

KnowItAll® Informatics Training

NMR Analysis Tools

NMR

Analyze NMR Multiplets and Store in a Database

Purpose

This exercise demonstrates how to label multiplets and coupling constants for NMR spectra, and how to assign the assessed multiplets when the structure associated with the spectrum is known. The NMR Tools in ProcessIt can be applied to ^1H -NMR, ^{13}C -NMR and X-NMR.

Objectives

This exercise will teach you:

- How to define multiplets for a processed NMR spectrum in Minelt
- How to edit multiplet assignments using the NMR Tools available in Minelt
- How to automatically generate an NMR Report

Background

Storing processed NMR spectra in a database is valuable for R&D, quality control, and quality assurance laboratories, and for verification of unknown chemical compounds. Adding assignments enhances the merit of the archived reference material.

Training Files Used in This Lesson



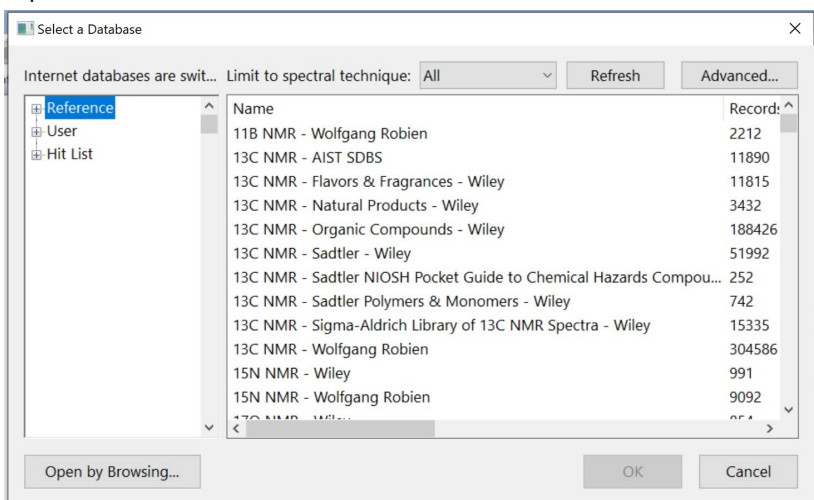
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- C14H10CINO3 H1.dsf
- C14H10CINO3 H1.sdbx

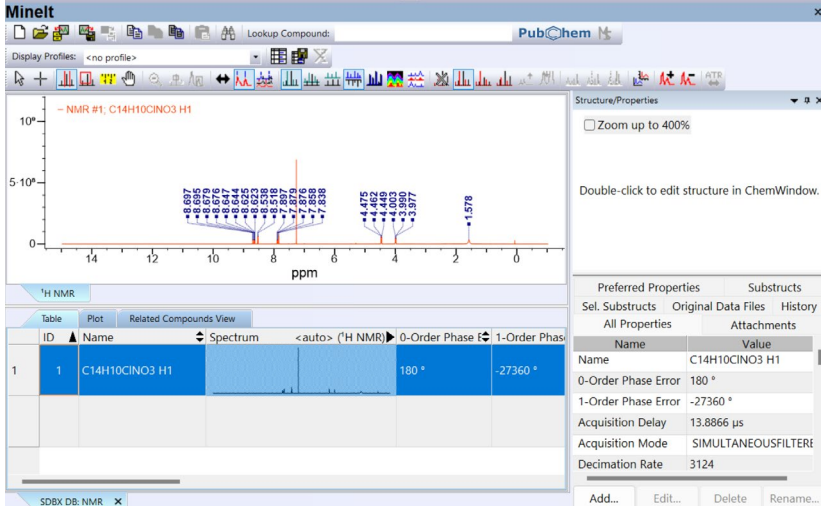
KnowItAll Applications Used

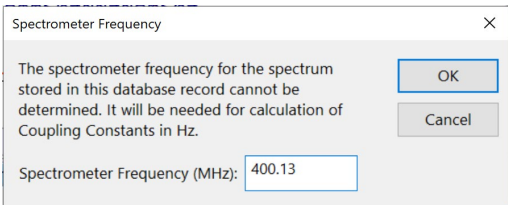
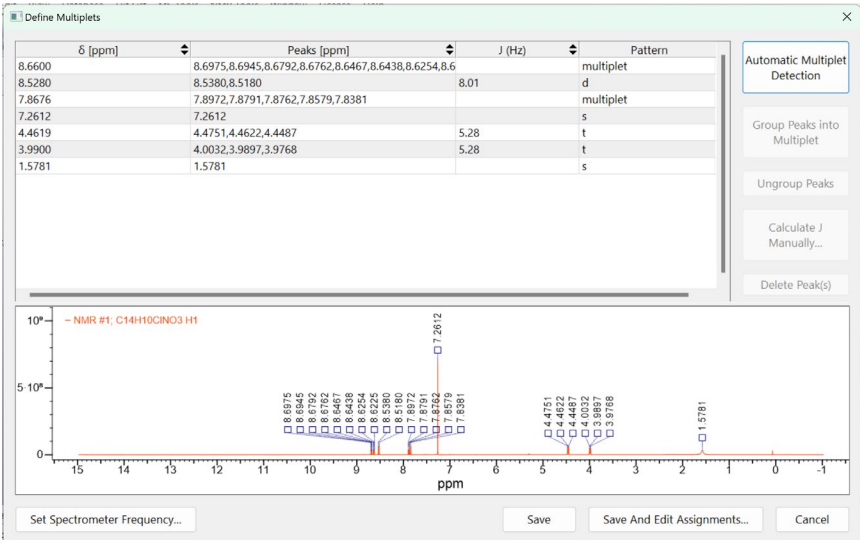
- Minelt
- ProcessIt

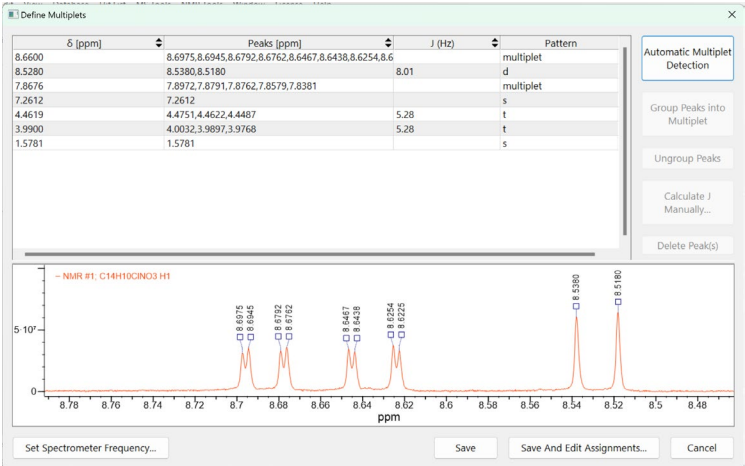
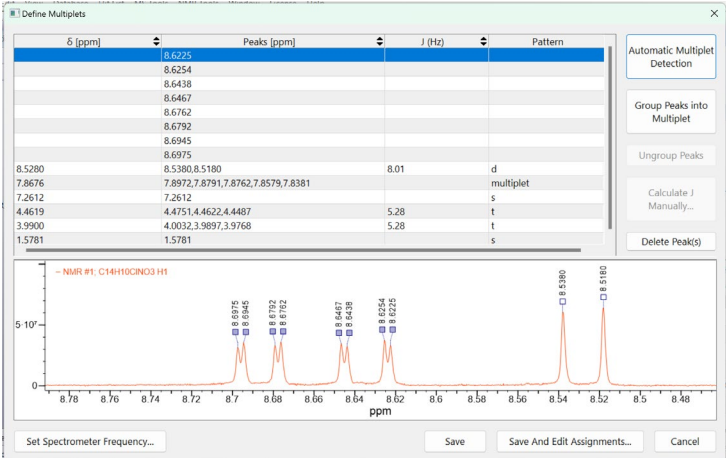
Calculate Spectrum Multiplets using NMR Tools

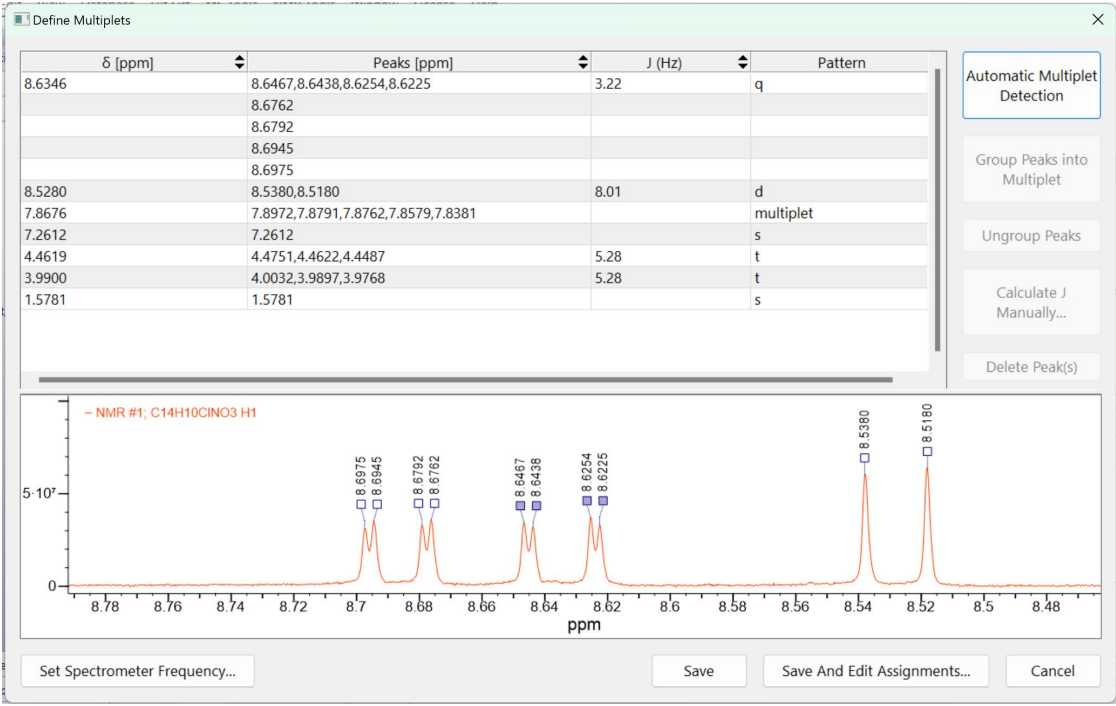
The Define Multiplets dialog in Minelt NMR Tools is used to calculate J-values and transition peak lists into defined multiplets with splitting patterns. The tool is available for ^1H , ^{13}C and X-NMR spectra.

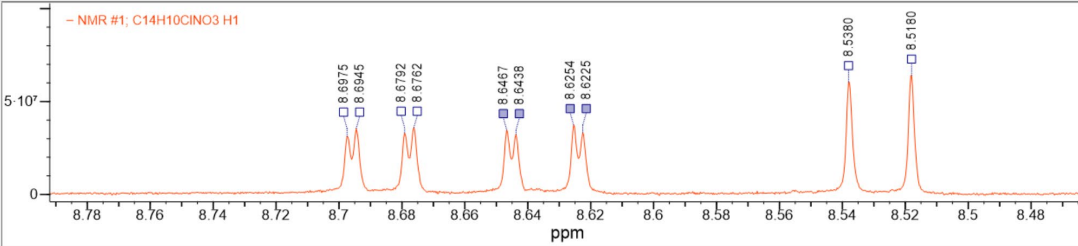
	Action	Result
1	Note: For this section, you will need a fully processed NMR spectrum. This training will apply the processed file from Chapter 13 stored in a Minelt user database.	
2	Open the Minelt application by clicking its icon, typically found in the Data toolbox. 	
3	Click the Open Database icon () and then click Open by Browsing on the Select a Database dialog.	Clicking the Open Database launches the Select a Database dialog. Clicking Open by Browsing launches a file explorer to select a file: 

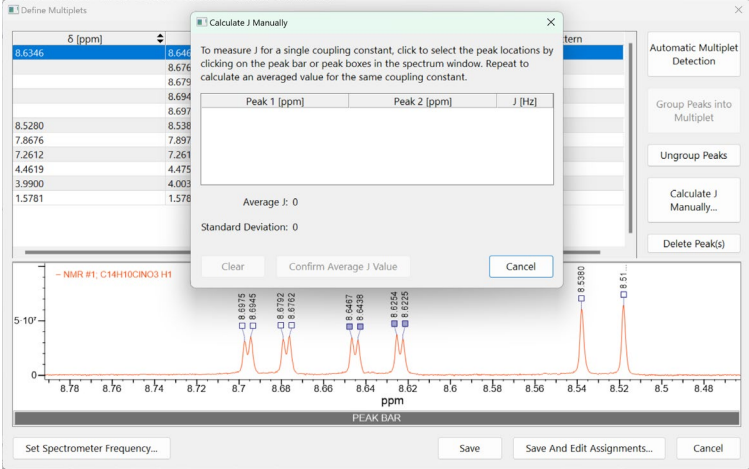
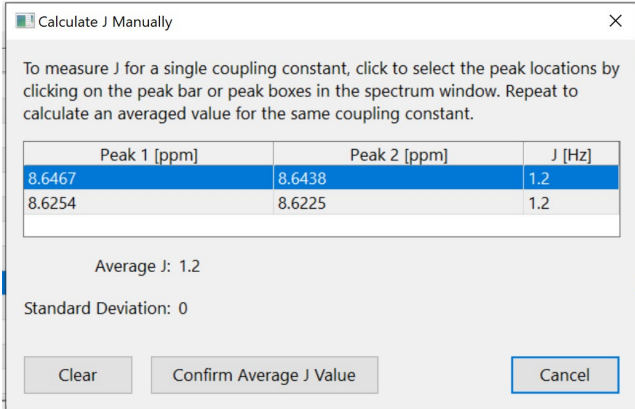
	Action	Result
4	Navigate to "C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\NMR\Bruker TopSpin\C14H10ClNO3 C14H10ClNO3 H1.sdbx". Double click to open the file.	<p>Upon opening the database, a processed NMR spectrum is displayed in Minelt:</p>  <p>The screenshot shows the Minelt software window. The main display is a 1H NMR spectrum for the sample C14H10ClNO3 H1. The x-axis represents chemical shift in ppm, ranging from 0 to 14. The y-axis represents intensity. Several peaks are visible, with their chemical shifts labeled: 1.578, 3.976, 4.407, 4.425, 4.448, 4.469, 4.490, 4.511, 4.532, 4.553, 4.574, 4.595, 4.616, 4.637, 4.658, 4.679, 4.700, 4.721, 4.742, 4.763, 4.784, 4.805, 4.826, 4.847, 4.868, 4.889, 4.910, 4.931, 4.952, 4.973, 4.994, 5.015, 5.036, 5.057, 5.078, 5.099, 5.120, 5.141, 5.162, 5.183, 5.204, 5.225, 5.246, 5.267, 5.288, 5.309, 5.330, 5.351, 5.372, 5.393, 5.414, 5.435, 5.456, 5.477, 5.498, 5.519, 5.540, 5.561, 5.582, 5.603, 5.624, 5.645, 5.666, 5.687, 5.708, 5.729, 5.750, 5.771, 5.792, 5.813, 5.834, 5.855, 5.876, 5.897, 5.918, 5.939, 5.960, 5.981, 5.999, 6.017, 6.035, 6.053, 6.071, 6.089, 6.107, 6.125, 6.143, 6.161, 6.179, 6.197, 6.215, 6.233, 6.251, 6.269, 6.287, 6.305, 6.323, 6.341, 6.359, 6.377, 6.395, 6.413, 6.431, 6.449, 6.467, 6.485, 6.503, 6.521, 6.539, 6.557, 6.575, 6.593, 6.611, 6.629, 6.647, 6.665, 6.683, 6.701, 6.719, 6.737, 6.755, 6.773, 6.791, 6.809, 6.827, 6.845, 6.863, 6.881, 6.899, 6.917, 6.935, 6.953, 6.971, 6.989, 7.007, 7.025, 7.043, 7.061, 7.079, 7.097, 7.115, 7.133, 7.151, 7.169, 7.187, 7.205, 7.223, 7.241, 7.259, 7.277, 7.295, 7.313, 7.331, 7.349, 7.367, 7.385, 7.403, 7.421, 7.439, 7.457, 7.475, 7.493, 7.511, 7.529, 7.547, 7.565, 7.583, 7.601, 7.619, 7.637, 7.655, 7.673, 7.691, 7.709, 7.727, 7.745, 7.763, 7.781, 7.799, 7.817, 7.835, 7.853, 7.871, 7.889, 7.907, 7.925, 7.943, 7.961, 7.979, 7.997, 8.015, 8.033, 8.051, 8.069, 8.087, 8.105, 8.123, 8.141, 8.159, 8.177, 8.195, 8.213, 8.231, 8.249, 8.267, 8.285, 8.303, 8.321, 8.339, 8.357, 8.375, 8.393, 8.411, 8.429, 8.447, 8.465, 8.483, 8.501, 8.519, 8.537, 8.555, 8.573, 8.591, 8.609, 8.627, 8.645, 8.663, 8.681, 8.699, 8.717, 8.735, 8.753, 8.771, 8.789, 8.807, 8.825, 8.843, 8.861, 8.879, 8.897, 8.915, 8.933, 8.951, 8.969, 8.987, 9.005, 9.023, 9.041, 9.059, 9.077, 9.095, 9.113, 9.131, 9.149, 9.167, 9.185, 9.203, 9.221, 9.239, 9.257, 9.275, 9.293, 9.311, 9.329, 9.347, 9.365, 9.383, 9.401, 9.419, 9.437, 9.455, 9.473, 9.491, 9.509, 9.527, 9.545, 9.563, 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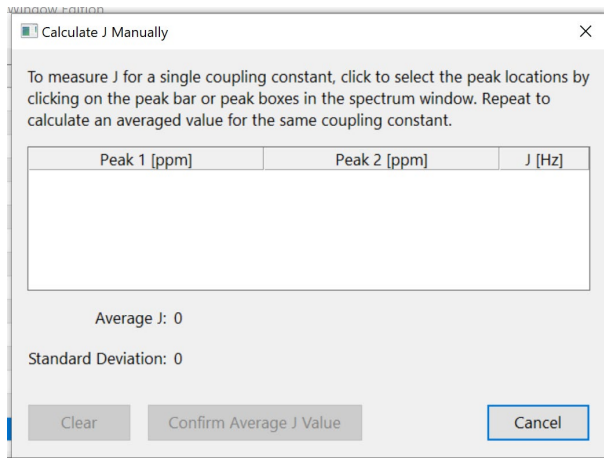
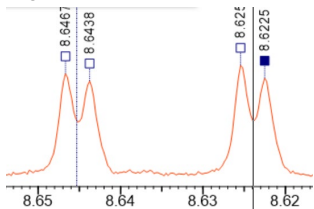
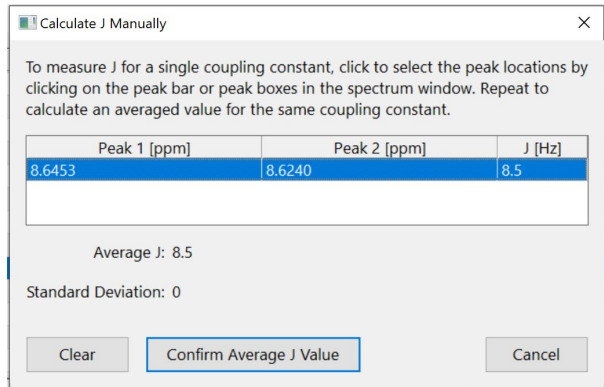
	Action	Result
6	<p>Note: If the record does not contain a property value for NMR Spectrometer Frequency, the Spectrometer Frequency dialog will appear before the Define Multiplets dialog is launched.</p>	<p>In this example, the Spectrometer Frequency dialog is bypassed because the record contains a property value for NMR Spectrometry Frequency. It can be relaunched directly from the Define Multiplets dialog by clicking Set Spectrometer Frequency:</p> 
7	<p>On the Define Multiplets dialog, select the button for Automatic Multiplet Detection.</p> <p>Note: The button for Automatic Multiplet Detection is only available for ¹H-NMR.</p>	<p>The peaks have been grouped into multiplets using an automatic algorithm. Note that the spectrum has 2 multiplets, 2 triplets (t), 1 doublet (d), and 2 singlets (s). Any incorrect assignments will be updated in the proceeding steps. For each multiplet:</p> <ul style="list-style-type: none"> • There is a shift value in the δ column • The peaks were assigned the default simple splitting pattern • The J-value for the simple splitting patterns were automatically calculated 

	Action	Result
8	<p>Click and hold the left mouse button on the spectrum at ~ 8.5 ppm. Drag the mouse across the region on the spectrum from ~ 8.5 ppm to ~ 8.8 ppm. Release the mouse button.</p> <p>Note: The zoom cursor should still be active. If not, you can activate it by right clicking on the spectrum and selecting Horizontal Zoom Mode.</p>	<p>Three groups of peaks are visible. The set of peaks near 8.5 ppm are correctly identified as a doublet (d), and the set of peaks near 8.6 ppm will become divided into two sets of doublet of doublets (dd).</p> 
9	<p>In the Define Multiplets dialog, click to select the row assigned as multiplet at 8.6600 ppm. Then click Ungroup Peaks button on the same dialog.</p>	<p>The set of peaks near 8.6 ppm have been ungrouped to enable further analysis.</p> 

	Action	Result
10	<p>Press and hold CTRL button on the keyboard. In the Multiplets Table, click on the four peaks near ~ 8.62 – 8.64 ppm (8.6225, 8.6254, 8.6438 and 8.6467). Click Group Peaks into Multiplet button.</p> <p>Note: Coupling constants (J) will automatically calculate for the simple splitting patterns: doublet (d), triplet (t), and quartet (q). Groups of 5 or more peaks will be labelled as “multiplet” for the splitting pattern. They can be reassigned if needed using the dropdown menu in the related cell.</p>	<p>In the Multiplets Table, the two peaks at 8.6346 ppm have been grouped together:</p> <ul style="list-style-type: none"> There is now a shift value in the δ column The peaks were assigned the default simple splitting pattern (q for quartet, which will be adjusted in a proceeding step) the J-value for the simple splitting pattern automatically calculated 

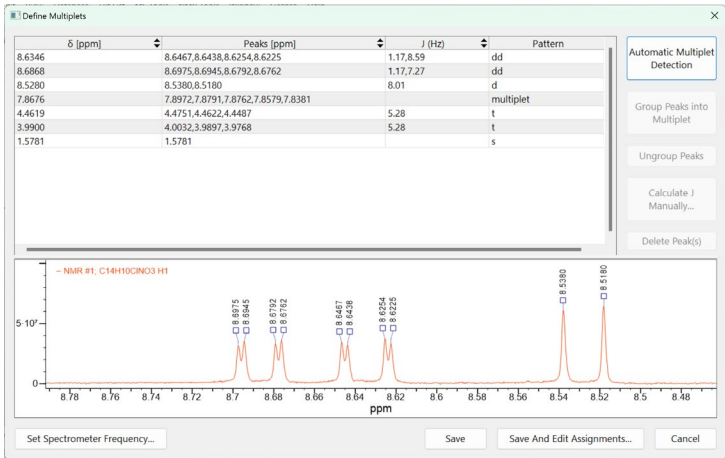
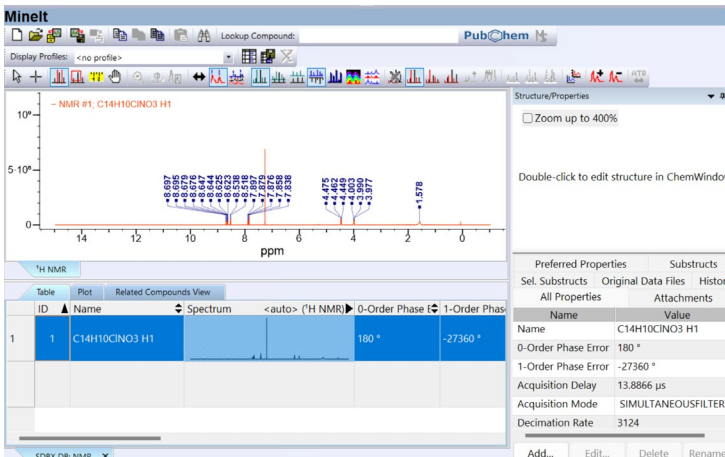
	Action	Result																																																
11	In the Multiplets Table , click on the Pattern cell for the multiplet at 8.6346 ppm to change it from a “q” to a “dd” using the dropdown menu.	<p>The pattern in the Multiplets Table for the multiplet at 8.6346 ppm now displays as dd. The cell for the J-value is blank.</p> <div><div>Define Multiplets</div><table><thead><tr><th>δ [ppm]</th><th>Peaks [ppm]</th><th>J (Hz)</th><th>Pattern</th></tr></thead><tbody><tr><td>8.6346</td><td>8.6467,8.6438,8.6254,8.6225</td><td></td><td>dd</td></tr><tr><td></td><td>8.6762</td><td></td><td></td></tr><tr><td></td><td>8.6792</td><td></td><td></td></tr><tr><td></td><td>8.6945</td><td></td><td></td></tr><tr><td></td><td>8.6975</td><td></td><td></td></tr><tr><td>8.5280</td><td>8.5380,8.5180</td><td>8.01</td><td>d</td></tr><tr><td>7.8676</td><td>7.8972,7.8791,7.8762,7.8579,7.8381</td><td></td><td>multiplet</td></tr><tr><td>7.2612</td><td>7.2612</td><td></td><td>s</td></tr><tr><td>4.4619</td><td>4.4751,4.4622,4.4487</td><td>5.28</td><td>t</td></tr><tr><td>3.9900</td><td>4.0032,3.9897,3.9768</td><td>5.28</td><td>t</td></tr><tr><td>1.5781</td><td>1.5781</td><td></td><td>s</td></tr></tbody></table><div><p>— NMR #1; C14H10ClNO3 H1</p><p>Set Spectrometer Frequency... Save Save And Edit Assignments... Cancel</p></div></div>	δ [ppm]	Peaks [ppm]	J (Hz)	Pattern	8.6346	8.6467,8.6438,8.6254,8.6225		dd		8.6762				8.6792				8.6945				8.6975			8.5280	8.5380,8.5180	8.01	d	7.8676	7.8972,7.8791,7.8762,7.8579,7.8381		multiplet	7.2612	7.2612		s	4.4619	4.4751,4.4622,4.4487	5.28	t	3.9900	4.0032,3.9897,3.9768	5.28	t	1.5781	1.5781		s
δ [ppm]	Peaks [ppm]	J (Hz)	Pattern																																															
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1.5781	1.5781		s																																															

	Action	Result
12	<p>Click Calculate J Manually in the Define Multiplets dialog.</p> <p>Note: The coupling constants (J) for complex splitting patterns (e.g., dd, td, dt, ddd, etc.) have to be manually calculated using the Calculate J Manually tool.</p>	<p>The Calculate J Manually dialog is launched:</p>  <p>This dialog will be used two times for this multiplet, to calculate two separate J-values for the dd.</p>
13	<p>Begin by calculating the smaller J-value: click on the peak boxes on the spectrum in the Define Multiplets dialog from left to right for the peaks at 8.6467, 8.6438, 8.6254 and 8.6225 ppm.</p>	<p>When the peak box is selected, its shift value adds to the Calculate J Manually table in the order that they are clicked. The J-value is calculated for the first two selected peaks (8.6467 and 8.6438) and then the second two selected peaks (8.6254 and 8.6225). The average J-value for all of the rows in the table is displayed as Average J:</p> 

	Action	Result
14	Click Confirm Average J Value to save the small J-value. Do not close the dialog.	<p>The J-value is committed to the record and the Calculate J Manually dialog is cleared:</p> 
15	<p>To calculate the larger J-value, use the Peak Bar to click on the centroid of the peaks for each of the two groups of peaks: once between 8.6467 and 8.6438 ppm, then again between 8.6254 and 8.6225 ppm. e.g., as shown below with lines:</p> 	<p>When the Peak Bar is clicked, the shift values adds to the Calculate J Manually table. The J-value is calculated as the central value for each of the two groups of peaks:</p> 

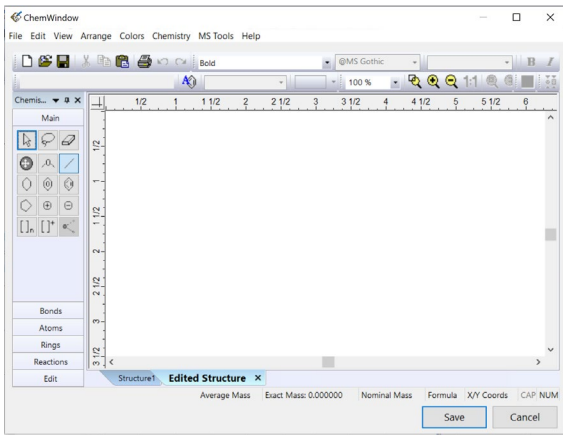
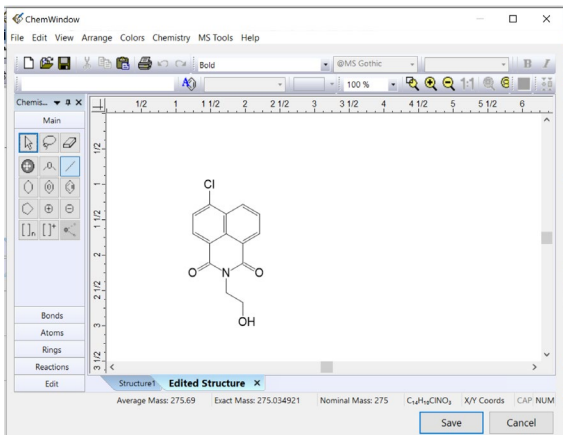
Action	Result
Click Confirm Average J Value to save the large J-value. Next, click Cancel to close the Calculate J Manually dialog.	Two J-values are displayed in the Define Multiplets table for the multiplet at 8.6346 ppm:

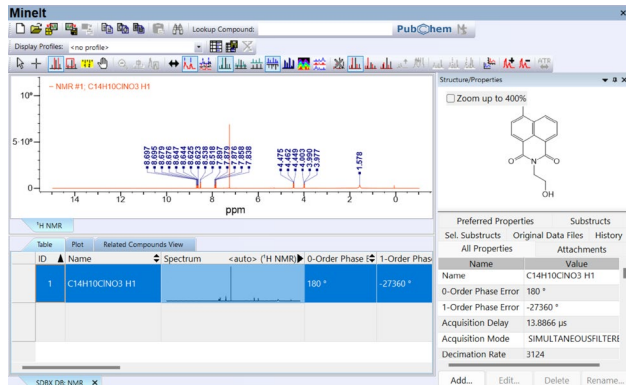
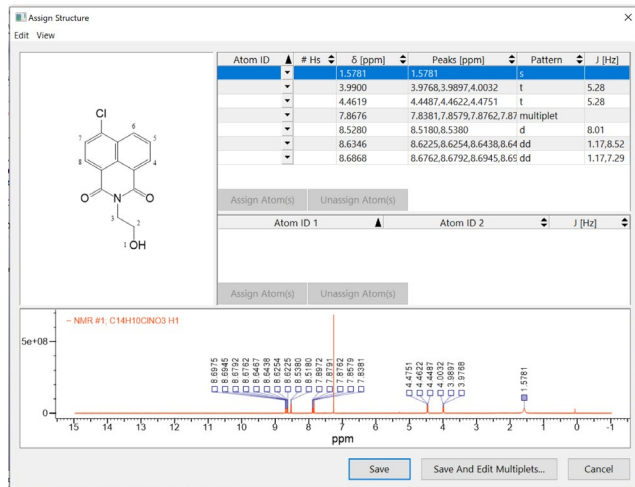
	Action	Result																																				
17	Repeat steps 10 to 16 to group the 4 peaks at ~ 8.67 – 8.70 ppm (8.6762, 8.6792, 8.6945 and 8.6975) into a dd with two coupling constants.	<p>The peaks are grouped into a multiplet at ~ 8.6868 ppm with dd as the splitting pattern. Two J-values for the multiplet are added to the table:</p> <div><div>Define Multiplets</div><table><thead><tr><th>δ [ppm]</th><th>Peaks [ppm]</th><th>J [Hz]</th><th>Pattern</th></tr></thead><tbody><tr><td>8.6346</td><td>8.6467, 8.6438, 8.6254, 8.6225</td><td>1.17, 8.59</td><td>dd</td></tr><tr><td>8.6868</td><td>8.6975, 8.6945, 8.6792, 8.6762</td><td>1.17, 7.27</td><td>dd</td></tr><tr><td>8.5280</td><td>8.5380, 8.5180</td><td>8.01</td><td>d</td></tr><tr><td>7.8676</td><td>7.8972, 7.8791, 7.8762, 7.8579, 7.8381</td><td></td><td>multiplet</td></tr><tr><td>7.2612</td><td>7.2612</td><td></td><td>s</td></tr><tr><td>4.4619</td><td>4.4751, 4.4622, 4.4487</td><td>5.28</td><td>t</td></tr><tr><td>3.9900</td><td>4.0032, 3.9897, 3.9768</td><td>5.28</td><td>t</td></tr><tr><td>1.5781</td><td>1.5781</td><td></td><td>s</td></tr></tbody></table><div><p>Automatic Multiplet Detection</p><p>Group Peaks into Multiplet</p><p>Ungroup Peaks</p><p>Calculate J Manually...</p><p>Delete Peak(s)</p></div><div><p>— NMR #1; C14H10ClNO3 H1</p><p>ppm</p><p>Set Spectrometer Frequency... Save Save And Edit Assignments... Cancel</p></div></div>	δ [ppm]	Peaks [ppm]	J [Hz]	Pattern	8.6346	8.6467, 8.6438, 8.6254, 8.6225	1.17, 8.59	dd	8.6868	8.6975, 8.6945, 8.6792, 8.6762	1.17, 7.27	dd	8.5280	8.5380, 8.5180	8.01	d	7.8676	7.8972, 7.8791, 7.8762, 7.8579, 7.8381		multiplet	7.2612	7.2612		s	4.4619	4.4751, 4.4622, 4.4487	5.28	t	3.9900	4.0032, 3.9897, 3.9768	5.28	t	1.5781	1.5781		s
δ [ppm]	Peaks [ppm]	J [Hz]	Pattern																																			
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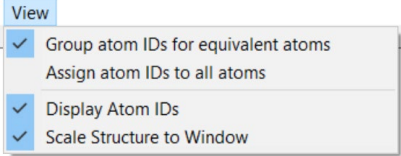
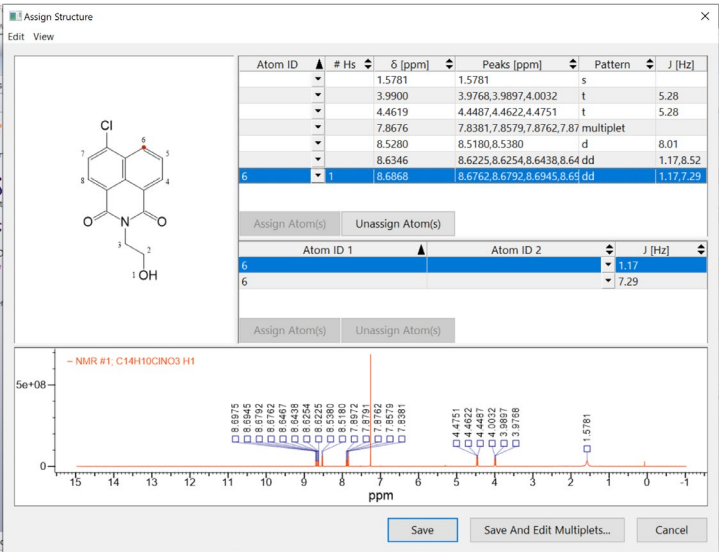
	Action	Result
18	Click to select the row at 7.2612 ppm which represents the solvent peak. Click Delete Peak(s) .	<p>The solvent peak (7.2612 ppm) is removed from the table:</p> 
19	Click Save to save the multiplets to the record and exit the Define Multiplets dialog.	<p>The dialog is closed and the Minelt record is displayed:</p> 

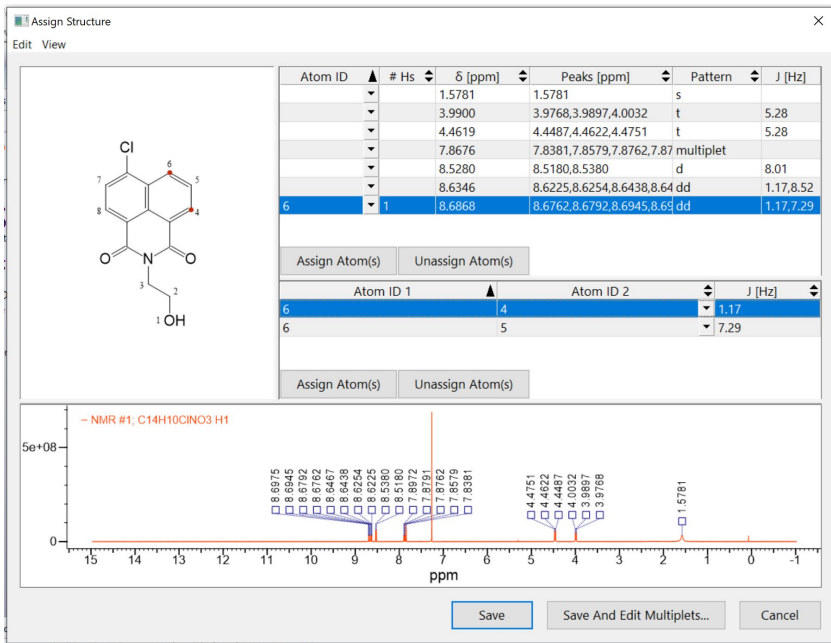
Assign Multiplets to a Structure using NMR Tools

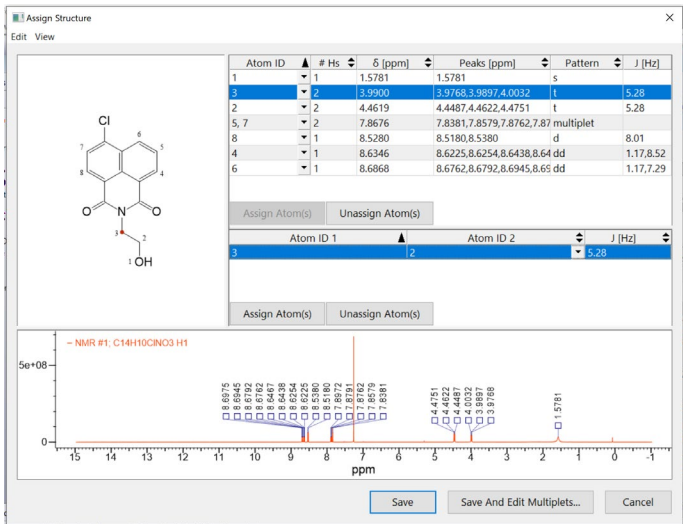
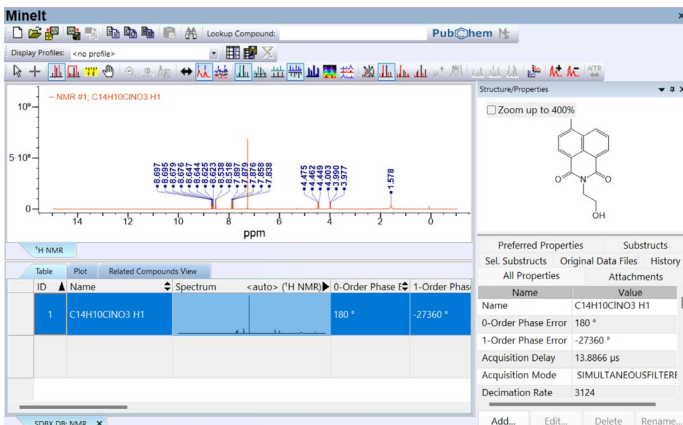
The Assign Multiplets dialog in Minelt NMR Tools allows for the assignment of peaks and multiplets to a structure in Minelt, for ^1H , ^{13}C and X-NMR.

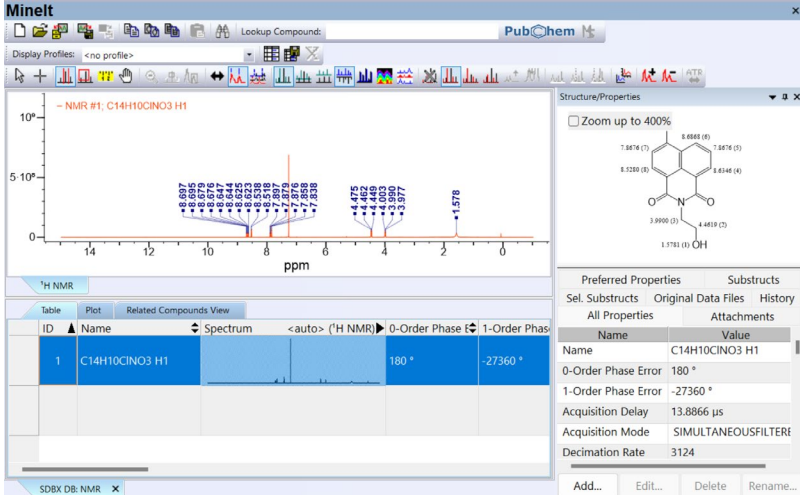
	Action	Result
1	<p>Select the Minelt record for the previous section.</p> <p>Click in the Structure/Properties window on the text “Double-click to edit structure in ChemWindow.”</p> <p>Note: To assign atoms to a structure, a structure must be attached to the Minelt Record.</p>	<p>ChemWindow is launched:</p> 
2	<p>Choose File > Open and open the structure for “C14H10ClNO3.dsf” located in</p> <p>“C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\NMR\Bruker TopSpin\C14H10ClNO3.dsf”.</p>	<p>The structure C14H10ClNO3.dsf opens in ChemWindow:</p> 

	Action	Result																																																
3	Click Save to add the structure to the Minelt record.	<p>The structure is attached to the Minelt record:</p>  <p>The screenshot shows the Minelt software window. On the left, an NMR spectrum is displayed with peaks labeled with chemical shifts (e.g., 1.5781, 3.9900, 4.4619, 7.8676, 8.5280, 8.6346, 8.6868). The x-axis is labeled 'ppm' and ranges from 14 to 0. On the right, the chemical structure of 1-(4-chlorophenyl)ethanol is shown. Below the structure, a table lists properties:</p> <table><tr><th>Name</th><th>Value</th></tr><tr><td>Name</td><td>C14H10ClNO3 H1</td></tr><tr><td>0-Order Phase Error</td><td>180 °</td></tr><tr><td>1-Order Phase Error</td><td>-27360 °</td></tr><tr><td>Acquisition Delay</td><td>13.8866 µs</td></tr><tr><td>Acquisition Mode</td><td>SIMULTANEOUSFILTER</td></tr><tr><td>Decimation Rate</td><td>3124</td></tr></table>	Name	Value	Name	C14H10ClNO3 H1	0-Order Phase Error	180 °	1-Order Phase Error	-27360 °	Acquisition Delay	13.8866 µs	Acquisition Mode	SIMULTANEOUSFILTER	Decimation Rate	3124																																		
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4	Choose NMR Tools > Assign Structure .	<p>The Assign Structure dialog is launched, and the multiplet information from the Define Multiplets dialog is prepopulated:</p>  <p>The screenshot shows the 'Assign Structure' dialog box. It contains a chemical structure of 1-(4-chlorophenyl)ethanol with atoms numbered 1 through 10. Below the structure is a table with peak and multiplet data:</p> <table><tr><th>Atom ID</th><th># Hs</th><th>δ [ppm]</th><th>Peaks [ppm]</th><th>Pattern</th><th>J [Hz]</th></tr><tr><td>1</td><td>1</td><td>1.5781</td><td>1.5781</td><td>s</td><td></td></tr><tr><td>2</td><td>2</td><td>3.9900</td><td>3.9768, 3.9897, 4.0032</td><td>t</td><td>5.28</td></tr><tr><td>3</td><td>2</td><td>4.4619</td><td>4.4487, 4.4622, 4.4751</td><td>t</td><td>5.28</td></tr><tr><td>4</td><td>2</td><td>7.8676</td><td>7.8381, 7.8579, 7.8762, 7.87</td><td>multiplet</td><td></td></tr><tr><td>5</td><td>2</td><td>8.5280</td><td>8.5180, 8.5380</td><td>d</td><td>8.01</td></tr><tr><td>6</td><td>2</td><td>8.6346</td><td>8.6225, 8.6254, 8.6438, 8.64</td><td>dd</td><td>1.17, 8.52</td></tr><tr><td>7</td><td>2</td><td>8.6868</td><td>8.6762, 8.6792, 8.6945, 8.65</td><td>dd</td><td>1.17, 7.29</td></tr></table> <p>Below the table are buttons for 'Assign Atom(s)', 'Unassign Atom(s)', and 'Assign Atom(s)'.</p> <p>The dialog also shows an NMR spectrum at the bottom with peaks labeled with chemical shifts (e.g., 1.5781, 3.9900, 4.4619, 7.8676, 8.5280, 8.6346, 8.6868). The x-axis is labeled 'ppm' and ranges from 15 to -1.</p> <p>The Assign Structure dialog is used to assign peaks and multiplets to atoms in the structure.</p>	Atom ID	# Hs	δ [ppm]	Peaks [ppm]	Pattern	J [Hz]	1	1	1.5781	1.5781	s		2	2	3.9900	3.9768, 3.9897, 4.0032	t	5.28	3	2	4.4619	4.4487, 4.4622, 4.4751	t	5.28	4	2	7.8676	7.8381, 7.8579, 7.8762, 7.87	multiplet		5	2	8.5280	8.5180, 8.5380	d	8.01	6	2	8.6346	8.6225, 8.6254, 8.6438, 8.64	dd	1.17, 8.52	7	2	8.6868	8.6762, 8.6792, 8.6945, 8.65	dd	1.17, 7.29
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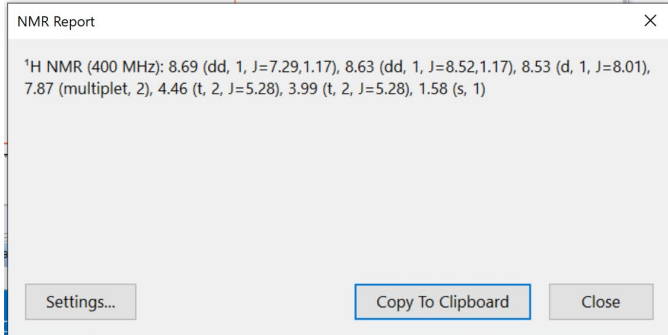
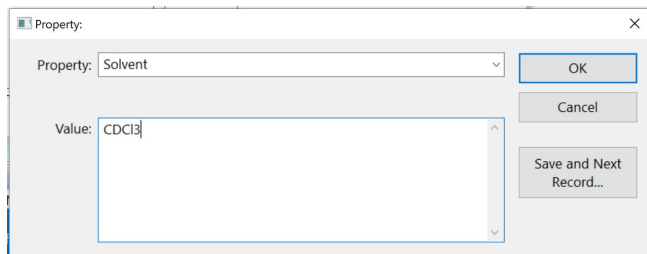
	Action	Result
5	Verify the Assign Structure dialog settings under View tab: <ul style="list-style-type: none"> • Group atom IDs for equivalent atoms should be selected with a checkmark • Assign atom IDs to all atoms should be deselected without a checkmark 	 <p>Group atom IDs for equivalent atoms is used to add/remove equivalent numeration for symmetrical structures. Assign atom IDs to all atoms is used to add/remove numeration for heteroatoms, which may be necessary to label cross-coupling in the spectrum (e.g., H-P).</p>
6	Click on the row with δ value 8.6868 ppm. Use the dropdown menu under Atom ID to select proton 6 for assignment to the multiplet. Click on the white space below the table to commit the change. <p>Note: More than one proton can be selected for assignment using this menu. Atom IDs can also be assigned to the cells using the numbers on a keyboard or using the Assign Atom(s) button and selecting an atom in the structure. Protons can be unassigned at any time by clicking Unassign Atom(s).</p>	<p>The Atom ID for the dd at 8.6868 is proton 6. # Hs is populated with the number of assigned protons:</p> 

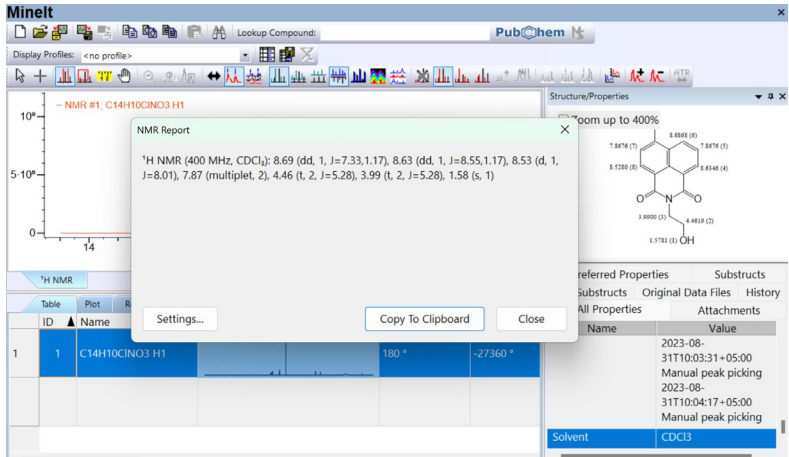
	Action	Result
7	In the lower table within the Assign Structure dialog, use the Atom ID 2 column and the dropdown menus within the cells to assign the small J-value (~1.17 Hz) to proton #4 and the large J-value (~7.29 Hz) to proton #5.	<p>The Atom ID 2 column in the lower table becomes populated with atoms #4 and #5:</p>  <p>The lower table is used to assign cross-coupling.</p>

	Action	Result																					
8	<p>Repeat steps 6 and 7 for each proton in the structure. Assign the following pairs:</p> <table border="1"> <thead> <tr> <th>δ</th><th>Atom ID</th><th>Atom ID 2</th></tr> </thead> <tbody> <tr> <td>1.5781</td><td>1</td><td>N/A</td></tr> <tr> <td>3.9900</td><td>3</td><td>2</td></tr> <tr> <td>4.4619</td><td>2</td><td>3</td></tr> <tr> <td>7.8676</td><td>5, 7</td><td>N/A</td></tr> <tr> <td>8.5280</td><td>8</td><td>7</td></tr> <tr> <td>8.6346</td><td>4</td><td>6 (1.17) 5 (8.52)</td></tr> </tbody> </table> <p>N/A means no value can be added in the lower table.</p>	δ	Atom ID	Atom ID 2	1.5781	1	N/A	3.9900	3	2	4.4619	2	3	7.8676	5, 7	N/A	8.5280	8	7	8.6346	4	6 (1.17) 5 (8.52)	<p>The Atom ID column for the Assign Structure dialog is filled:</p> 
δ	Atom ID	Atom ID 2																					
1.5781	1	N/A																					
3.9900	3	2																					
4.4619	2	3																					
7.8676	5, 7	N/A																					
8.5280	8	7																					
8.6346	4	6 (1.17) 5 (8.52)																					
9	Click Save to commit the changes to the record.	<p>Upon clicking Save, the dialog is closed and the Minelt record is displayed.</p> 																					

	Action	Result																																																		
10	To view the assignments on the structure, choose View > Assignment Information > Both .	<p>The atom IDs are displayed on the structure in the Structure/Properties window:</p>  <p>The screenshot shows the Minelt software interface. The main window displays the ¹H NMR spectrum of C14H10ClNO3 H1. The x-axis represents the chemical shift in ppm, ranging from 0 to 14. The y-axis represents the intensity. Peaks are labeled with their chemical shift values: 8.6346, 8.6868, 8.5280, 7.8676, 4.4619, 3.9900, and 1.5781. The chemical structure of the compound is shown on the right, with atom IDs assigned to each proton. The Structure/Properties window is open, displaying the chemical structure and a table of properties.</p> <table><tr><th>Name</th><th>Value</th></tr><tr><td>Name</td><td>C14H10ClNO3 H1</td></tr><tr><td>0-Order Phase Error</td><td>180 °</td></tr><tr><td>1-Order Phase Error</td><td>-27360 °</td></tr><tr><td>Acquisition Delay</td><td>13.8866 µs</td></tr><tr><td>Acquisition Mode</td><td>SIMULTANEOUSFILTER</td></tr><tr><td>Decimation Rate</td><td>3124</td></tr></table>	Name	Value	Name	C14H10ClNO3 H1	0-Order Phase Error	180 °	1-Order Phase Error	-27360 °	Acquisition Delay	13.8866 µs	Acquisition Mode	SIMULTANEOUSFILTER	Decimation Rate	3124																																				
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11	To view the cross-coupling information, choose View > Windows/Tables > Coupling Data Table .	<table><tr><th colspan="5">Coupling Data Table</th></tr><tr><th>Pos (ppm)</th><th>Multiplicity</th><th>Atom #</th><th>Atom #</th><th>J (Hz)</th></tr><tr><td>8.6346</td><td>dd</td><td>4</td><td>6</td><td>1.17</td></tr><tr><td>8.6346</td><td>dd</td><td></td><td></td><td>8.55</td></tr><tr><td>8.6868</td><td>dd</td><td></td><td></td><td>7.33</td></tr><tr><td>8.5280</td><td>d</td><td>8</td><td>7</td><td>8.01</td></tr><tr><td>7.8676</td><td>m</td><td></td><td></td><td></td></tr><tr><td>4.4619</td><td>t</td><td>2</td><td>3</td><td>5.28</td></tr><tr><td>3.9900</td><td>t</td><td>3</td><td>2</td><td>5.28</td></tr><tr><td>1.5781</td><td>s</td><td></td><td></td><td></td></tr></table>	Coupling Data Table					Pos (ppm)	Multiplicity	Atom #	Atom #	J (Hz)	8.6346	dd	4	6	1.17	8.6346	dd			8.55	8.6868	dd			7.33	8.5280	d	8	7	8.01	7.8676	m				4.4619	t	2	3	5.28	3.9900	t	3	2	5.28	1.5781	s			
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Viewing the NMR Multiplet Report

	Action	Result
1	<p>In Minelt, choose NMR Tools > Multiplet Report.</p> <p>Note: Clicking Copy to Clipboard will copy the report information in the dialog to the clipboard.</p>	<p>The Multiplet Report is prefilled with the information saved to the record using the Define Multiplets dialog. The integral information is attached from the Assign Structure dialog:</p>  <p>The NMR Report will automatically generate for all NMR spectra (^1H, ^{13}C and X-NMR). The specific settings for the NMR Report for these can be adjusted by clicking Settings.</p>
2	<p>Click Close on the dialog. In the Structure/Properties window, click Add. Choose "Solvent" in the dropdown list. Enter "CDCl₃" as the value.</p>	<p>The Property dialog is launched:</p> 

	Action	Result								
3	Click OK on the Property dialog to add the Solvent to the Minelt record. Relaunch the NMR Report dialog (NMR Tools > Multiplet Report).	<p>The NMR Report now displays the NMR solvent for the specific record:</p>  <p>The screenshot shows the Minelt software interface. The main window displays the chemical structure of the compound, the NMR spectrum, and the NMR data table. The NMR data table shows the chemical shift (delta) and the multiplicity (m) for each peak. The NMR solvent is listed as CDCl3.</p> <table><tr><th>ID</th><th>Name</th><th>Chemical Shift (delta)</th><th>Multiplicity (m)</th></tr><tr><td>1</td><td>C14H10ClNO3 H1</td><td>100 *</td><td>-2/360 *</td></tr></table>	ID	Name	Chemical Shift (delta)	Multiplicity (m)	1	C14H10ClNO3 H1	100 *	-2/360 *
ID	Name	Chemical Shift (delta)	Multiplicity (m)							
1	C14H10ClNO3 H1	100 *	-2/360 *							

NMR

Generate an NMR Spectrum

Purpose

This exercise demonstrates how to generate an NMR spectrum using peak lists or an NMR report for a decoupled spectrum.

Objectives

This exercise will teach you:

- How to import peak lists to Minelt

Background

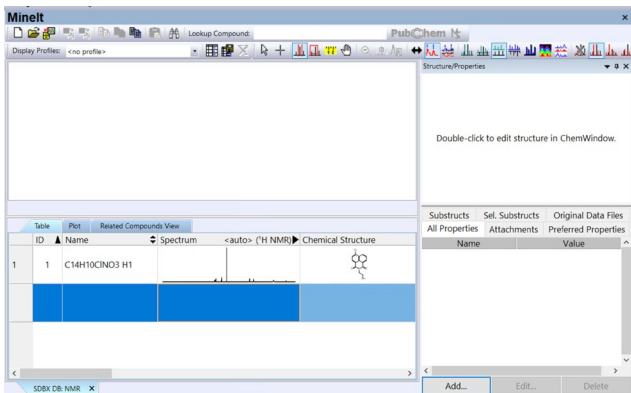
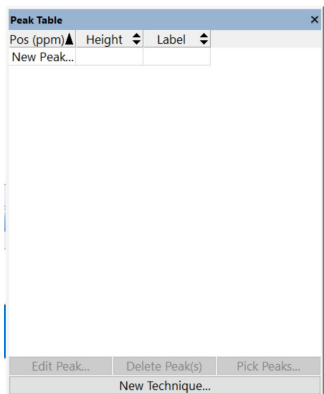
Being able to overlay reference material to experimental spectra is important for confirmation of compounds and identification of impurities. Through importing tabulated peak lists from reference material such as NMR reports into Minelt user databases, the spectra for these compounds can be directly overlaid, subtracted and searched against experimental data.

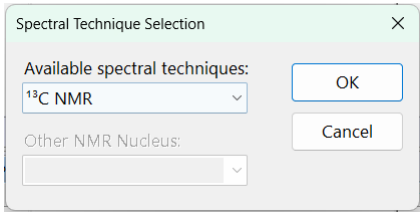
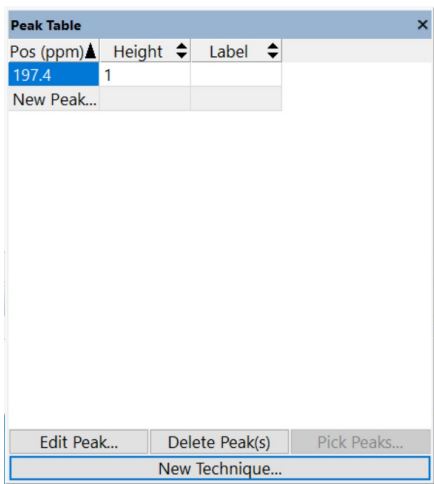
KnowItAll Applications Used

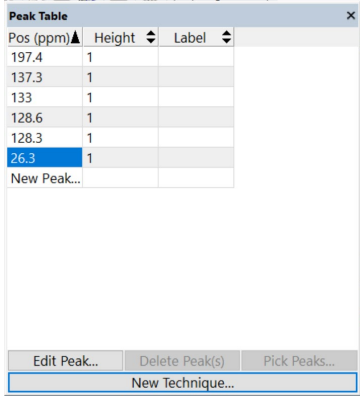
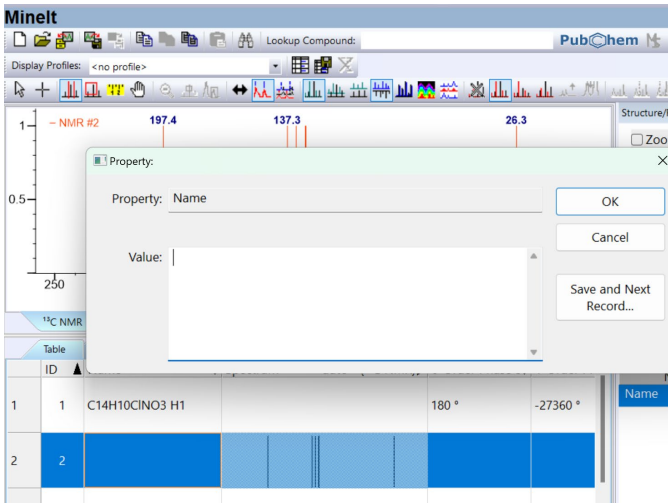
- Minelt

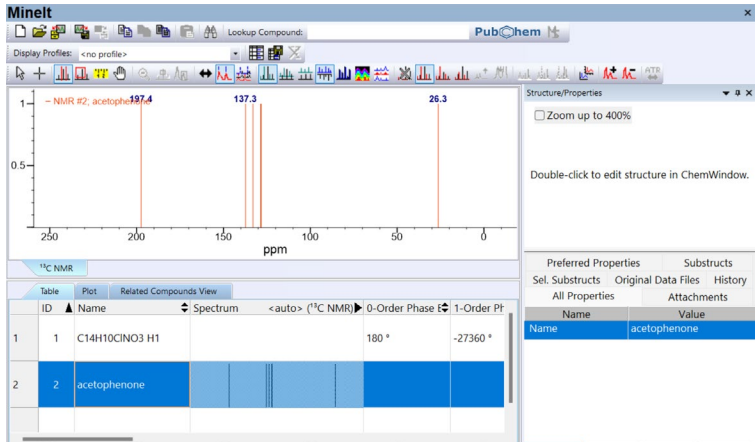
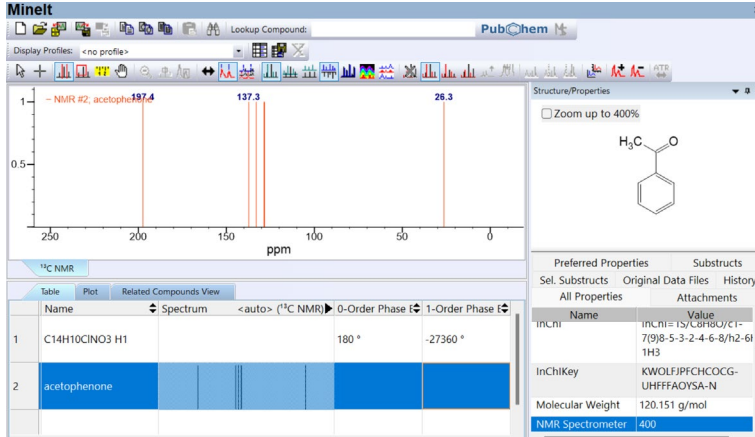
Generating a Database Record from NMR Report or Peak List

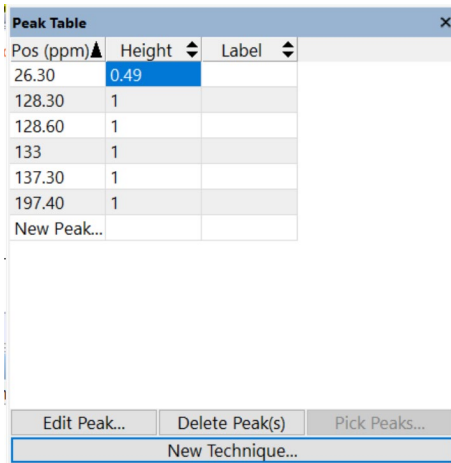
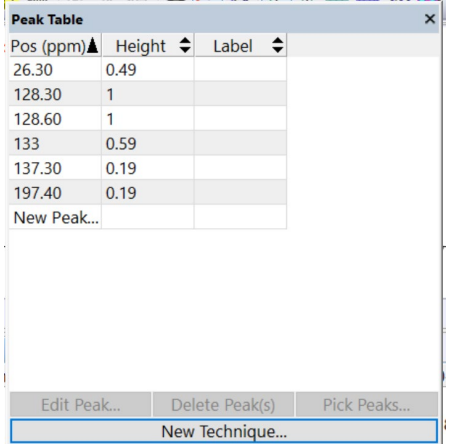
This section shows how an NMR peak spectrum can be generated from peak list information.

	Action	Result
1	Using the user database from the previous section, click on the blank row in the Table section. This is currently the second row for the opened database.	<p>A blank record is displayed:</p> 
2	Choose View > Windows/Tables > Peak Table	<p>A blank Peak Table dialog opens:</p> 

	Action	Result
3	Click New Technique to choose the spectrum type on the Peak Table dialog.	<p>The Spectral Technique Selection dialog opens:</p> 
4	Use the Available spectral techniques dropdown menu to choose ^{13}C NMR, then click OK .	The Spectral Technique Selection dialog is closed and the blank Peak Table remains visible.
5	Double click on the cell that reads "New Peak" in the Peak Table and enter the value 197.4. Click the down arrow to begin a new row.	<p>The Peak Table displays 197.4 as a peak in the first cell, with a default peak height of 1:</p> 

	Action	Result
6	<p>Repeat step 5 for each of the following peaks: 137.3, 133, 128.6, 128.3, 26.3.</p> <p>Note: This simulates the spectrum for the NMR Report: ¹³C NMR (80 MHz): 197.4, 137.3, 133.0, 128.6, 128.3, 26.3".</p>	<p>The Peak Table is filled with the peaks:</p> 
7	<p>Click the X button to close the Peak Table dialog, then double click on the Name cell for the active record.</p>	<p>The Peak Table closes. Upon clicking the Name cell, Minelt refreshes and the generated spectrum displays. The Property dialog appears:</p> 

	Action	Result
8	Enter "acetophenone" as in the Value box and click OK .	<p>The simulated spectrum is displayed with name of record "acetophenone":</p>  <p>The screenshot shows the Minelt software window. The main plot area displays a simulated ¹³C NMR spectrum with three prominent peaks labeled at 197.4, 137.3, and 26.3 ppm. Below the plot is a table with two rows. The first row is for 'C14H10ClNO3 H1' and the second row is for 'acetophenone'. To the right of the table is a 'Structure/Properties' panel. It shows the chemical structure of acetophenone (a benzene ring with an acetyl group) and lists various properties including InChI, InChIKey, Molecular Weight, and NMR Spectrometer frequency.</p>
9	<p>Note: The chemical structure and NMR Spectrometer Frequency can be attached to the record by applying skills previously reviewed in this document.</p>	<p>The chemical structure and NMR spectrometer frequency information have been attached to the simulated spectrum:</p>  <p>This screenshot is similar to the previous one but shows additional information in the 'Structure/Properties' panel. The chemical structure of acetophenone is displayed. Below it, a table lists properties: InChI, InChIKey, Molecular Weight, and NMR Spectrometer. The NMR Spectrometer value is 400.</p>

	Action	Result																								
10	<p>Peak Height information can also be included in the simulation.</p> <p>Choose View > Windows/Tables > Peak Table.</p> <p>Double click on the cell for Height in the row next to the peak 26.30 ppm. Enter 0.49 and press Enter on the keyboard.</p> <p>Note: Clicking enter jumps to the cell below.</p>	<p>The peak height value is displayed in the Peak Table:</p>  <table border="1"> <thead> <tr> <th>Pos (ppm)</th> <th>Height</th> <th>Label</th> </tr> </thead> <tbody> <tr> <td>26.30</td> <td>0.49</td> <td></td> </tr> <tr> <td>128.30</td> <td>1</td> <td></td> </tr> <tr> <td>128.60</td> <td>1</td> <td></td> </tr> <tr> <td>133</td> <td>1</td> <td></td> </tr> <tr> <td>137.30</td> <td>1</td> <td></td> </tr> <tr> <td>197.40</td> <td>1</td> <td></td> </tr> <tr> <td>New Peak...</td> <td></td> <td></td> </tr> </tbody> </table>	Pos (ppm)	Height	Label	26.30	0.49		128.30	1		128.60	1		133	1		137.30	1		197.40	1		New Peak...		
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New Peak...																										
11	<p>Repeat step 10 to enter the following values: 0.59 (133 ppm), 0.19 (137.30 ppm), 0.19 (197.40 ppm).</p>	<p>The peak height values are displayed in the Peak Table:</p>  <table border="1"> <thead> <tr> <th>Pos (ppm)</th> <th>Height</th> <th>Label</th> </tr> </thead> <tbody> <tr> <td>26.30</td> <td>0.49</td> <td></td> </tr> <tr> <td>128.30</td> <td>1</td> <td></td> </tr> <tr> <td>128.60</td> <td>1</td> <td></td> </tr> <tr> <td>133</td> <td>0.59</td> <td></td> </tr> <tr> <td>137.30</td> <td>0.19</td> <td></td> </tr> <tr> <td>197.40</td> <td>0.19</td> <td></td> </tr> <tr> <td>New Peak...</td> <td></td> <td></td> </tr> </tbody> </table>	Pos (ppm)	Height	Label	26.30	0.49		128.30	1		128.60	1		133	0.59		137.30	0.19		197.40	0.19		New Peak...		
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