Quick Start Guide

ACD/2D NMR Processor: Basic Training

Version 12

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Introduction

The following document outlines how to utilize ACD/2D NMR Processor for processing, assigning, and reporting 2D NMR spectra.

Approximate Time to Proficiency: ~ **20 Minutes**

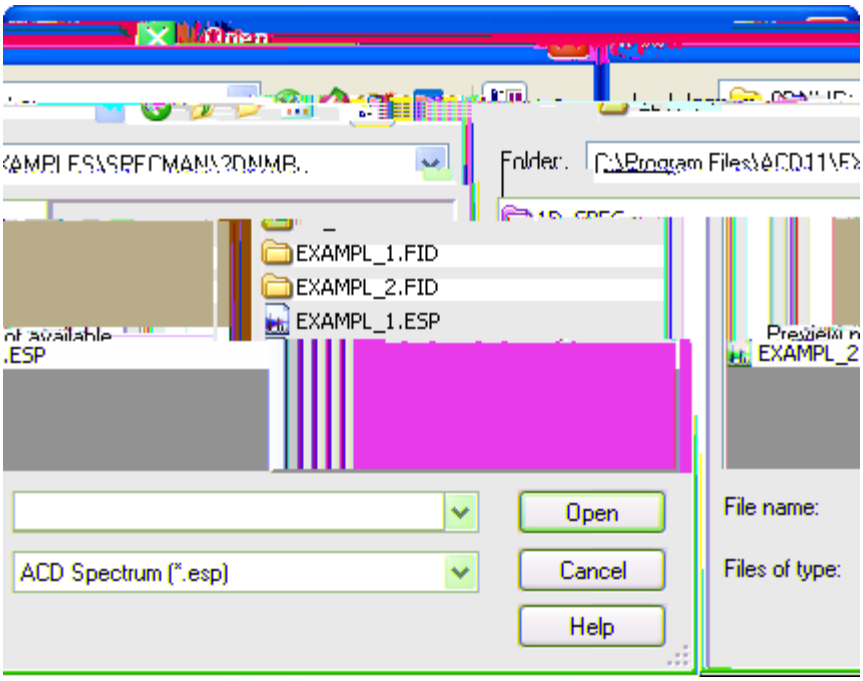
How-to Instructions

Importing Raw Data

- Start the ACD/2D 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.



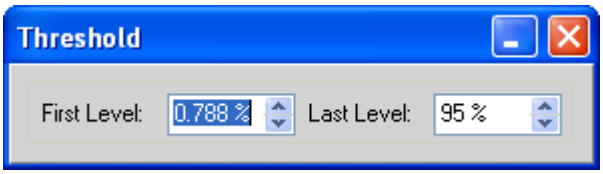
> **Note** If an expected data file is not shown in the folder content list, select **(Autodetect)** in the **File of Type** list. This will show all files irrespective of extension.

Practice Task:

Contour Display Thresholds

To adjust the threshold for the contour display

1. From the **View** menu, choose **Threshold**.
2. In the **Threshold** dialog box, choose the first level and last level values.
3. Press ENTER to apply the current threshold.

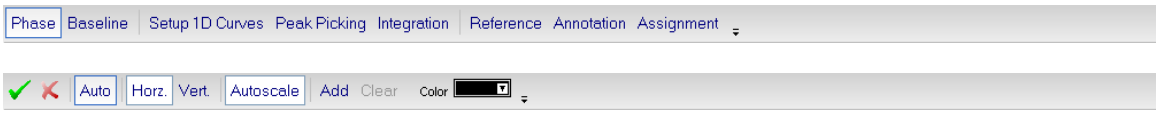


The initial minimal level threshold is set according to the noise level calculated using the auto-detect.

> **Note** An alternate way of changing this number is to press the PAGE UP and PAGE DOWN keys on your keyboard or by using the scroll wheel on the mouse.

Practice Task:
Set the first level threshold to 5%.

Phase Correction

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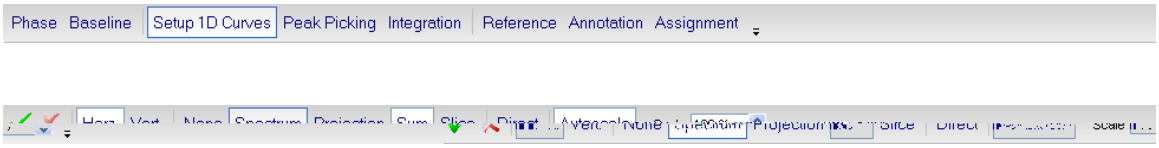
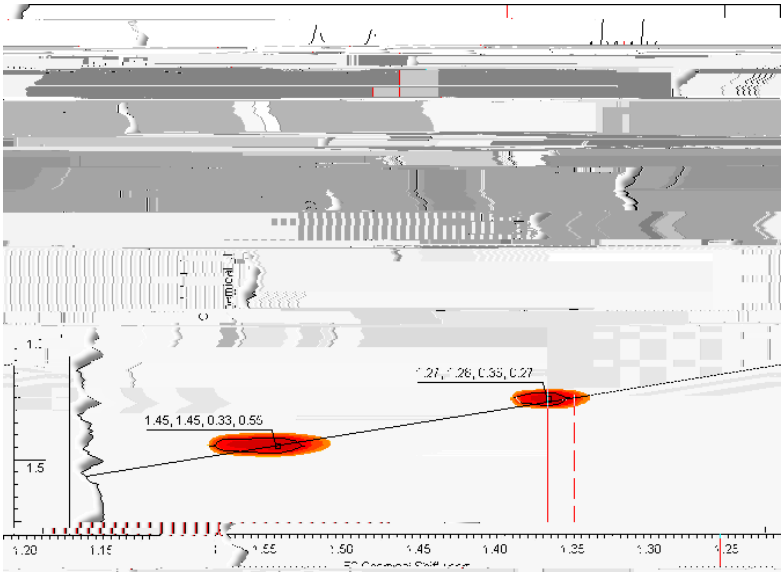
Attaching and Referencing 1D NMR Spectra to 2D NMR



To attach and reference a 1D NMR spectrum with respect to the 2D NMR data

1. From the **Tools** menu, choose **Setup 1D Curves**.
2. On the Setup 1D Curves toolbar, click Horz. or Vert. according to the desired axis orientation, and then click Spectrum to open a 1D NMR spectrum that you have saved as an .ESP file already.
3. Click on any peak in the 2D spectrum and drag left or right to align the 1D and 2D NMR. Ensure that the red line intersects the required peak on the 1D NMR.

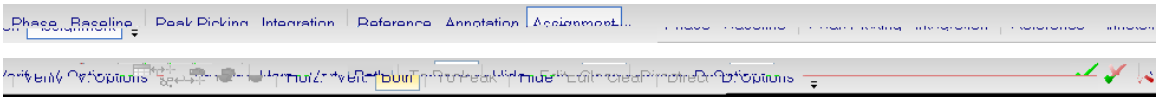


Practice Task:

Attach the ^{1}H spectrum of strychnine on the horizontal axis. This ^{1}H spectrum can be found in the ACD/Labs example folder:

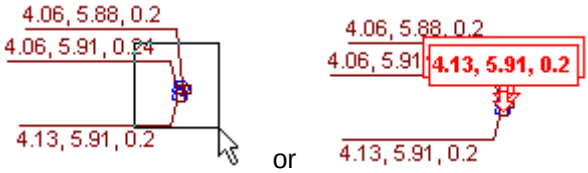
…\ACD11\EXAMPLES\SPECMAN\2DNMR\1D_SPEC\1H.ESP

Manual Structure Assignment

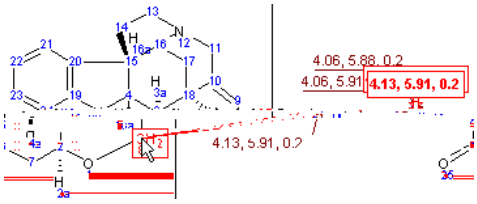


To make a structure-to-spectrum assignment

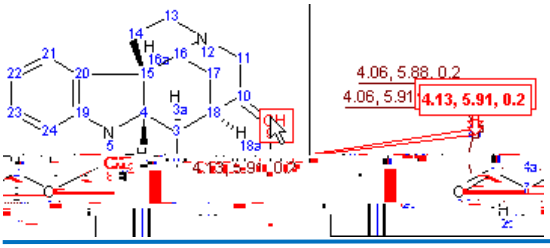
1. On the Operation toolbar, click Assignment.
2. On the spectrum, select the peak to be assigned by lassoing or clicking the peak when the red label appears.



3. On the structure, click the atom (or atom group) to make the assignment. A red line will connect the selected peak and atoms in the assignment.
4. If the program prompts you for additional assignment details, select the appropriate one.



5. Click the other atom involved in the correlation to finish the assignment.



> **Note** If a correlation is between the proton and carbon on a single atom group (in a HSQC for example), the assignment is made by clicking twice on the same group, or double-clicking.

Practice Task:

Make two practice assignments.

To show the a structure-to-spectrum assignment table

- On the General toolbar, click  to show the Table of Assignments.

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 then choose **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

Conclusion

The process described above is a very basic overview of the main workflow in ACD/2D NMR Processor. Many more processing options exist that may be valuable in your process.

More in-depth instructions are available in the *ACD/2D NMR Processor Reference Manual*. The User's Guide can be accessed in Adobe PDF format from the Processor window (Help>Documents>2D 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.**

2D NMR Processor Quick Start Summary Sheet

Importing Raw Data

To import spectral data

1. On the main toolbar, click  to

Attaching a Chemical Structure to a Spectrum

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.

To clear a chemical structure from a spectrum

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

Attaching 1D NMR Spectra and Referencing the 2D NMR data

To attach and reference a 1D NMR spectra relative to a 2D NMR spectrum

1. On the Operations toolbar, click Setup 1D Curves.
2. On the Setup 1D Curves toolbar, click Horz. or Vert. according to the desired axis orientation, and then click Spectrum to open a 1D NMR spectrum that you have saved as an .ESP file already.
3. Click on any peak in the 2D spectrum and drag left or right to align the 1D and 2D NMR. Ensure that the red line intersects the required peak on the 1D NMR.

Manual Structure Assignment

To make a structure-to-spectrum assignment

1. On the Operation toolbar, click Assignment.
2. On the spectrum, select the peak to be assigned by lassoing or clicking the peak when the red label appears.
3. On the structure, click the atom (or atom group) to make the assignment. A red line will connect the selected peak and atoms in the assignment.
4. If the program prompts you for additional assignment details, select the appropriate one.
5. Click the other atom involved in the correlation to finish the assignment.

Preparing a Report

To preview a report in the ChemSketch editor

- From the **Edit** menu of 1D NMR Processor, point to **Create Report**, and then choose **Standard**.

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, choose **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 choose **Standard**.

   —OR—

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