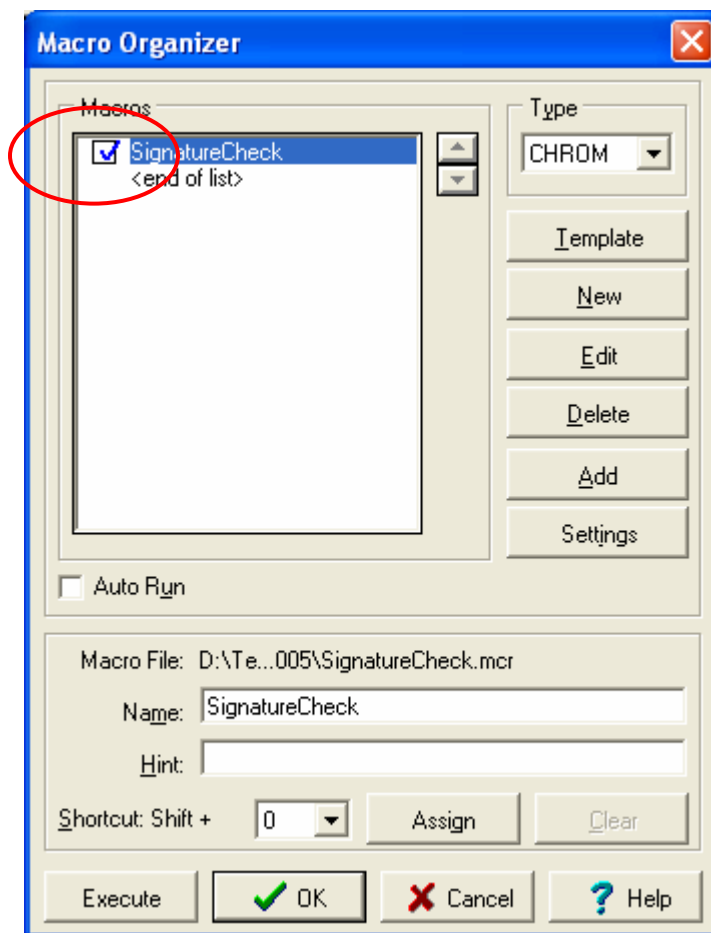


Figure 12: The Organizer with the macro checked-off.

Executing the Macro

Near the top left corner, directly above the spectrum, a SignatureCheck button is available. Click this button to execute the macro on the active chromatogram.

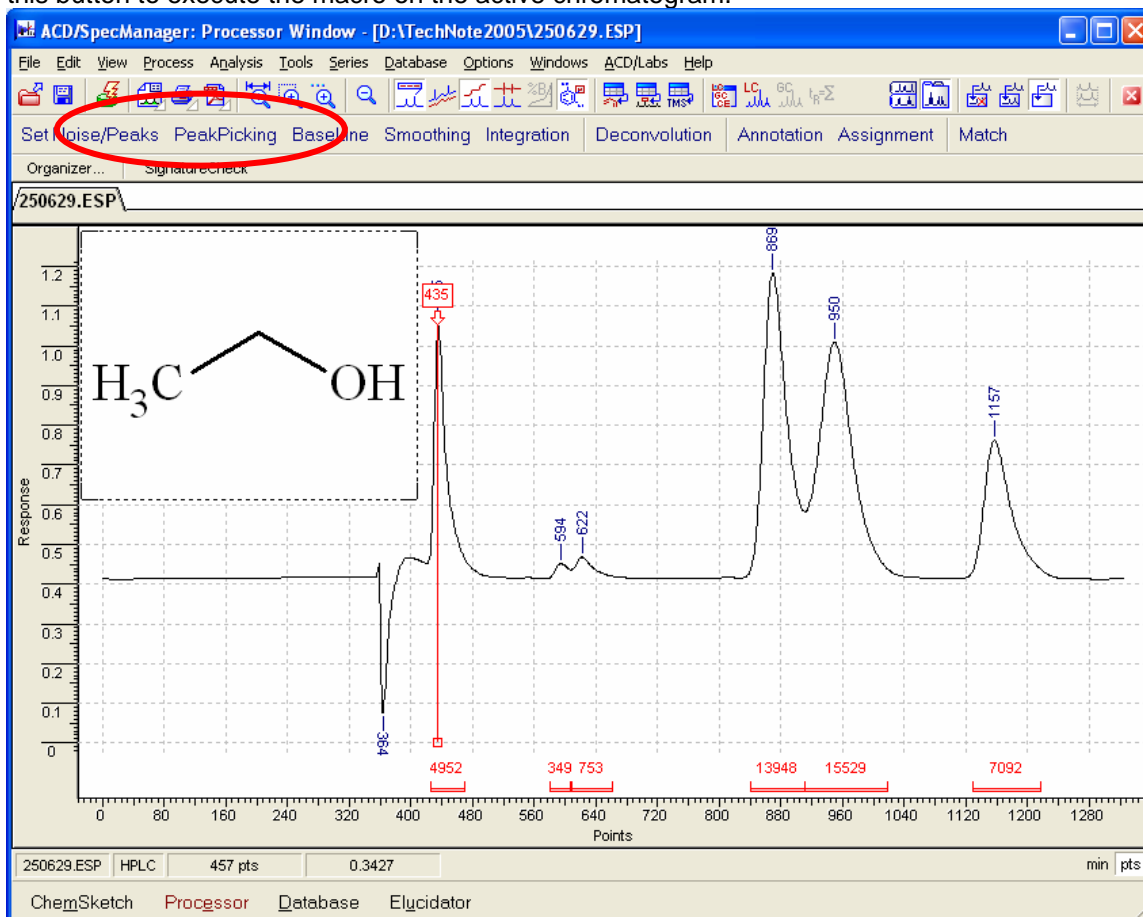


Figure 13: Locating the macro button.

Once the macro has completed, the macro protocol should be checked to ensure all commands were executed. See Figure 14 for a completed macro execution.

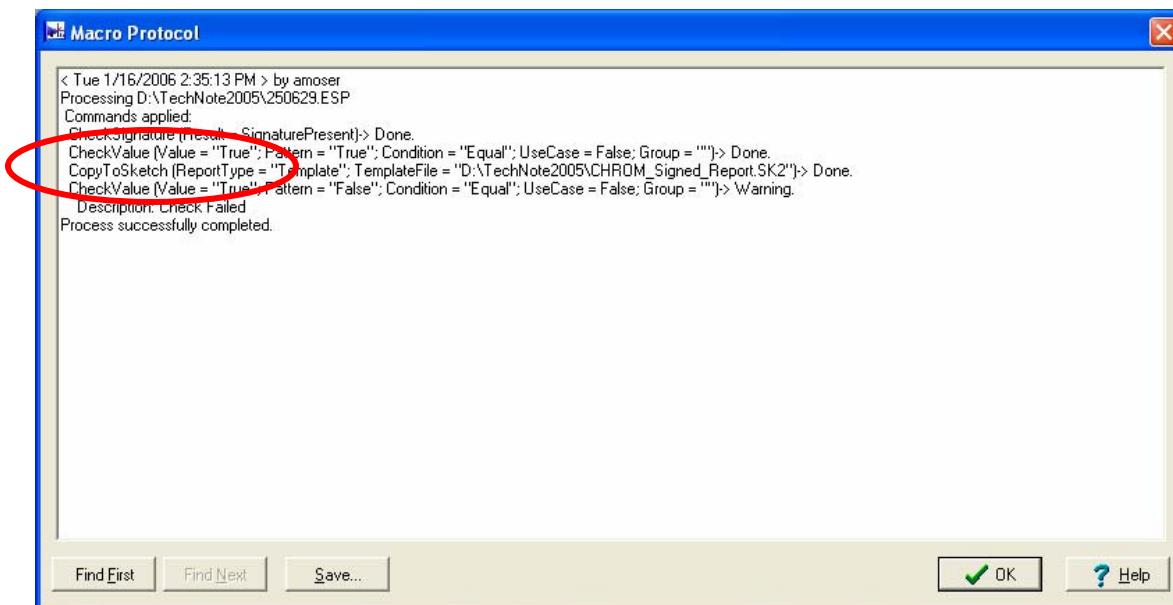


Figure 14: The Macro protocol showing the successful completion of the macro.

Click **OK** on the macro protocol. To view the report, click **ChemSketch** located on the Windows Switching bar.

Figure 15 and 16 illustrate the completed reports with Company logo, Chromatogram data, chromatogram, and Table of Structures. The report can be copied to Microsoft Word for further manipulation.

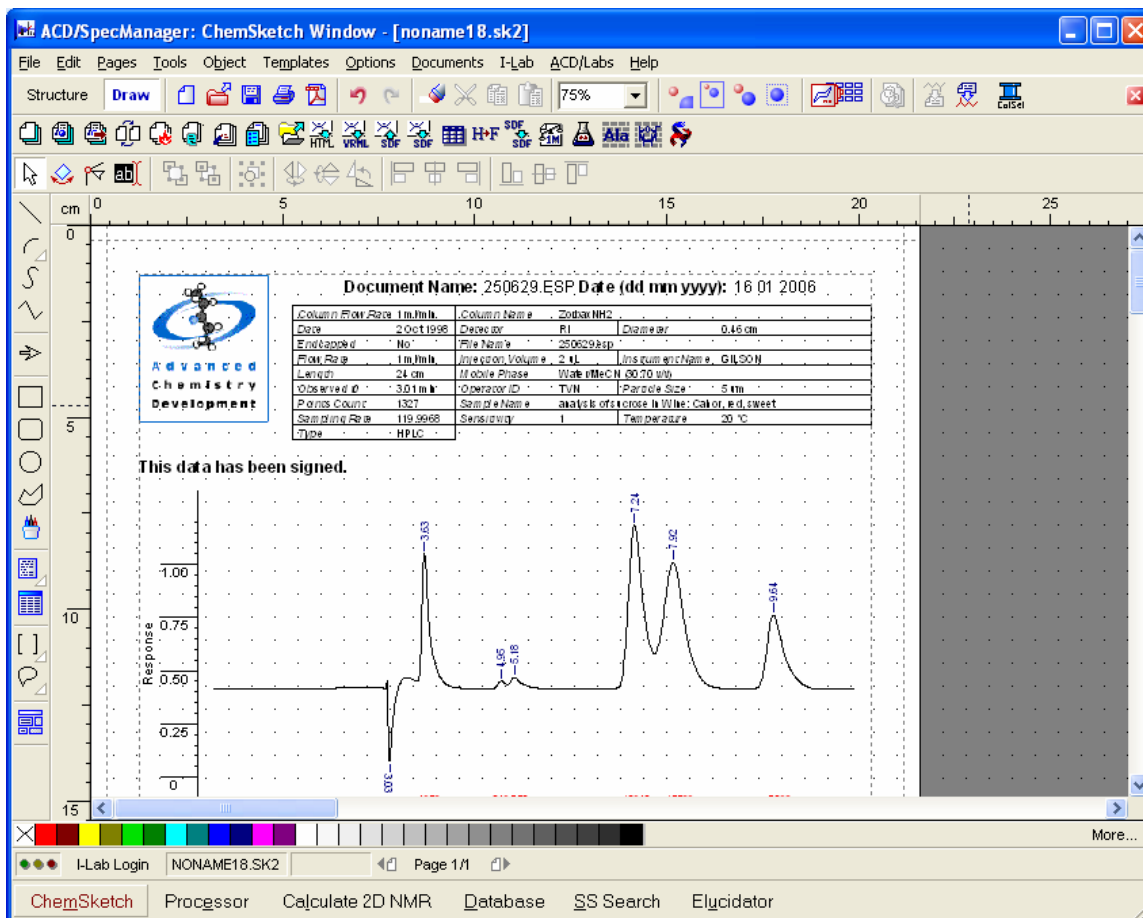


Figure 15: The report created for a signed chromatogram.

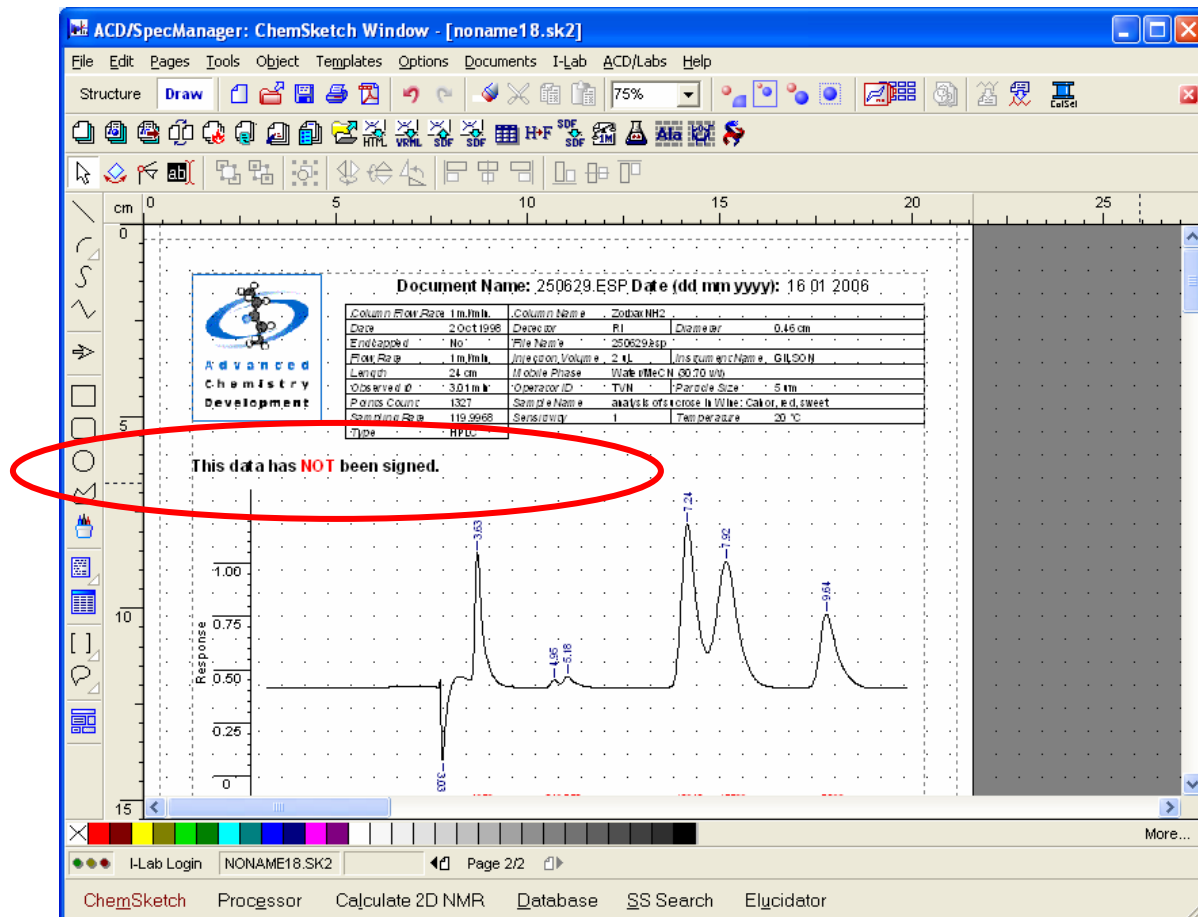


Figure 16: The report created for an unsigned chromatogram.

Conclusion

With ACD/ChromProcessor version 9, it is possible to create a macro with a conditional statement for multiple reporting. This offers faster report creations and easier data management. The macro is included in the download with the Technical Note.

References

1. ACD/SpecManager. www.acdlabs.com/specmanager/. 3 May 2006
2. ACD/ChromManager. www.acdlabs.com/chrommanager/. 3 May 2006
3. ACD/Curve Manager. www.acdlabs.com/curve/. 3 May 2006
4. ACD/MS Manager. www.acdlabs.com/msmanager/. 3 May 2006
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7. ACD/UV-IR Manager. www.acdlabs.com/uvir/. 3 May 2006