

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 ([page 2](#))

Fourier Transform, ([page 3](#))

Contour Display Threshold ([page 4](#))

Phase Correction ([page 4](#))

Peak Picking ([page 5](#))

Attaching Structure to Spectrum ([page 6](#))

Attaching & Referencing 1D NMR Spectra Relative to 2D NMR ([page 7](#))

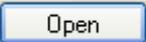
Peak to Structure Assignment ([page 8](#))

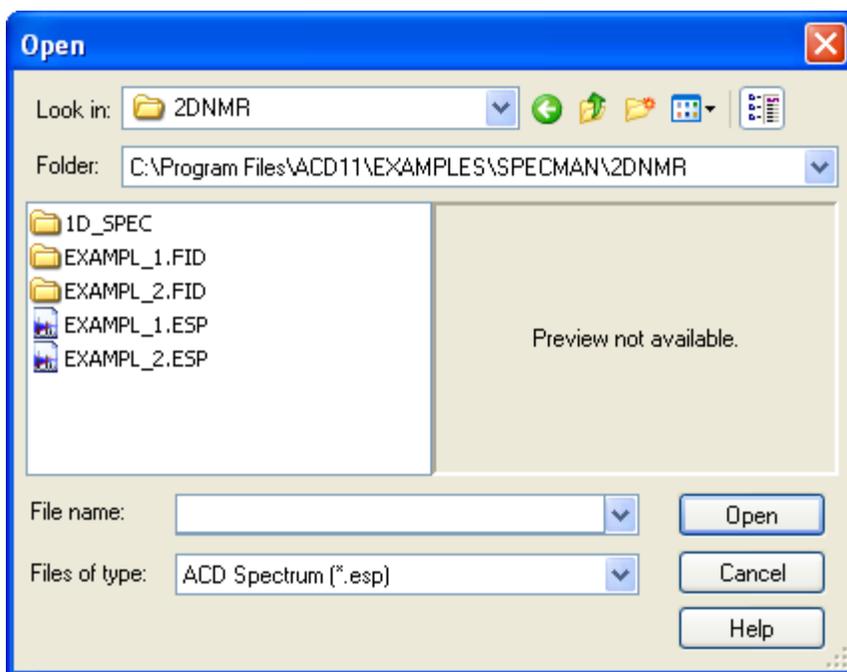
Creating Reports ([page 9](#))

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 .



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 Example_1 FID file. This file is located in the ACD/Labs example folder
 ... \ACD11\EXAMPLES\SPECMAN\2DNMR\EXAMPLE_1.FID\FID

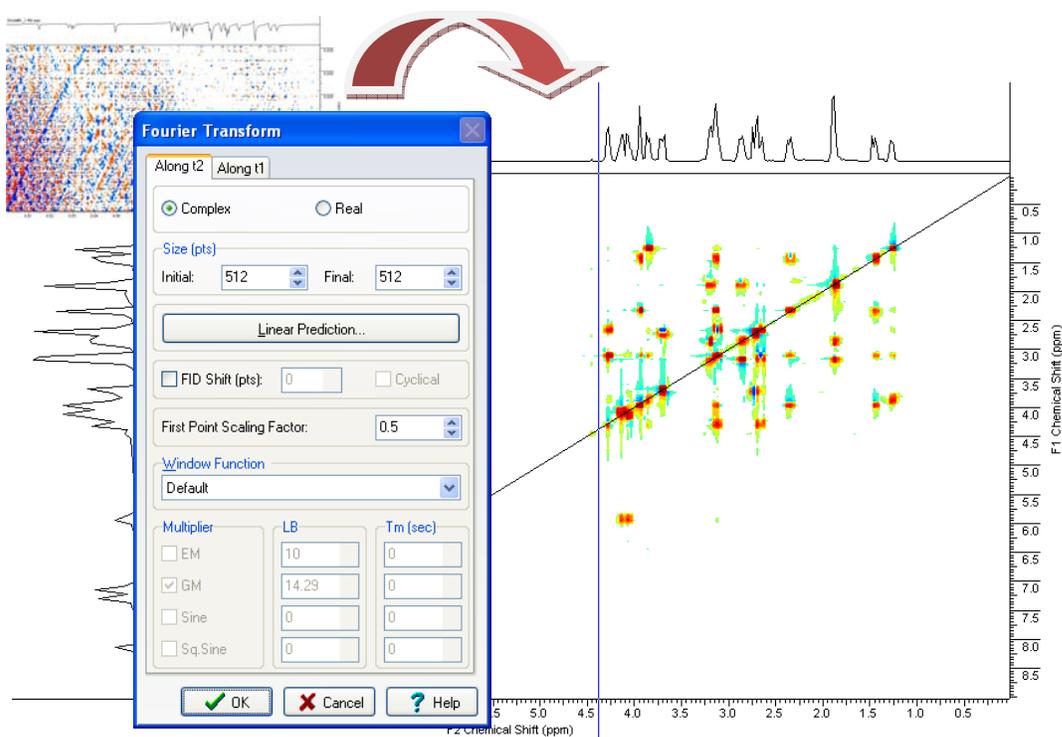
It is recommended that you save this file as "2DNMRPractice1".

Fast Fourier Transform

Interactive FT | FT along t2 | Full FT

To Fourier transform an FID file

1. On the Fourier Transform toolbar, click .
2. In the **Fourier Transform** dialog box, review and adjust settings if necessary, and click .
3. Click  to accept.



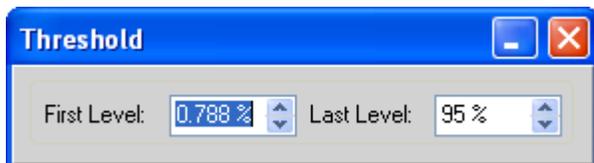
Practice Task:

Fourier transform the "2DNMRPractice1" FID according to the default settings.

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



To automatically phase correct the spectrum

1. On the Operation toolbar, click **Phase**.
2. On the Phase Correction toolbar, click **Auto**.
3. Click  to accept the current phase correction.

Practice Task:

Apply the automatic phase correction to the currently loaded spectrum.

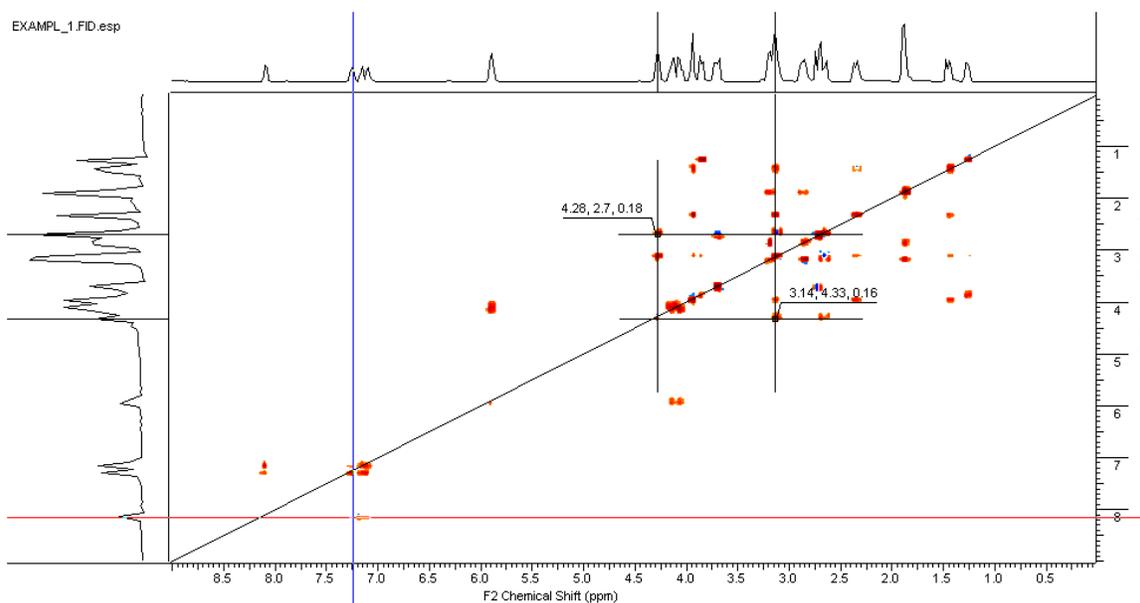
Peak Picking

Phase Baseline Setup 1D Curves **Peak Picking** Integration Reference Annotation Assignment

✓ ✗ Auto **Manual** Area Gridlines Clear Options Resolve Uncertainties

To pick peaks in a spectrum

1. On the Operations toolbar, click **Peak Picking**.
2. On the Peak Picking toolbar, click **Manual**.
3. Using the colored crosshair line and the 1D spectra as guides, click a peak contour to label it.



Manual peak picking can optionally be set to display gridlines as shown above. As a peak picking aid, you can choose to snap to existing gridlines.

Note Peak picking is a necessary tool if you wish to use the structure-to-spectrum assignment tools.

To remove a picked peak label in a spectrum

- In manual Peak Picking mode, click on a peak that has already been labeled to remove the label.

Practice Task:

Peak pick the 2D spectrum.

Attaching a Chemical Structure to a Spectrum

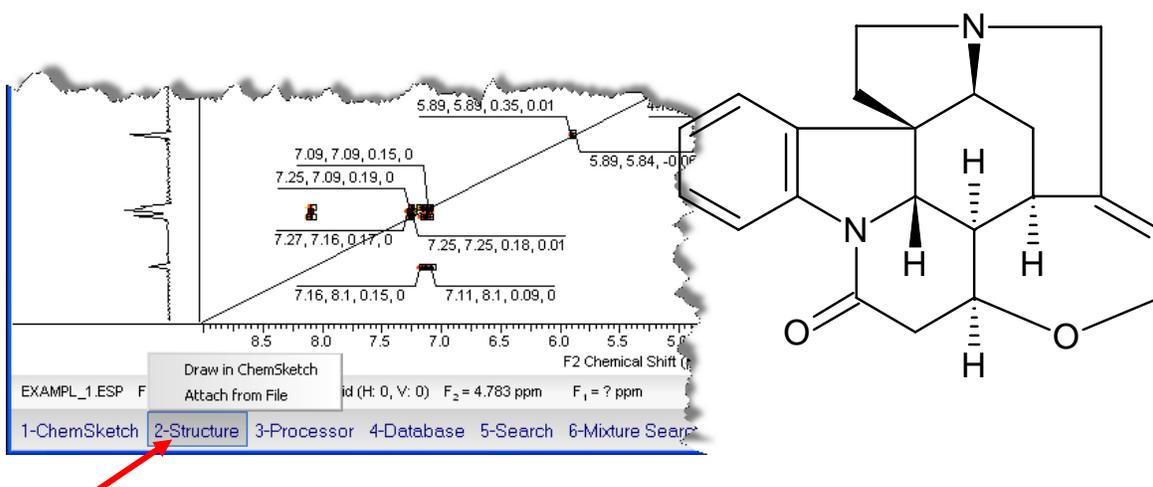
Once attached to a spectrum, the structure information is imbedded directly in the ACD/Labs spectral data format, making it less likely that the identity information will be misplaced or lost.

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. On the button menu, click **Draw in ChemSketch** to use the built-in structure drawing package.
3. Draw a structure, and on the Switching bar, click the Processor button to open the button list, and click **Attach to Structure to Spectrum**.

—OR—

On the button menu, click **Attach from File** to open an import structure 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 choose **Structure**.

Practice Task:

Attach the structure of strychnine to the spectrum.

Hint! Instead of drawing the chemical structure for strychnine and other well known compounds by hand, check 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.



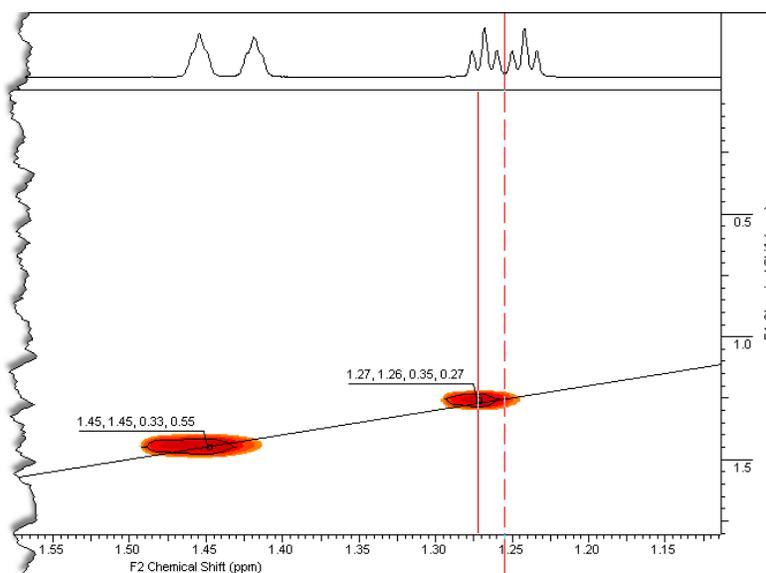
Attaching and Referencing 1D NMR Spectra to 2D NMR

Phase Baseline **Setup 1D Curves** Peak Picking Integration Reference Annotation Assignment

✓ ✗ Horz. Vert. None **Spectrum** Projection Sum Slice Direct Autoscale Scale 100%

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

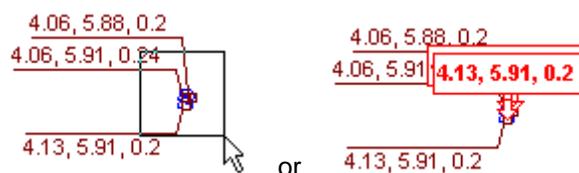
...\ACD11\EXAMPLES\SPECMAN\2DNMR\1D_SPEC\1H.ESP

Manual Structure Assignment

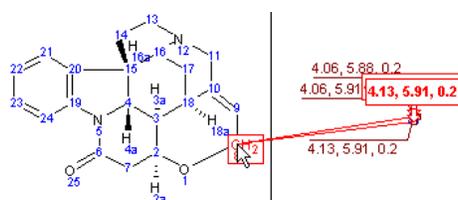


To make a structure-to-spectrum assignment

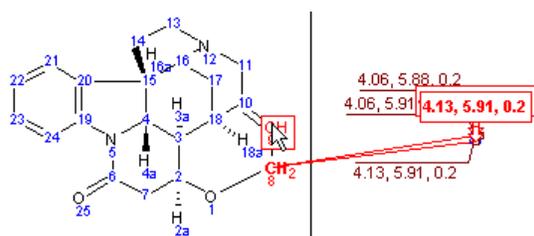
1. On the Operation toolbar, click **Assignment**.
2. On the spectrum, select the peak to be assigned by lassoing or clicking the peak when the red label appears.



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

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.
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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—
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Practice Task

Create a PDF report.

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).

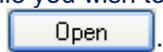
A detailed User's Guide for the ACD/ChemSketch structure editor is also available. To access the ChemSketch user guide, you must be in the ChemSketch window (Help>Documents>Guides).

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

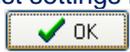
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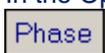
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—OR—

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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

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