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 ^{1}H NMR or ^{13}C spectrum.

Approximate Time to Proficiency: ~ **12 Minutes**

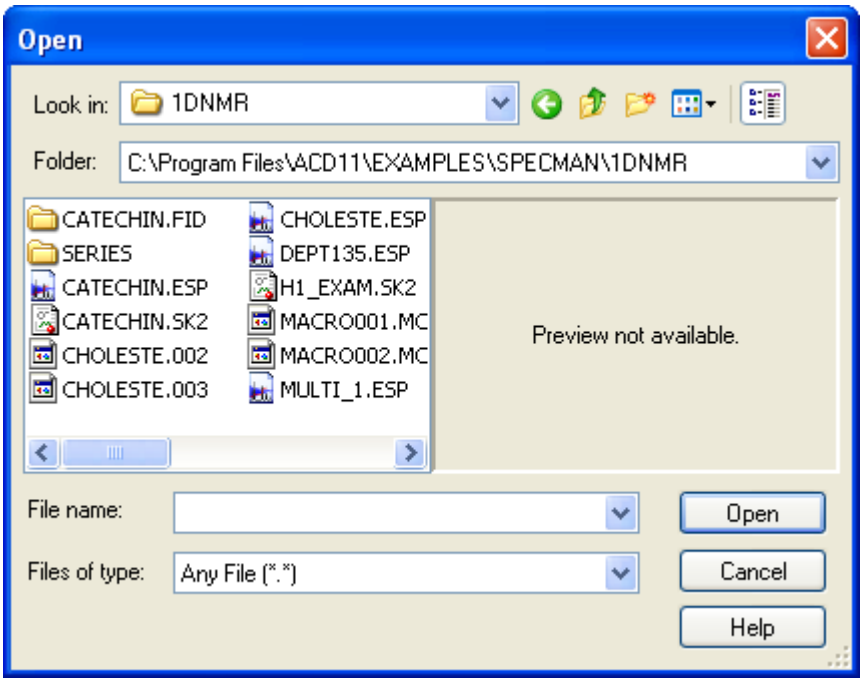
How-to Instructions

Importing Raw Data

- Start the ACD/1D NMR Processor or Manager software.

To import spectral data

1. On the main toolbar, click  to open the **Import** dialog box.
2. In the **Look In** list, locate the folder containing the instrumental data files.
3. Select the data file you wish to import, and click Open.



> **Note** If an expected data file is not shown in the folder content list, select **(Autodetect)** in the **File of Type** list. This will show all files irrespective of extension.

Practice Task:

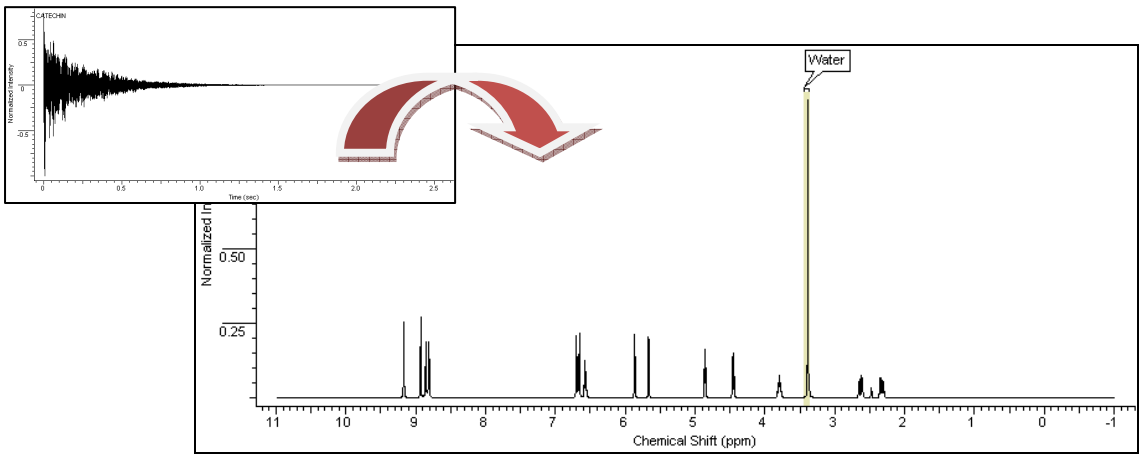
Open the catechin FID file. This file is located in the ACD/Labs example folder …\ACD11\EXAMPLES\SPECMAN\1DNMR\CATECHIN.FID\FID

It is recommended that you save this file as "*NMRPractice1*".

Fast Fourier Transform, Baseline, and Phase Corrections

To automatically Fourier transform, baseline correct, and phase correct

- On the Operations toolbar, click Shortcut.

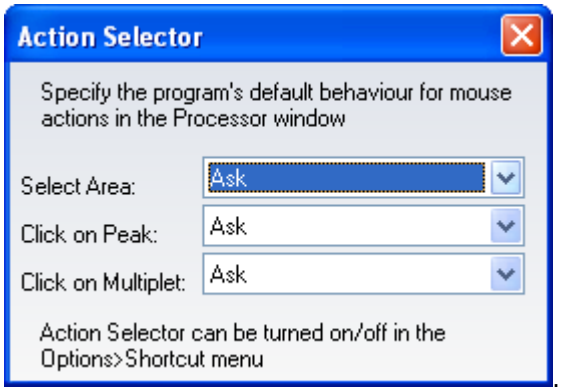


Strong extraneous signals such as water, TMS, DMSO, and Methanol in the spectrum are detected automatically, and are designated as dark regions. Dark regions are indicated by a colored rectangular area. Signals in the dark regions are generally ignored during subsequent processing and analysis.

Practice Task:

Fourier transform, baseline correct, and phase correct the catechin FID file according to the default settings.

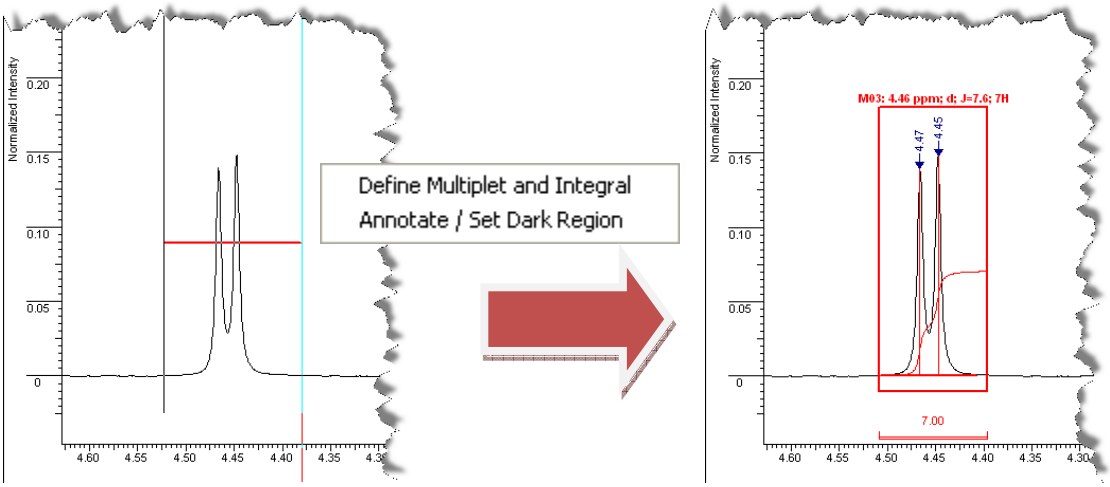
Note Ensure the **Action Selector** dialog box settings are as follows:



Peak Picking, Integration, and Multiplet Creation

To define a multiplet, peak pick, and integrate it in one step

- Drag horizontally across the spectral feature area of the multiplet, and vertically to set the selection threshold.



Note Ensure that noise and extraneous signals lie below the threshold and that real signals cross above the threshold.

Peaks detected above the horizontal line will be automatically picked, the signal integrated. Furthermore, the coupling pattern and constants for the multiplet will automatically analyzed if recognized by the software interpretation algorithms.

Practice Task:
Define multiplet regions in the catechin example.

Attaching a Chemical Structure to a Spectrum

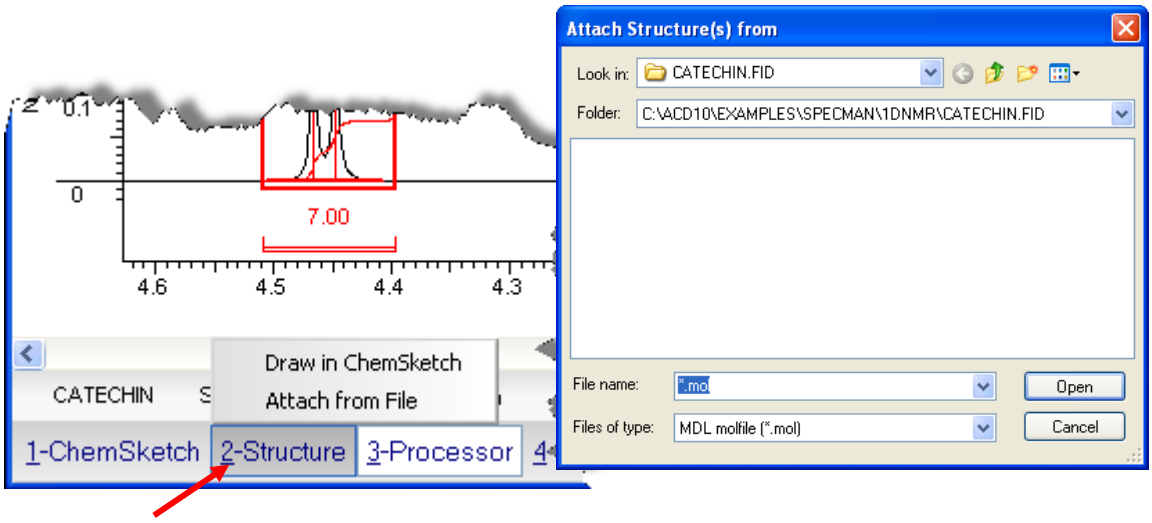
Once attached to a spectrum, the structure information is imbedded directly in the ACD/Labs spectral data format making it less likely that the identity information will be misplaced or lost.

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.

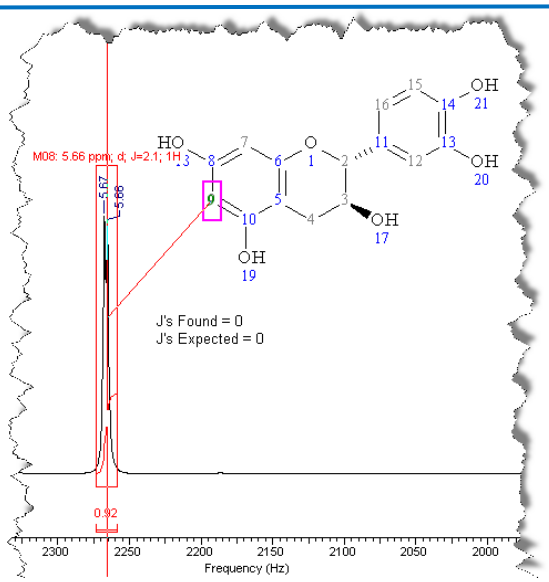
Peak Assignment

To assign peaks to corresponding proton (or carbon) in the structure

1. On the Operation toolbar, click Assignment to enter Assignment mode.
2. On the Assignment toolbar, click By Multiplet.
3. Click an atom in the structure, and then click a multiplet in the spectrum to create the assignment.

   —OR—

   Click a multiplet in the spectrum, and then click the atom to assign it.



If you select the atom first, a red line will go from the cursor to this atom. As well, a vertical bar will indicate your position on the spectrum and the nearest multiplet near this point will get highlighted. Similar functionality exists in assigning from multiplet to atom.

> **Note** To abort an assignment, click an empty background area.

Practice Task:
Assign a multiplet in the spectrum to an atom.

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

1. 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

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To clear a chemical structure from a spectrum

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

Manual Structure Assignment

To assign peaks to corresponding proton (or carbon) in the structure

1. On the Operation toolbar, click Assignment to enter Assignment mode.
2. On the Assignment toolbar, click By Multiplet.
3. Click an atom in the structure, and then click the corresponding multiplet in the spectrum.

—OR—

Click a multiplet in the spectrum, and then click the atom to assign it.

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