

# 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 <sup>11</sup>

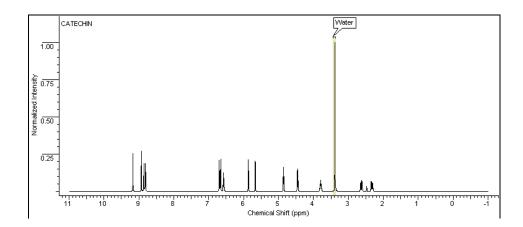


# **Fast Fourier Transform, Baseline, and Phase Corrections**

Shortcut Zero Filling FID Shift LinearPred WFunctions FourierTr. Apodization Manual Offset

#### To automatically Fourier transform, baseline correct, and phase correct

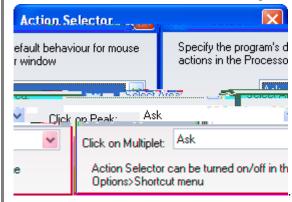
On the Operations toolbar, click Shortcut







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



Peak Picking, Integration, and Multiplet Creation



#### Attaching a Chemical Structure to a Spectrum

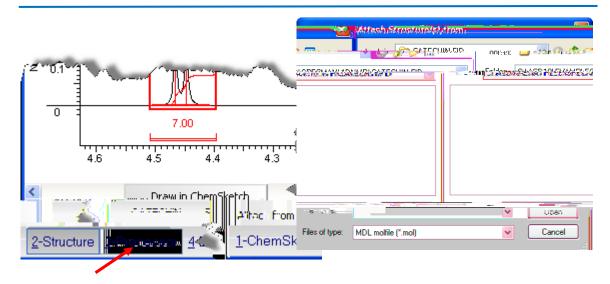
Once attached to a spectrum, the structure information is imbedded directly in the ACD/Labs spectral data format making it less likely that the identity information will be misplaced or lost.

#### 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.
- 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.

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#### 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 Microsoft® Word or other applications

- 1. Select the object (or objects) to be copied.
- 2. From the Edit menu, click Copy or use the CTRL+C shortcut.
- 3. Switch to the third-party application and use the CTRL+V shortcut.

#### To create a report in PDF format

 On the Edit menu of ACD/1D NMR Processor, point to Export to PDF, and then click Standard.

-OR-

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

Practice Task

Create a PDF report.





#### 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

On the main toolbar, click



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Preparing a Report