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.

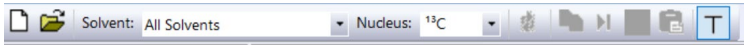
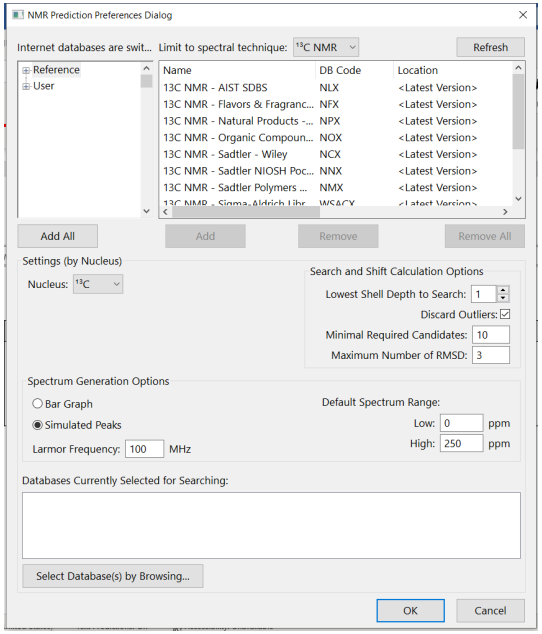
Training Files Used in This Lesson

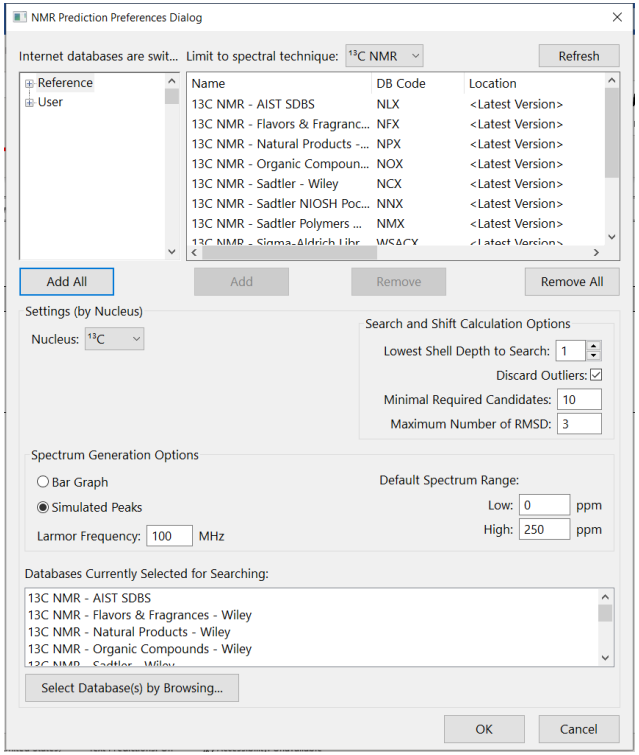
- C:\Users\Public\Public Documents\Wiley\KnowItAll\ Samples\Structures\p-Methoxycarbanilic acid, 2-ethoxyethyl ester.dsf

KnowItAll Applications Used

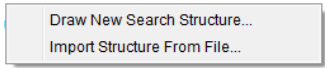
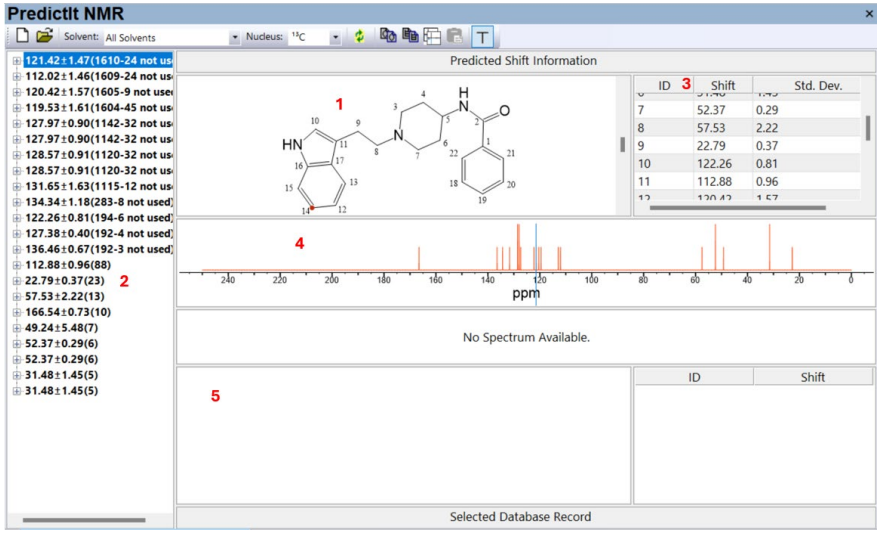
- PredictIt NMR
- ChemWindow
- MineIt

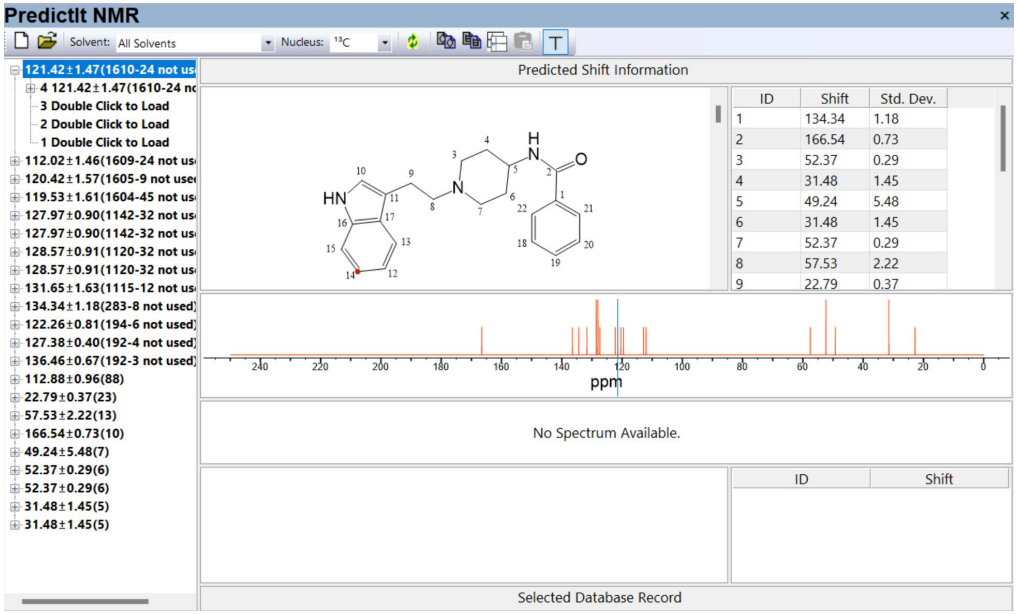
Set PredictIt NMR preferences

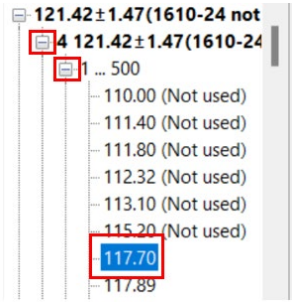
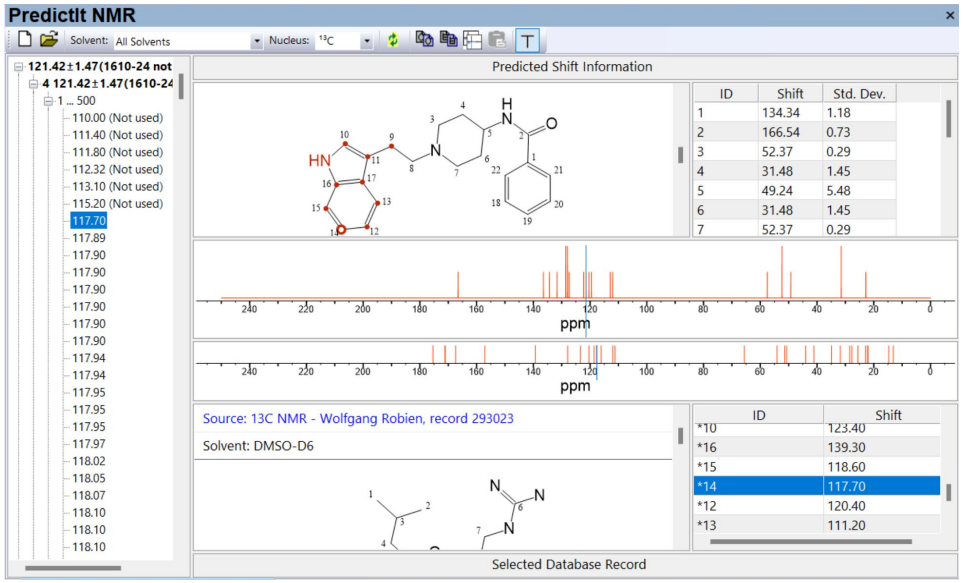
	Action	Result
1	Open the **PredictIt NMR** application by clicking its icon, typically found in the **Spectral Analysis** group.	
2	Examine the entries in the **Solvent** and **Nucleus** drop-down lists on the **Standard Toolbar**. Change the mention option to **^{13}C**.	The **Nucleus** displays **^{13}C**:  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: 

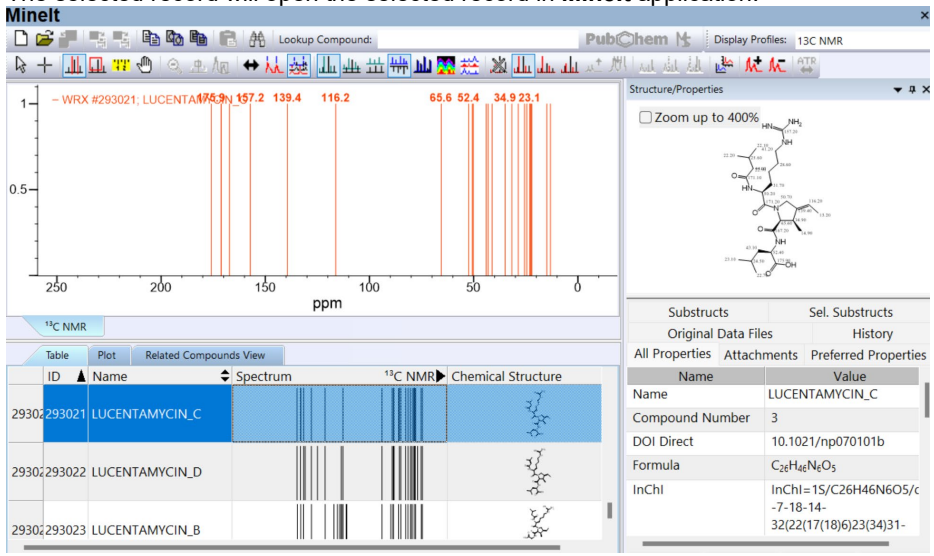
	Action	Result
4	In the **NMR Prediction Preferences Dialog**, set the **Settings (by Nucleus)** to **^{13}C**. Under **Limit to spectral technique**, choose **^{13}C NMR**. Click the **Add All** button followed by **OK**.	The selected databases will be used when a prediction is performed. Upon clicking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

Load a structure and perform a prediction

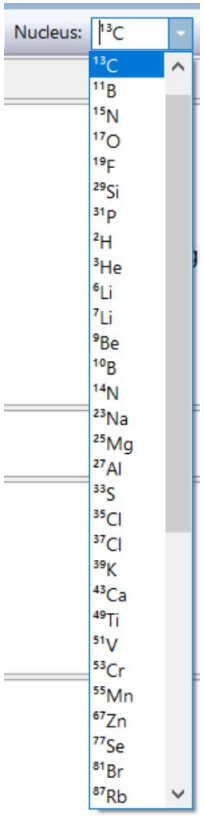
	Action	Result
5	Right-click in the box that reads **Right click to add structure.**	A pop-up menu opens: 
6	Select **Import Structure From File**.	A standard Windows **Open** dialog box appears.
7	Navigate to **C:\Users\Public\Public Documents\Wiley\KnowItAll\ Samples\Structures**. Select "**N-[1-(2-Indol-3-ylethyl)(4-piperidyl)]benzamide.mol**". Click **Open**.	After calculating, the results are displayed in **PredictIt NMR**:  • **1**: The structure is displayed with a red tag on the selected atom. Click to select another atom. • **2**: The corresponding row is highlighted in the **Tree Control**. • **3**: The computed chemical shifts are displayed in the **Shift Table**. • **4**: A line spectrum is generated for the computed spectrum. • **5**: When a lower level row is selected in the **Tree Control**, a database record that participated in the computation for the selected atom will display in this region. More on this below.

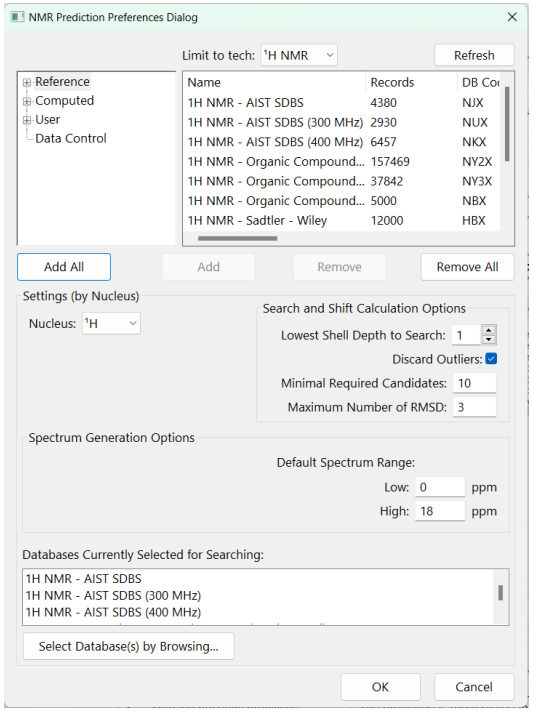
	Action	Result
8	Click on the plus icon ( ) in the **Tree Control** to expand it.	Upon clicking the first plus box, a series of rows is expanded below in the **Tree Control**:  To compute a prediction, the program searches the database(s) for specific chemical environments, which are described by **HOSE (Hierarchically Ordered Spherical description of Environment)** code - a topology code used to describe the chemical surroundings of an atom in a molecular structure. See “W. Bremser, “HOSE - A Novel Substructure Code," *Anal. Chim. Acta* (1978), 103:355-365”.

	Action	Result
9	For the first row in the **Tree Control**, click on the plus icons ( ) for the lower two levels to display records which participated in the calculation. Click on one of the bottom rows, such as “117.70”.  **Note:** Specific row values will depend on the selected databases that participated in the computation.	Upon selecting a record in the **Tree Control**, a record that was involved in the calculation of the chemical shift is displayed:  • Each row in the **Tree Control** represents a record that participated in the computation for the highlighted atom. • The **Tree Control** gives you access to the structures, spectra, and chemical shifts from the database records upon which the predictions are based to give you confidence in the accuracy of the prediction. • At the top level of the predicted values in the **Tree Control**, a coefficient of value **4**, **3**, **2** or **1** is provided, which represents the number of shells shared between the computed structure and the database record. **KnowItAll** averages the database records which match the atom environment to the 4th shell, 3rd shell, *etc.* • If an exact match(es) are found in the databases for the computed structure, then these NMR shifts will be listed first before shells from similar structures. • When a record row reads “Not used”, it represents a database value that is determined to be an **Outlier**. This feature is controlled in the **Preferences** dialog (**File > Preferences**).

	Action	Result
10	For any record, click on the **record ID** shown in blue text as "Source: 13C NMR.  Return to **PredictIt NMR**.	The selected record will open the selected record in **MineIt** application:  This allows for further investigation of the NMR database record which participated in the computation.
11	Filter the prediction 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
12	The above example is for ^{13}C NMR predictions. To predict for another nuclei, change the selection in the **Nucleus** drop down menu.	

	Action	Result
13	**Note:** The databases must be updated for the selected technique. Choose **File > Preferences**. Click **Remove All** to remove existing databases used for the prediction. Modify the selection for **Limit spectral technique 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: 
14	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.