Quick Start Guide

ACD/1D NMR Processor: Basic Training

Version 12

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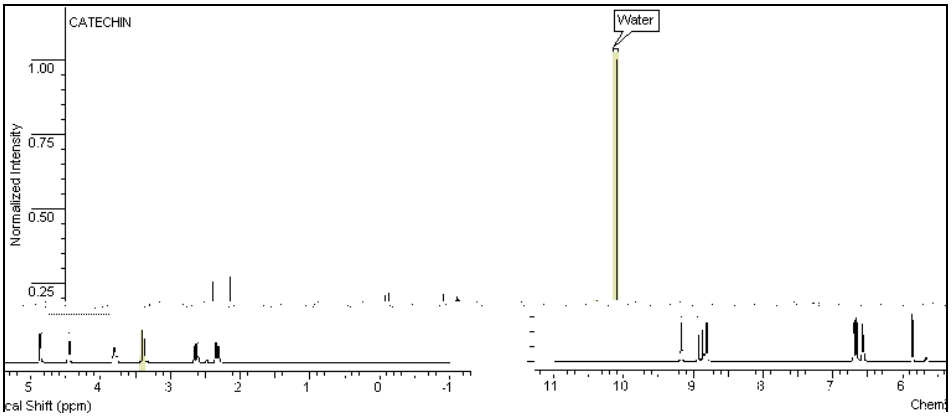
Introduction

The following document outlines how to utilize ACD/1D NMR Processor for processing, assigning, and reporting a [11]

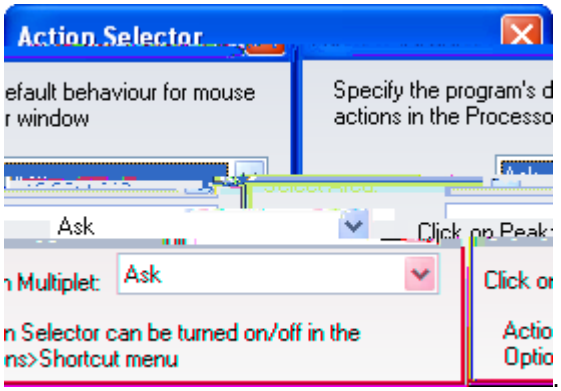
Fast Fourier Transform, Baseline, and Phase Corrections

To automatically Fourier transform, baseline correct, and phase correct

- On the Operations toolbar, click Shortcut.



Note Ensure the **Action Selector** dialog box settings are as follows:



Peak Picking, Integration, and Multiplet Creation

Attaching a Chemical Structure to a Spectrum

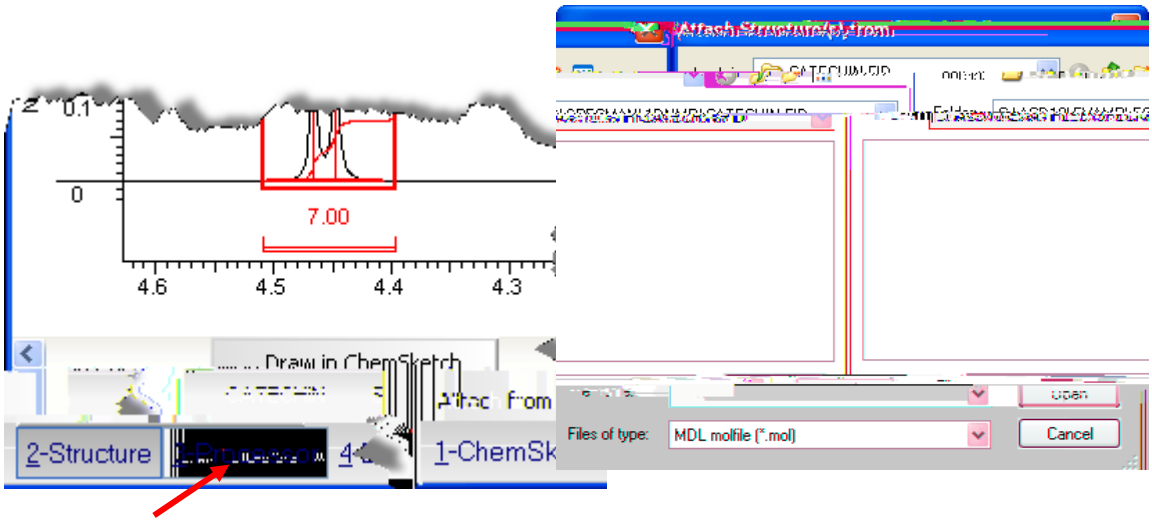
Once attached to a spectrum, the structure information is imbedded directly in the ACD/Labs spectral data format making it less likely that the identity information will be misplaced or lost.

To attach a chemical structure to a spectrum

1. On the bottom Switching bar, rest the cursor on 2-Structure to show the button menu.
2. From the button menu, choose **Draw in ChemSketch** to use the built-in structure drawing package.

   —OR—

   From the button menu, choose **Attach from File** to open the Attach Structure(s) from dialog box.



Chemical structures associated with a spectrum can be automatically included in publication quality reports. The attached chemical structure is used for facilitating spectral assignments and verification.

To clear a chemical structure from a spectrum

- On the **Edit** menu, point to **Clear**, and then click **Structure**.

Practice Task:

Attach the structure of catechin to the spectrum.

Hint! Instead of drawing the chemical structure for catechin and other well known compounds by hand, check the ACD/Dictionary first. Search for compounds by name by clicking the **Dictionary** button on the right-side vertical toolbar. Found structures can be pasted directly in the workspace.

Preparing a Report

To preview a report in the ChemSketch editor

- On the **Edit** menu of ACD/1D NMR Processor, point to **Create Report**, and click **Standard**.

From ChemSketch you can print the report as shown, save it in ChemSketch format, or produce a PDF version.

> **Note** Larger reports automatically create a multipage report. On the bottom bar, use the 
>
> controls to navigate between the pages of the report. .

To paste segments of a ChemSketch report to

Conclusion

The process described above is a very basic overview of the main workflow in ACD/1D NMR Processor. Many more processing options exist that may be valuable in your process.

More in-depth instructions are available in the *ACD/1D NMR Processor Reference Manual*. The User's Guide can be accessed in Adobe PDF format from the Processor window (Help>Documents>1D NMR>Reference Manual).

A detailed User's Guide for the ACD/ChemSketch structure editor is also available. To access the ChemSketch user guide, you must be in the ChemSketch window (Help>Documents>Guides).

Whenever prompted, you are encouraged to watch the technical movies that are included in the software. **These movies cover important material that is not included in this guide.**

1D NMR Processor Quick Start Summary Sheet

Importing Raw Data

To import spectral data

1. On the main toolbar, click 

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Preparing a Report