# KnowItAll® Informatics Training

## NMR Predictions



WILEY

# Predict NMR

## How to Predict NMR Spectra

### Purpose

This exercise demonstrates how to use the KnowItAll Informatics System's PredictIt NMR application to generate a predicted NMR spectrum from a chemical structure.

### Objectives

These exercises will teach you:

- How to set database and solvent preferences
- How to open a structure in PredictIt NMR
- How to perform a prediction
- How to interpret the predicted results

### Background

The PredictIt NMR application allows the prediction of $^{1}H$, $^{13}C$, and other NMR shifts for a structure by searching the database(s) for specific chemical environments. These are described by a Hierarchical Organization of Spherical Environments (HOSE) code that is used to characterize the chemical surroundings of an atom in a molecular structure.

Because the PredictIt NMR application allows you to choose from a list of common solvents. Predictions can be solvent-specific, if desired.

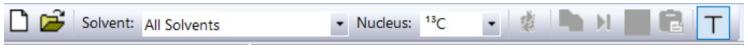
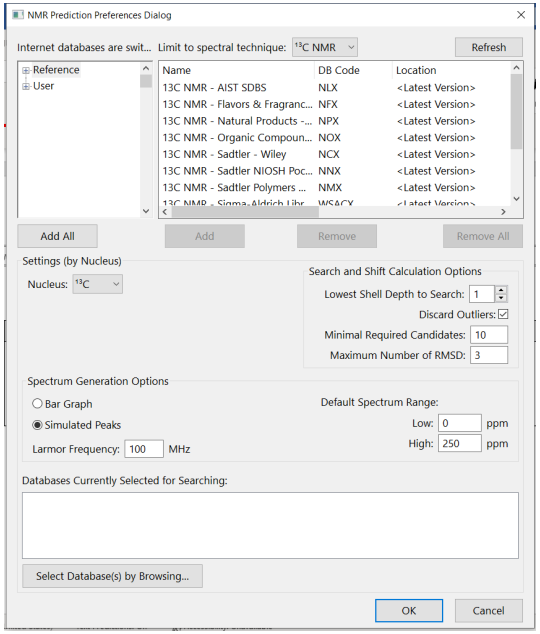
***Training Files Used in This Lesson***

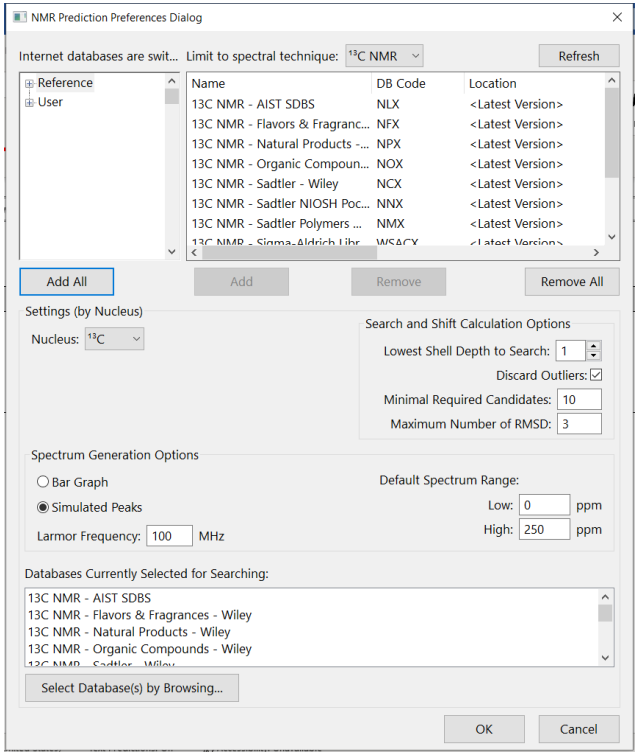
- C:\Users\Public\Public Documents\Wiley\KnowItAll\ Samples\Structures\p-Methoxycarbanilic acid, 2-ethoxyethyl ester.dsf

***KnowItAll Applications Used***

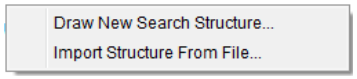
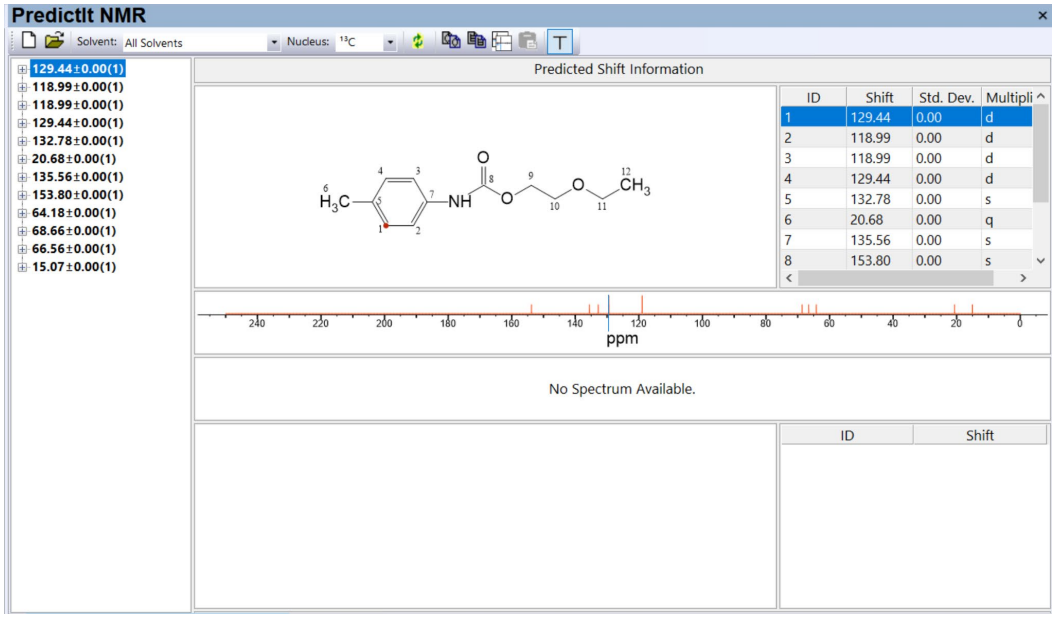
- PredictIt™ NMR
- ChemWindow®
- MineIt™

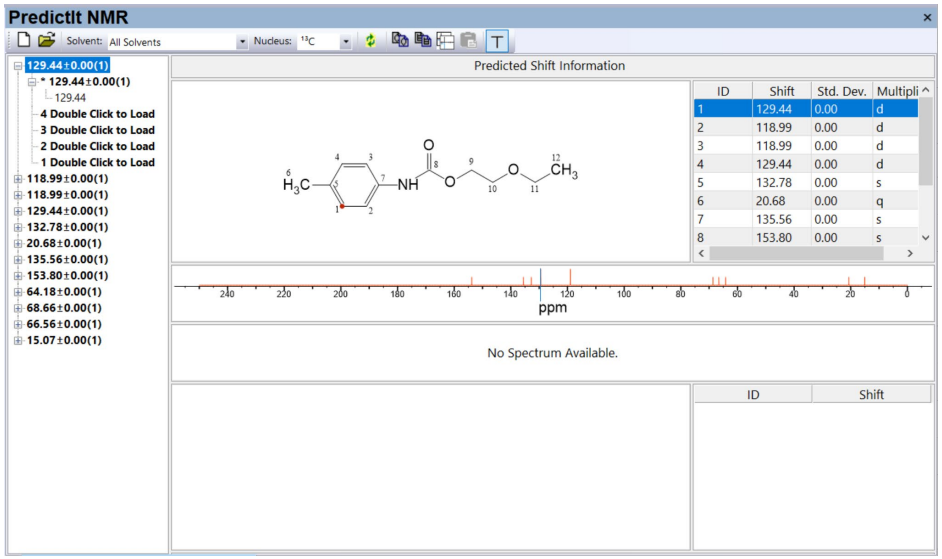
# Set PredictIt NMR preferences

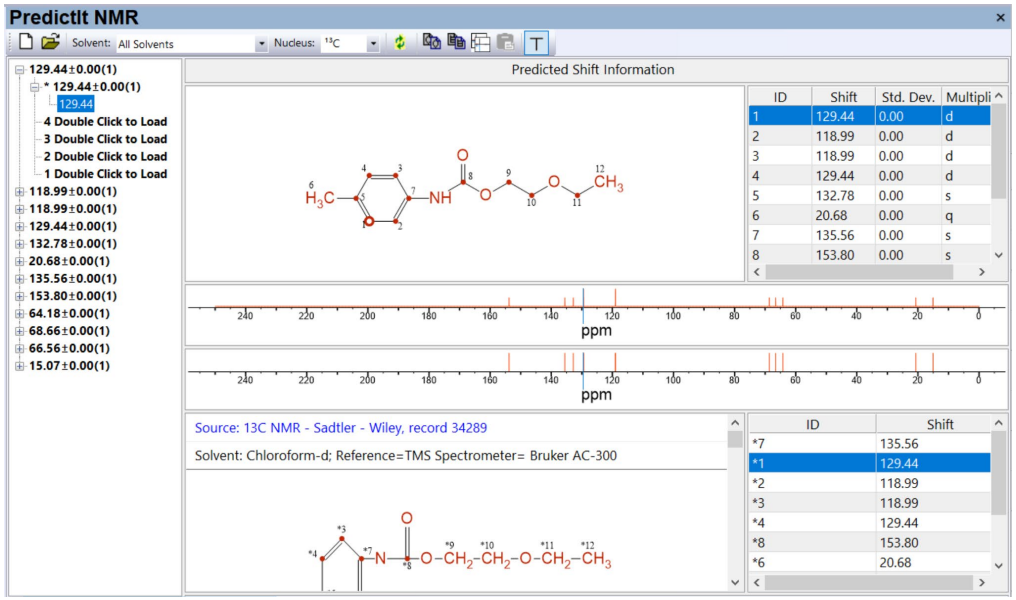
| | Action | Result |
|---|---|---|
| 1 | Open the **PredictIt NMR** application by clicking its icon, typically found in the **Spectral Analysis** group. |  |
| 2 | Examine the entries in the **Solvent** and **Nucleus** drop-down lists on the **Standard Toolbar**. Change the Nucleus type to $^{13}C$. | The **Nucleus** type displays $^{13}C$:<br>  <br>The **PredictIt NMR** application performs predictions for the solvent and nucleus specified using the toolbar. |
| 3 | Choose **File > Preferences**. | The **PredictIt NMR Preferences Dialog** box opens:<br>  |

| | Action | Result |
|---|---|---|
| 4 | In the **NMR Prediction Preferences Dialog**, set the **Settings (by Nucleus)** to $^{13}C$. Under **Limit to spectral technique**, choose $^{13}C$. Click the **Add All** button followed by **OK**. | The selected databases will be used when a prediction is performed. Upon clicking **OK**, the dialog closes.<br>  <br><br>**Note:** Specific availability of databases will depend on your package. DEMOX may be the only database available. |

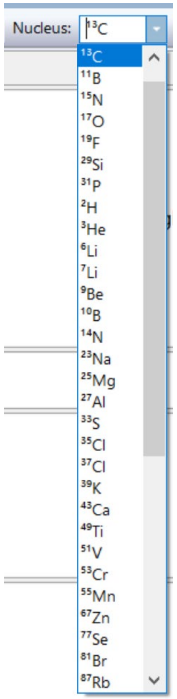
## Load a structure and perform a prediction

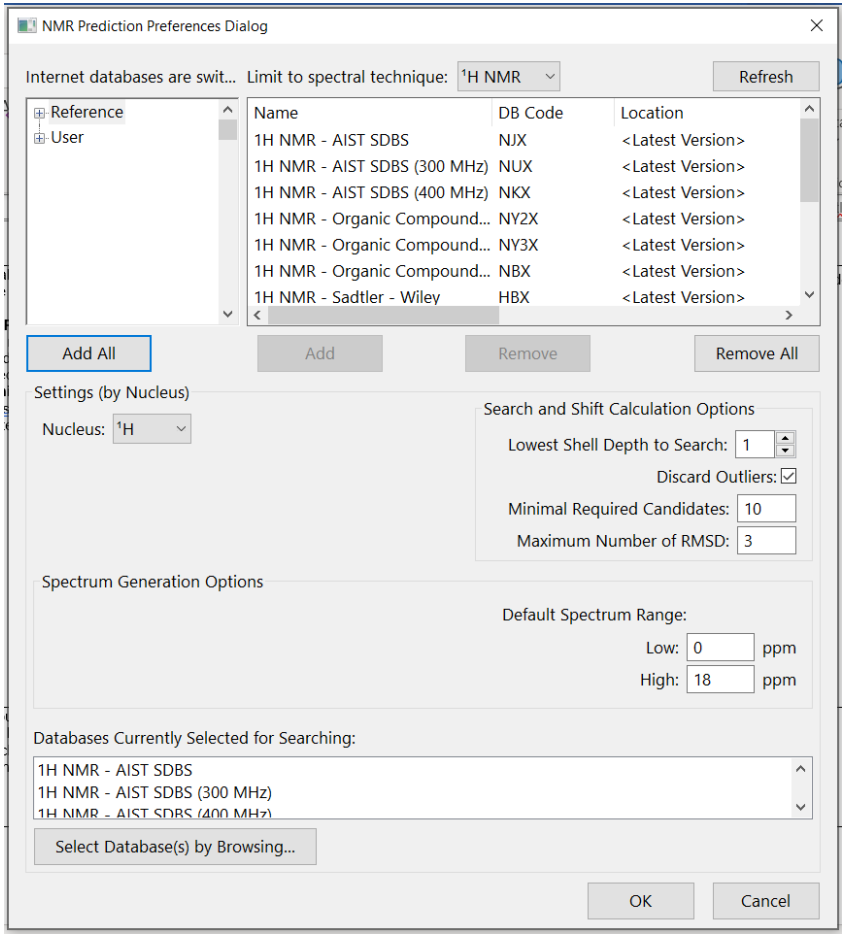
| | Action | Result |
|---|---|---|
| 5 | Right-click in the box that reads **Right click to add structure.** | A pop-up menu opens:<br>  |
| 6 | Select **Import Structure From File**. | A standard Windows **Open** dialog box appears. |
| 7 | Navigate to C:\Users\Public\Public Documents\Wiley\KnowItAll\ Samples\Structures. Select “p-Methoxycarbanilic acid, 2-ethoxyethyl ester.dsf”. Click **Open**. | After calculating, the results are displayed in the main **PredictIt NMR** window:<br>  <br>The structure is displayed with a red tag on the selected atom. The corresponding row is highlighted in the **Peak Table**. The chemical shifts are displayed in the **Shift Table**. |

| | Action | Result |
|---|---|---|
| 8 | Click on the plus sign in the **Peak Table** tree to expand it. Click on the plus sign in the branch one level lower to expand it. | Upon clicking the first plus box, a series of rows is expanded below in a tree. Upon clicking on the second plus box, a row is displayed that reveals the records which contributed to the specific calculation.<br>  <br><br>KnowItAll averages the database records which match the atom environment to the 4th shell, 3rd shell, *etc*. |

| | Action | Result |
|---|---|---|
| 9 | Click on the row that reads 129.44 to display the record.<br><br>**Note:** Clicking on the record ID (shown in blue text as "Source: 13C NMR") will open the selected record in **MineIt** application. | Upon selecting a record in the **Peak Table** tree, a record which was involved in the calculation of the chemical shift is displayed.<br>  <br>The tree control gives you access to the structures, spectra, and chemical shifts from the databases upon which the predictions are based to give you confidence in the accuracy of the prediction. |
| 10 | The prediction can be filtered according to a specific solvent by using the **Solvent** dropdown menu. | Upon filtering the solvent, the calculation will be repeated using data only for the selected solvent. |

## Perform a prediction for other nuclei

| | Action | Result |
|---|---|---|
| 1 | The above example is for $^{13}C$ NMR predictions. To predict for another nuclei, change the selection in the **Nucleus** drop down menu. |   |

| | | |
|---|---|---|
| 2 | **Note:** The databases must be updated for the selected technique.<br><br>Choose **File > Preferences**. Click **Remove All** to remove existing databases used for the prediction. Modify the selection for **Limit spectral technique to** to the desired nucleus, and click **Add All** to add the related databases. | The **NMR Prediction Preferences Dialog** opens. In the example below, the $^{1}$H NMR databases were added:<br>  |

| | | |
|---|---|---|
| 3 | With the previous prediction opened, select **Edit > Repeat Prediction** or click the **Repeat Prediction** icon on the **Standard Toolbar**.  | The prediction is recalculated for the selected nucleus. |