Quick Start Guide

System Training for ACD/C+H NMR Predictors and DB
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Introduction
This short guide will demonstrate the steps required to add an assigned spectrum to a C+H NMR database to train NMR predictions with NMR spectra of in-house compounds.

Create a Database
1. From the main ACD/C+H NMR Predictors window, click on (Database) in the navigation toolbar at the bottom.
2. Select (User) in the left corner, then go to the Database menu and select New...
3. Input an appropriate filename and select the type: ACD/C+H NMR Predictors Database (*.NMRUDB).
4. Click (Save). The new DB will be open and in update mode ( ).

Add Assigned Spectrum
1. From the ACD/Labs menu in the top toolbar select Spectrus.
2. Load a processed spectrum or open a spectrum and structure and perform the necessary analysis and assignment.

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Tip: The Assignment: Auto tool ( ) can be used to peak pick, integrate, and assign signals to a structure in one step.

3. Go to the Database menu and select Update C+H NMR Database.

4. A window entitled Not Assigned Peaks will appear. This is a list of peaks in the spectrum that were not assigned to the structure included. Updating the database with peaks from impurities and solvents is not recommended; click OK to ignore this window.
5. A new database entry is displayed along with an indication that it will be included in future calculations.

Calculate a Spectrum from ChemSketch

1. Navigate to ChemSketch using the icon navigation toolbar (1-ChemSketch).
2. Input a structure then select (3-Calc HNMR).
3. In the ACD/C+H NMR... window, right click on any atom in the structure to observe the calculation protocol. You will see that the table indicates the values were determined based on a User database.

Note: You can hover your cursor over the source cell to see which specific database the values came from.
Calculate a Spectrum from Spectrus Processor

The first time you choose to include the user C+H NMR databases in calculations, you will need to begin by performing a default spectrum prediction in order to access the necessary options.

1. Click ( ) to open the chemical structure window and input a structure.
2. Locate the ( ) icon (you may need to view more buttons using the double arrows) and choose which spectrum you would like to calculate. Since the above example created a proton NMR database, we will choose HNMR.
3. Go to Options > Spectra Calculation Parameters...
4. Under Shift Calculation Method click ( ) and select Corrected Weighted Average Experimental. Click OK.
5. Place a check mark next to Use Training Database(s) and click ( ) to select the appropriate database(s). Click OK.

6. Click OK to close the Calculation Options window.
The next time you generate a predicted spectrum, the user database will be employed in the calculation protocol. To view the protocol, right click on any atom in the structure and select **Show 1H (HOSE) Calculation Protocol**...

**Note:** To automatically share NMR training Database(s) across your organization, please use Synchronization Server. Please contact ACD/Labs technical support for details.

**Conclusion**

This guide is intended as a brief overview of training in NMR Predictors. You can learn more about these tools by choosing [Help] when applicable or by going to the **Help** menu within ACD/C+H NMR Predictors and DB.

Please also visit [www.acdlabs.com](http://www.acdlabs.com) for more details. If your software is on a computer connected to the internet, our technical support team can be easily contacted by selecting **Send Bug Report/Feature Request**... under the ACD/Labs menu, filling out the appropriate information and sending via Web or Mail.