

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.

Objectives

This exercise will teach you:

- How to define multiplets for a processed NMR spectrum in Minelt
- How to edit shift 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

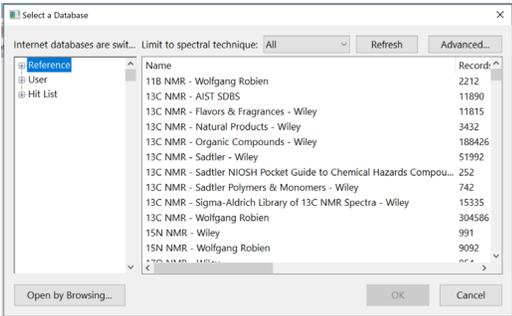
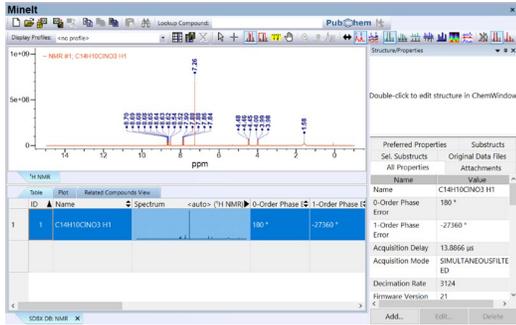
C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\NMR\Bruker TopSpin\ C14H10CINO3\

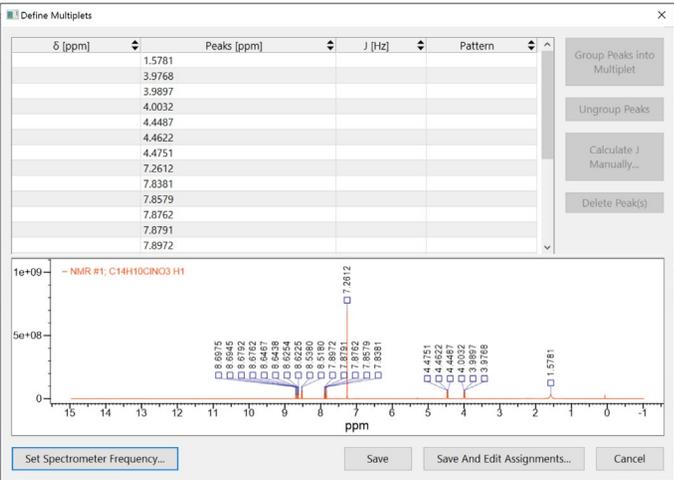
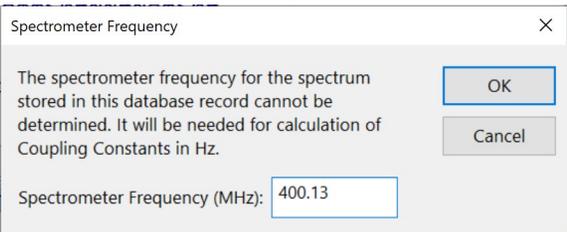
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- C14H10CINO3 H1.dsf
- C14H10CINO3 H1.sdbx

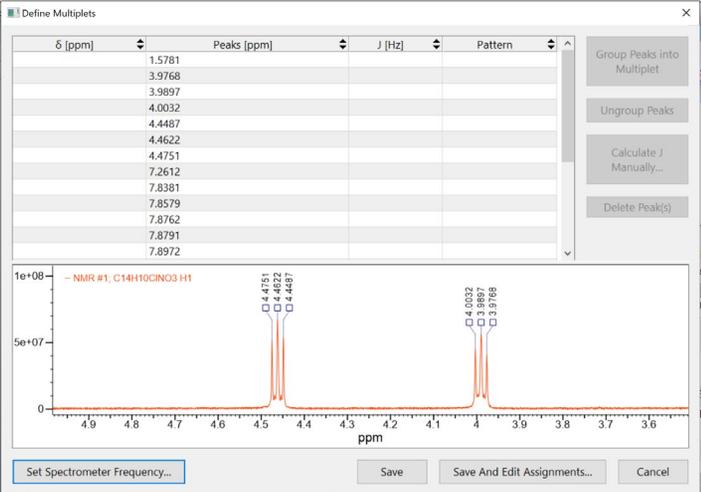
KnowItAll Applications Used

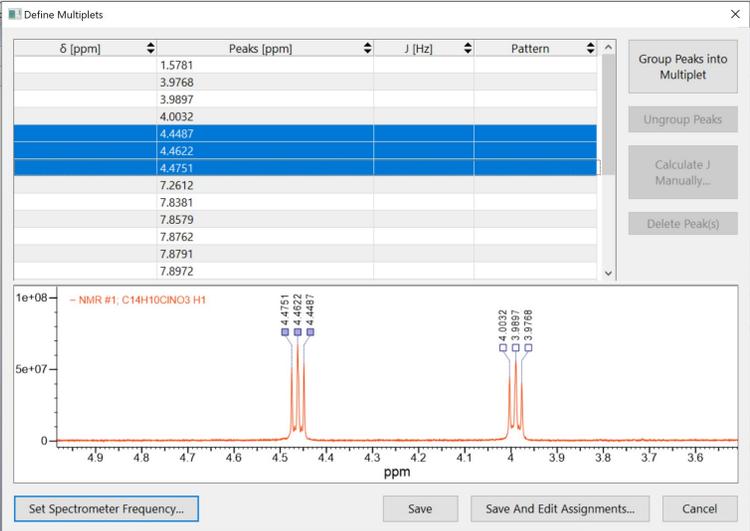
- Minelt™
- ProcessIt™

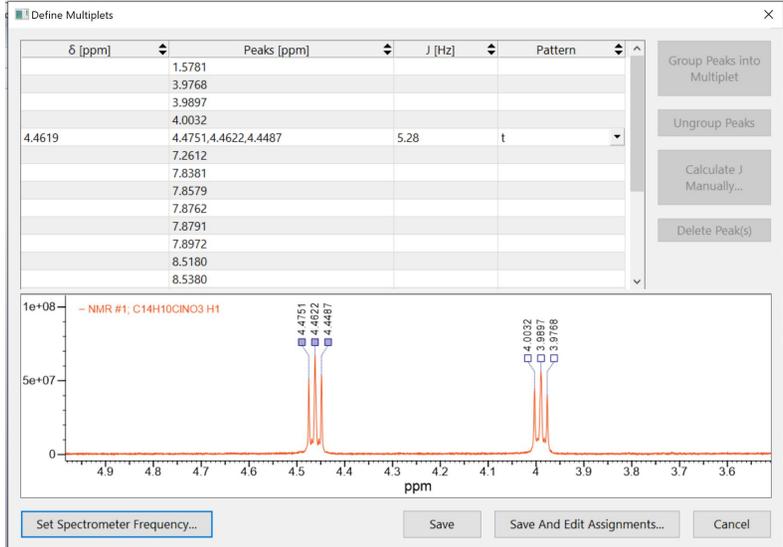
Calculate Spectrum Multiplets using NMR Tools

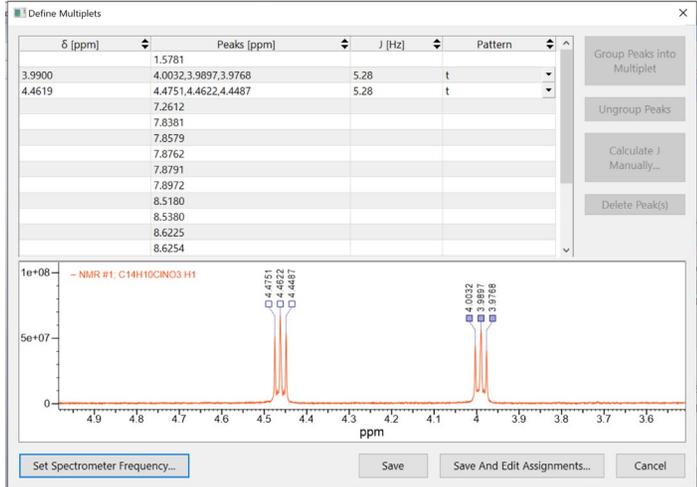
	Action	Result
1	Open the Minelt application by clicking its icon, typically found in the Data toolbox.  Minelt/Create Database	
2	Click Open Database button using the icon.  Then click Open by Browsing on the Select a Database dialog.	Clicking the Open Database launches the Select a Database dialog. Clicking Open by Browsing launches a file explorer to select a file: 
3	Navigate to "C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\NMR\Bruker TopSpin\C14H10ClNO3\C14H10ClNO3 H1.sdbx".	Upon opening the database, a processed NMR spectrum is displayed in Minelt.  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.

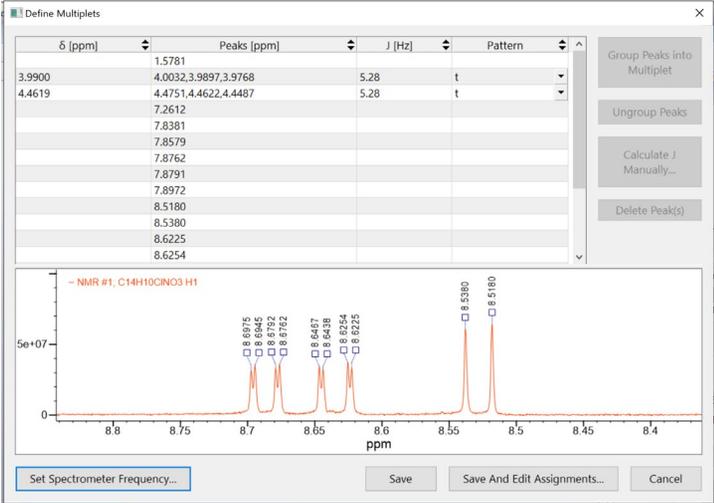
	Action	Result
4	<p>Choose NMR Tools > Define Multiplets.</p> <p>Note: The Define Multiplets window is used to calculate J-values and transition peak lists into defined multiplets with splitting patterns.</p>	<p>The Define Multiplets dialog is launched:</p> 
5	<p>Note: If the record does not contain a 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. It can be relaunched directly from the Define Multiplets dialog by clicking Set Spectrometer Frequency:</p> 

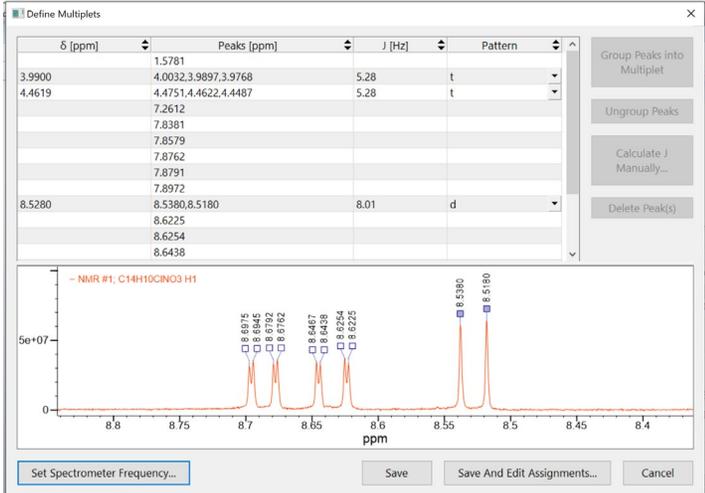
	Action	Result																																																								
6	<p>Click on the spectrum in the Define Multiplets dialog and hold the mouse button. Drag across the region from ~ 3.5 ppm to 5 ppm, then release the mouse button.</p> <p>Note: When the Define Multiplets dialog is first launched, the horizontal zoom cursor is preselected.</p>	<p>Two groups of peaks are visible in the spectrum:</p>  <table border="1" data-bbox="659 418 1228 646"><thead><tr><th>δ [ppm]</th><th>Peaks [ppm]</th><th>J [Hz]</th><th>Pattern</th></tr></thead><tbody><tr><td>1.5781</td><td></td><td></td><td></td></tr><tr><td>3.9768</td><td></td><td></td><td></td></tr><tr><td>3.9897</td><td></td><td></td><td></td></tr><tr><td>4.0032</td><td></td><td></td><td></td></tr><tr><td>4.4487</td><td></td><td></td><td></td></tr><tr><td>4.4622</td><td></td><td></td><td></td></tr><tr><td>4.4751</td><td></td><td></td><td></td></tr><tr><td>7.2612</td><td></td><td></td><td></td></tr><tr><td>7.8381</td><td></td><td></td><td></td></tr><tr><td>7.8579</td><td></td><td></td><td></td></tr><tr><td>7.8762</td><td></td><td></td><td></td></tr><tr><td>7.8791</td><td></td><td></td><td></td></tr><tr><td>7.8972</td><td></td><td></td><td></td></tr></tbody></table>	δ [ppm]	Peaks [ppm]	J [Hz]	Pattern	1.5781				3.9768				3.9897				4.0032				4.4487				4.4622				4.4751				7.2612				7.8381				7.8579				7.8762				7.8791				7.8972			
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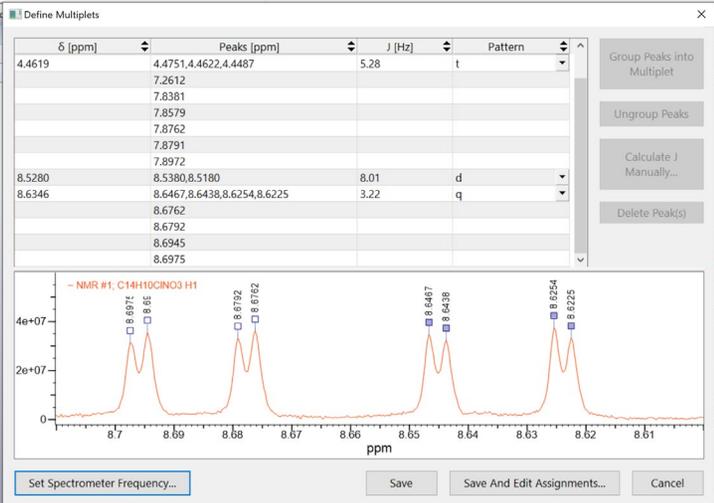
	Action	Result
7	Press and hold CTRL button on the keyboard. In the Multiplets Table , click on the three peaks at ~4.4 ppm (4.4487, 4.4622 and 4.4751). Release CTRL button.	<p>Three peaks are highlighted in the Multiplets Table and three boxes are highlighted on the spectrum corresponding to the selected peaks:</p> 

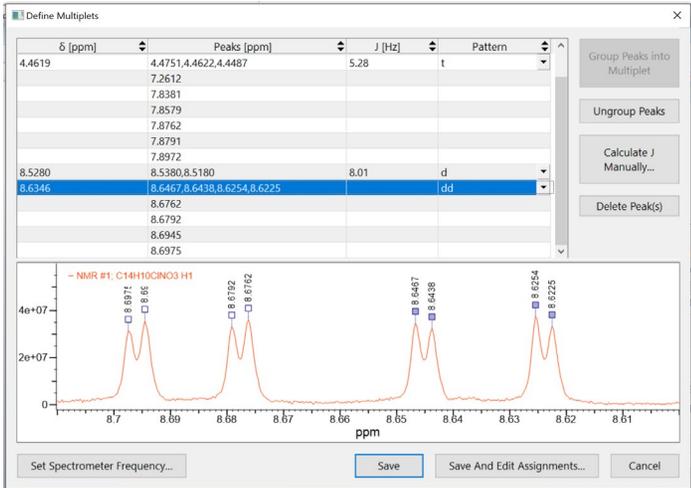
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8	<p>Click Group Peaks into Multiplet button.</p> <p>Note: Coupling constants (J) will automatically calculate for simple splitting patterns d, t, q. Groups of 5 or more peaks will be assigned "multiplet" as the splitting pattern. They can be reassigned as needed.</p>	<p>In the Multiplets Table, the three peaks at 4.4619 ppm have been grouped together. There is now a shift value in the δ column. The peaks were assigned the a default simple splitting pattern (t) and the J-value for the simple splitting pattern automatically calculated:</p>  <table border="1" data-bbox="653 440 1436 727"> <thead> <tr> <th>δ [ppm]</th> <th>Peaks [ppm]</th> <th>J [Hz]</th> <th>Pattern</th> </tr> </thead> <tbody> <tr> <td>1.5781</td> <td></td> <td></td> <td></td> </tr> <tr> <td>3.9768</td> <td></td> <td></td> <td></td> </tr> <tr> <td>3.9897</td> <td></td> <td></td> <td></td> </tr> <tr> <td>4.0032</td> <td></td> <td></td> <td></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>7.2612</td> <td></td> <td></td> <td></td> </tr> <tr> <td>7.8381</td> <td></td> <td></td> <td></td> </tr> <tr> <td>7.8579</td> <td></td> <td></td> <td></td> </tr> <tr> <td>7.8762</td> <td></td> <td></td> <td></td> </tr> <tr> <td>7.8791</td> <td></td> <td></td> <td></td> </tr> <tr> <td>7.8972</td> <td></td> <td></td> <td></td> </tr> <tr> <td>8.5180</td> <td></td> <td></td> <td></td> </tr> <tr> <td>8.5380</td> <td></td> <td></td> <td></td> </tr> </tbody> </table>	δ [ppm]	Peaks [ppm]	J [Hz]	Pattern	1.5781				3.9768				3.9897				4.0032				4.4619	4.4751, 4.4622, 4.4487	5.28	t	7.2612				7.8381				7.8579				7.8762				7.8791				7.8972				8.5180				8.5380			
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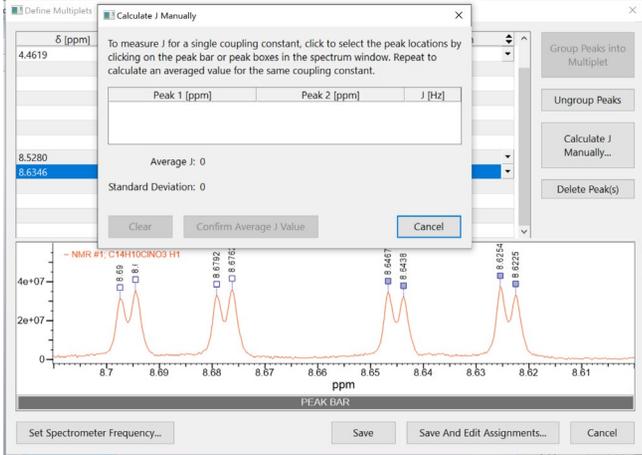
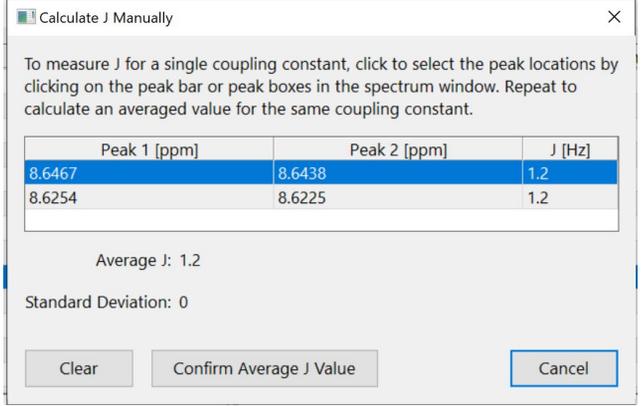
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9	Repeat steps 7 and 8 for the peaks at ~4.0 ppm (3.9768, 3.9897 and 4.0032).	<p>In the Multiplets Table, the three peaks at 3.9900 ppm have been grouped together. There is now a shift value in the δ column. The peaks were assigned a default simple splitting pattern (t) and the J-value for the simple splitting pattern automatically calculated:</p>  <table border="1" data-bbox="653 440 1228 695"><thead><tr><th>δ [ppm]</th><th>Peaks [ppm]</th><th>J [Hz]</th><th>Pattern</th></tr></thead><tbody><tr><td>1.5781</td><td></td><td></td><td></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>4.4619</td><td>4.4751, 4.4622, 4.4487</td><td>5.28</td><td>t</td></tr><tr><td>7.2612</td><td></td><td></td><td></td></tr><tr><td>7.8381</td><td></td><td></td><td></td></tr><tr><td>7.8579</td><td></td><td></td><td></td></tr><tr><td>7.8762</td><td></td><td></td><td></td></tr><tr><td>7.8791</td><td></td><td></td><td></td></tr><tr><td>7.8972</td><td></td><td></td><td></td></tr><tr><td>8.5180</td><td></td><td></td><td></td></tr><tr><td>8.5380</td><td></td><td></td><td></td></tr><tr><td>8.6225</td><td></td><td></td><td></td></tr><tr><td>8.6254</td><td></td><td></td><td></td></tr></tbody></table> <p>Buttons: Set Spectrometer Frequency..., Save, Save And Edit Assignments..., Cancel</p>	δ [ppm]	Peaks [ppm]	J [Hz]	Pattern	1.5781				3.9900	4.0032, 3.9897, 3.9768	5.28	t	4.4619	4.4751, 4.4622, 4.4487	5.28	t	7.2612				7.8381				7.8579				7.8762				7.8791				7.8972				8.5180				8.5380				8.6225				8.6254			
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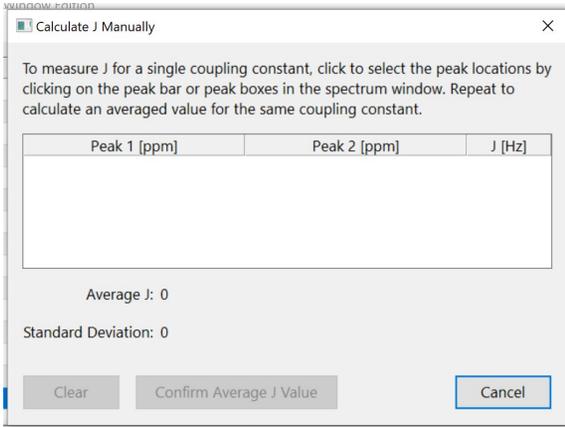
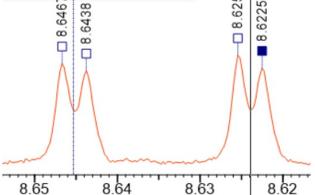
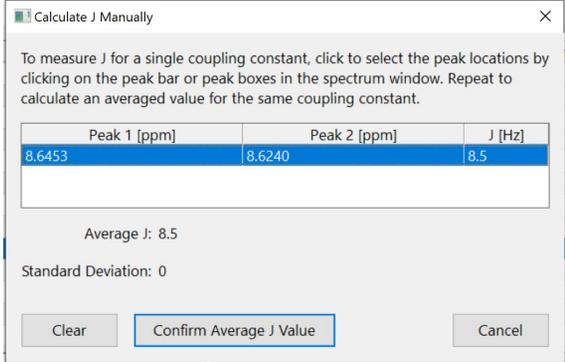
	Action	Result												
10	<p>Right click on the spectrum in the Define Multiplets dialog and select Zoom Out. Click on the spectrum and hold the left mouse button. Drag the mouse across the region on the spectrum from ~ 8.4 ppm to 8.8 ppm. Release the mouse button.</p> <p>Note: The zoom cursor should 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:</p>  <table border="1" data-bbox="667 418 1245 649"> <thead> <tr> <th>δ [ppm]</th> <th>Peaks [ppm]</th> <th>J [Hz]</th> <th>Pattern</th> </tr> </thead> <tbody> <tr> <td>3.9900</td> <td>1.5781 4.0032, 3.9897, 3.9768</td> <td>5.28</td> <td>t</td> </tr> <tr> <td>4.4619</td> <td>4.4751, 4.4622, 4.4487 7.2612 7.8381 7.8579 7.8762 7.8791 7.8972 8.5180 8.5380 8.6225 8.6254</td> <td>5.28</td> <td>t</td> </tr> </tbody> </table> <p>The spectrum below the table shows three groups of peaks. The x-axis is labeled 'ppm' and ranges from 8.8 to 8.4. The y-axis is labeled '5e+07' and '0'. The peaks are labeled with their chemical shifts: 8.6975, 8.6845, 8.6782, 8.6752, 8.6687, 8.6658, 8.6625, 8.6525, 8.5380, and 8.5180.</p>	δ [ppm]	Peaks [ppm]	J [Hz]	Pattern	3.9900	1.5781 4.0032, 3.9897, 3.9768	5.28	t	4.4619	4.4751, 4.4622, 4.4487 7.2612 7.8381 7.8579 7.8762 7.8791 7.8972 8.5180 8.5380 8.6225 8.6254	5.28	t
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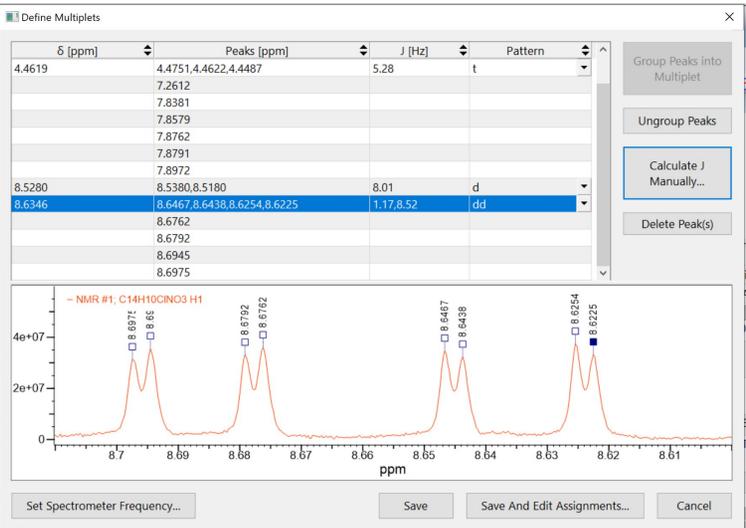
	Action	Result
11	Repeat steps 7 and 8 for the two peaks at ~ 8.5 ppm (8.5180 and 8.5380).	<p>In the Multiplets Table, the two peaks at 8.5280 ppm have been grouped together. There is now a shift value in the δ column. The peaks were assigned the a default simple splitting pattern (d) and the J-value for the simple splitting pattern automatically calculated:</p> 

	Action	Result
12	<p>Zoom in further to ~ 8.6 ppm to 8.71 ppm. Repeat steps 7 and 8 for the four peaks near ~ 8.62 – 8.64 ppm (8.6225, 8.6254, 8.6438 and 8.6467).</p> <p>Note: The pattern will automatically be assigned to the simple splitting pattern for 4 peaks (q). This will get corrected in the next step.</p>	<p>In the Multiplets Table, the two peaks at 8.6346 ppm have been grouped together. There is now a shift value in the δ column. The peaks were assigned the a default simple splitting pattern (q) and the J-value for the simple splitting pattern automatically calculated:</p> 

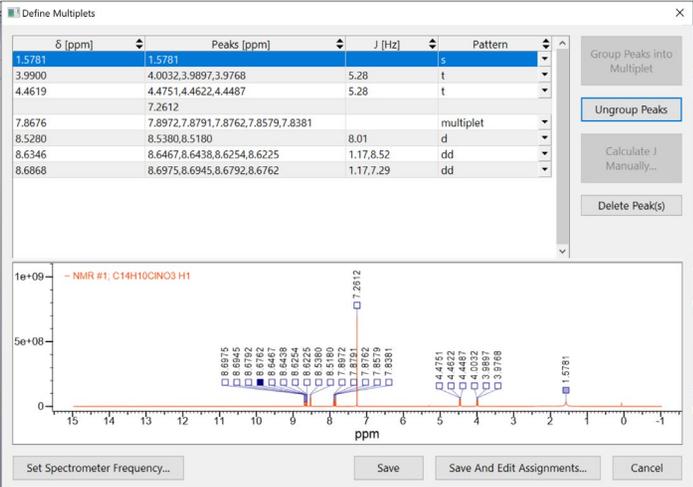
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13	<p>In the Multiplets Table, click on the Pattern for the multiplet at 8.6346 ppm to change it from a “q” to a “dd” using the dropdown menu for the cell.</p> <p>Note: You may need to resize the Define Multiplets dialog to choose the pattern on the dropdown menu.</p>	<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 now blank.</p>  <table border="1" data-bbox="655 410 1346 665"> <thead> <tr> <th>δ [ppm]</th> <th>Peaks [ppm]</th> <th>J [Hz]</th> <th>Pattern</th> </tr> </thead> <tbody> <tr> <td>4.4619</td> <td>4.4751,4.4622,4.4487</td> <td>5.28</td> <td>t</td> </tr> <tr> <td></td> <td>7.2612</td> <td></td> <td></td> </tr> <tr> <td></td> <td>7.8381</td> <td></td> <td></td> </tr> <tr> <td></td> <td>7.8579</td> <td></td> <td></td> </tr> <tr> <td></td> <td>7.8762</td> <td></td> <td></td> </tr> <tr> <td></td> <td>7.8791</td> <td></td> <td></td> </tr> <tr> <td></td> <td>7.8972</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 style="background-color: #e0f0ff;"> <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> </tbody> </table> <p>The screenshot also shows an NMR spectrum plot with peaks labeled at 8.6971, 8.695, 8.6792, 8.6762, 8.6467, 8.6438, 8.6254, and 8.6225 ppm. The plot title is '- NMR #1, C14H10ClNO3 H1'.</p>	δ [ppm]	Peaks [ppm]	J [Hz]	Pattern	4.4619	4.4751,4.4622,4.4487	5.28	t		7.2612				7.8381				7.8579				7.8762				7.8791				7.8972			8.5280	8.5380,8.5180	8.01	d	8.6346	8.6467,8.6438,8.6254,8.6225		dd		8.6762				8.6792				8.6945				8.6975		
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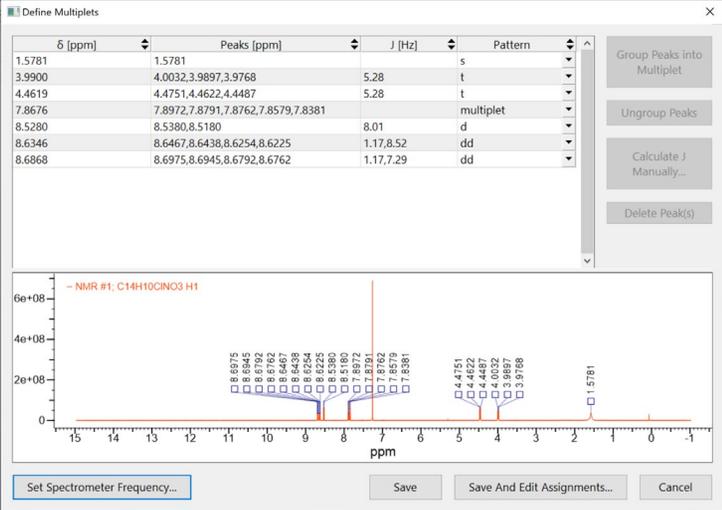
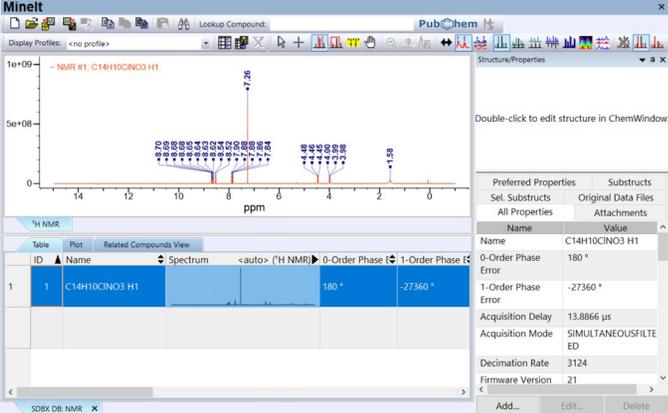
	Action	Result
14	<p>Click Calculate J Manually in the Define Multiplets dialog.</p> <p>Note: The coupling constants (J) for complex splitting patterns (e.g., dd, td, dt, ddd, etc.) have to be manually calculated using the Calculate J Manually tool.</p>	<p>The Calculate J Manually dialog is launched.</p>  <p>This dialog will be used two times for this multiplet, to calculate two separate J-values for the dd.</p>
15	<p>To calculate the smaller J-value, click on the peak boxes on the spectrum in the Define Multiplets dialog from left to right. Repeat for all 4 peaks in the multiplet, shown here as 8.6467, 8.6438, 8.6254 and 8.6225.</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>  <p>Average J:</p>

	Action	Result
16	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> 
17	<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> 

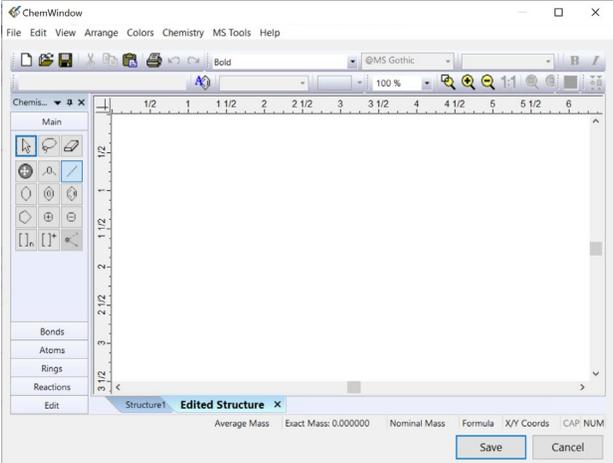
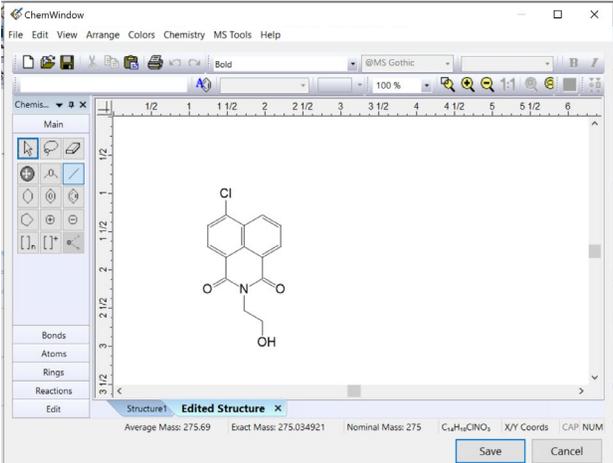
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18	Click Confirm Average J Value to save the large J-value. Next, click Cancel to close the Calculate J Manually dialog.	<p>Two J-values are displayed in the Define Multiplets table for the multiplet at 8.6346 ppm:</p>  <table border="1" data-bbox="661 414 1270 657"> <thead> <tr> <th>δ [ppm]</th> <th>Peaks [ppm]</th> <th>J [Hz]</th> <th>Pattern</th> </tr> </thead> <tbody> <tr> <td>4.4619</td> <td>4.4751, 4.4622, 4.4487</td> <td>5.28</td> <td>t</td> </tr> <tr> <td></td> <td>7.2612</td> <td></td> <td></td> </tr> <tr> <td></td> <td>7.8381</td> <td></td> <td></td> </tr> <tr> <td></td> <td>7.8579</td> <td></td> <td></td> </tr> <tr> <td></td> <td>7.8762</td> <td></td> <td></td> </tr> <tr> <td></td> <td>7.8791</td> <td></td> <td></td> </tr> <tr> <td></td> <td>7.8972</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>8.6346</td> <td>8.6467, 8.6438, 8.6254, 8.6225</td> <td>1.17, 8.52</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> </tbody> </table> <p>The plot shows the NMR spectrum with peaks labeled at 8.6874, 8.66, 8.6792, 8.6792, 8.6467, 8.6438, 8.6254, and 8.6225 ppm. The y-axis ranges from 0 to 4e+07.</p>	δ [ppm]	Peaks [ppm]	J [Hz]	Pattern	4.4619	4.4751, 4.4622, 4.4487	5.28	t		7.2612				7.8381				7.8579				7.8762				7.8791				7.8972			8.5280	8.5380, 8.5180	8.01	d	8.6346	8.6467, 8.6438, 8.6254, 8.6225	1.17, 8.52	dd		8.6762				8.6792				8.6945				8.6975		
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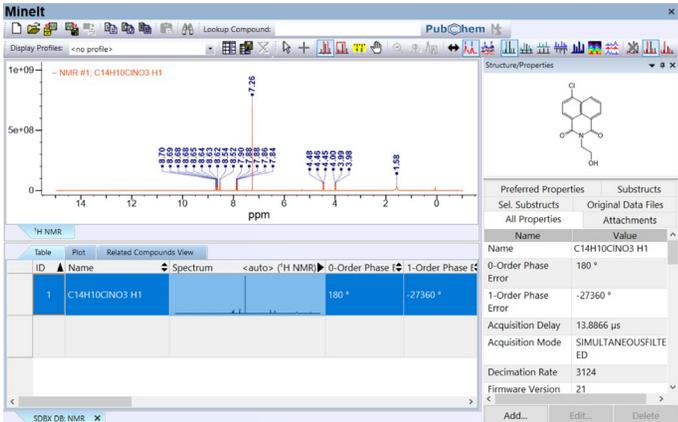
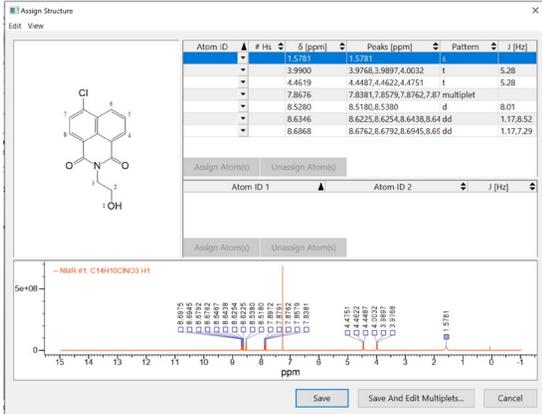
	Action	Result																																																				
19	<p>Repeat steps 12 to 18 to group the 4 peaks at ~ 8.67 – 8.70 ppm (8.6762, 8.6792, 8.6945 and 8.6975) into a dd with two coupling constants.</p> <p>Note: You may need to resize the Define Multiplets dialog to choose the pattern on the dropdown menu.</p>	<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> <table border="1" data-bbox="661 414 1344 665"> <thead> <tr> <th>δ [ppm]</th> <th>Peaks [ppm]</th> <th>J [Hz]</th> <th>Pattern</th> </tr> </thead> <tbody> <tr> <td>1.5781</td> <td></td> <td></td> <td></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>4.4619</td> <td>4.4751,4.4622,4.4487</td> <td>5.28</td> <td>t</td> </tr> <tr> <td>7.2612</td> <td></td> <td></td> <td></td> </tr> <tr> <td>7.8381</td> <td></td> <td></td> <td></td> </tr> <tr> <td>7.8579</td> <td></td> <td></td> <td></td> </tr> <tr> <td>7.8762</td> <td></td> <td></td> <td></td> </tr> <tr> <td>7.8791</td> <td></td> <td></td> <td></td> </tr> <tr> <td>7.8972</td> <td></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>8.6346</td> <td>8.6467,8.6438,8.6254,8.6225</td> <td>1.17,8.52</td> <td>dd</td> </tr> <tr style="background-color: #e0f0ff;"> <td>8.6868</td> <td>8.6975,8.6945,8.6792,8.6762</td> <td>1.17,7.29</td> <td>dd</td> </tr> </tbody> </table>	δ [ppm]	Peaks [ppm]	J [Hz]	Pattern	1.5781				3.9900	4.0032,3.9897,3.9768	5.28	t	4.4619	4.4751,4.4622,4.4487	5.28	t	7.2612				7.8381				7.8579				7.8762				7.8791				7.8972				8.5280	8.5380,8.5180	8.01	d	8.6346	8.6467,8.6438,8.6254,8.6225	1.17,8.52	dd	8.6868	8.6975,8.6945,8.6792,8.6762	1.17,7.29	dd
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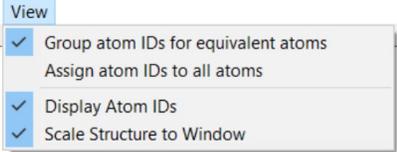
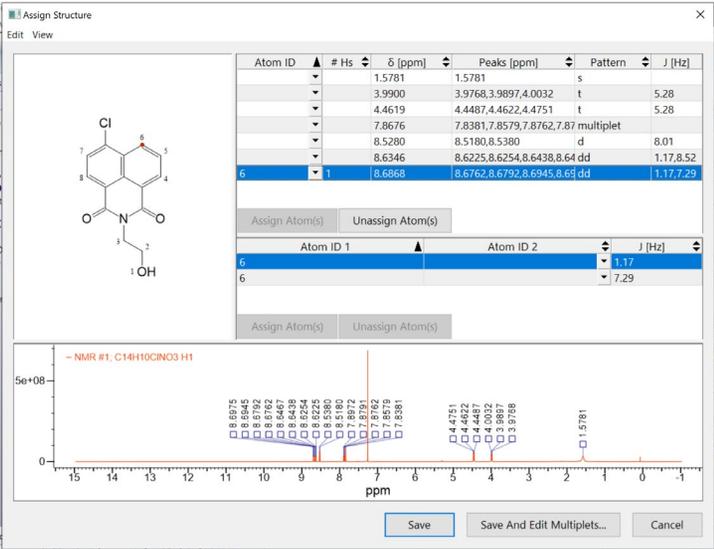
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20	<p>Right click on the spectrum in the Define Multiplets dialog and select View Entire Spectrum. Repeat steps 7 and 8 for the remaining groups of peaks: the 5 peaks at ~ 7.84 to 7.90 ppm (7.8381, 7.8579, 7.8762, 7.8791 and 7.8972) are grouped together, and the single peak at 1.5781 ppm is 'grouped' together.</p> <p>Note: The Multiplets Table requires that singlets become grouped as a single peak, to classify them with the correct Pattern (s).</p>	<p>The peaks at 7.8676 ppm are grouped into a multiplet. The peak at 1.5781 ppm is grouped into a singlet (s). Neither multiplets have a coupling constant due to nature of the pattern:</p>  <table border="1" data-bbox="659 412 1218 665"> <thead> <tr> <th>δ [ppm]</th> <th>Peaks [ppm]</th> <th>J [Hz]</th> <th>Pattern</th> </tr> </thead> <tbody> <tr> <td>1.5781</td> <td>1.5781</td> <td></td> <td>s</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>4.4619</td> <td>4.4751,4.4622,4.4487</td> <td>5.28</td> <td>t</td> </tr> <tr> <td></td> <td>7.2612</td> <td></td> <td></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>8.5280</td> <td>8.5380,8.5180</td> <td>8.01</td> <td>d</td> </tr> <tr> <td>8.6346</td> <td>8.6467,8.6438,8.6254,8.6225</td> <td>1.17,8.52</td> <td>dd</td> </tr> <tr> <td>8.6868</td> <td>8.6975,8.6945,8.6792,8.6762</td> <td>1.17,7.29</td> <td>dd</td> </tr> </tbody> </table>	δ [ppm]	Peaks [ppm]	J [Hz]	Pattern	1.5781	1.5781		s	3.9900	4.0032,3.9897,3.9768	5.28	t	4.4619	4.4751,4.4622,4.4487	5.28	t		7.2612			7.8676	7.8972,7.8791,7.8762,7.8579,7.8381		multiplet	8.5280	8.5380,8.5180	8.01	d	8.6346	8.6467,8.6438,8.6254,8.6225	1.17,8.52	dd	8.6868	8.6975,8.6945,8.6792,8.6762	1.17,7.29	dd
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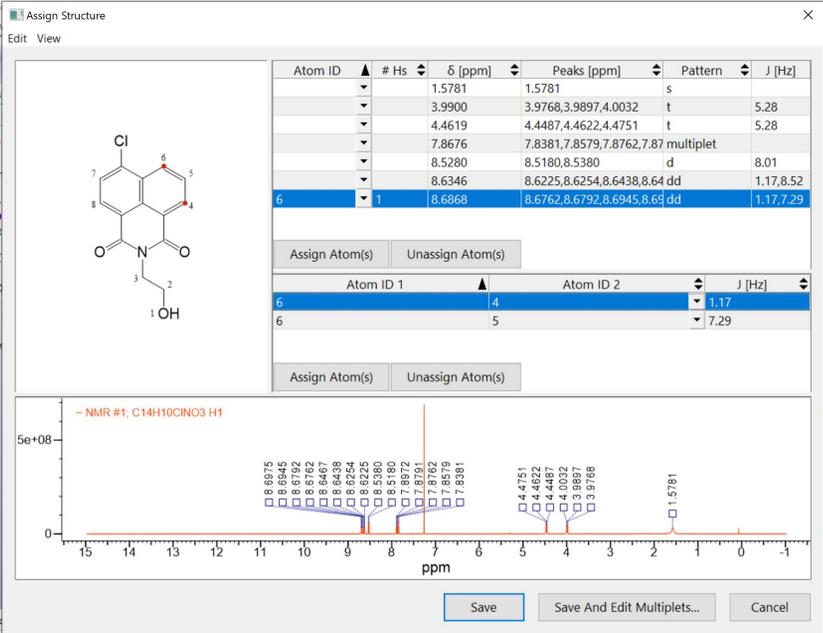
	Action	Result
21	The peak at 7.26 ppm does not belong to the structure and can be deleted by clicking Delete Peak(s) .	<p>The peak at 7.2612 ppm is removed from the Multiplets Table:</p> 
22	Click Save to save the multiplets to the record and exit the Define Multiplets dialog.	<p>The dialog is closed and the Minelt record is displayed:</p> 

Assign Multiplets to a Structure using NMR Tools

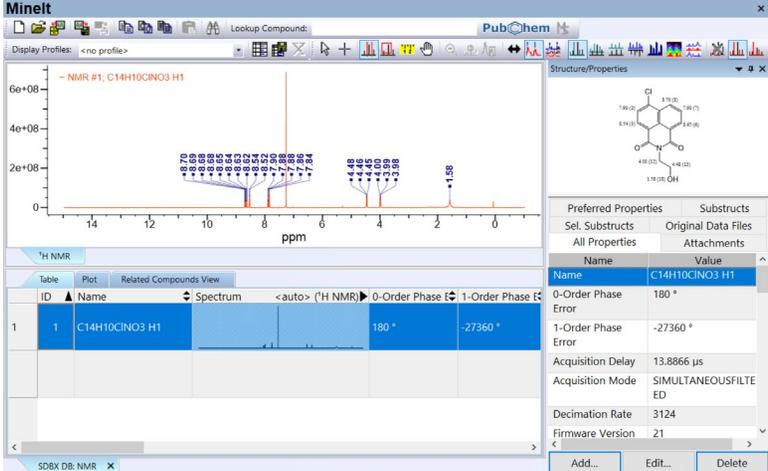
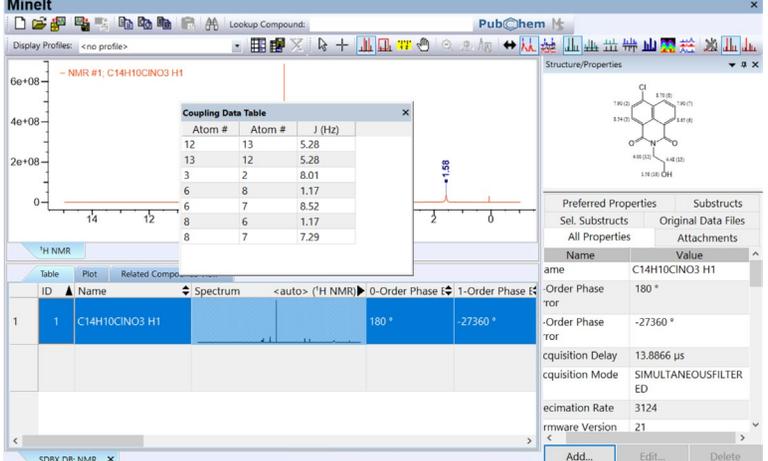
	Action	Result
1	<p>Select the Minelt record for the previous section. Click in the Structure/Properties window on the text "Double-click to edit structure in ChemWindow."</p> <p>Note: To assign protons or carbons to a structure, a structure must be attached to the Minelt Record.</p>	<p>ChemWindow is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

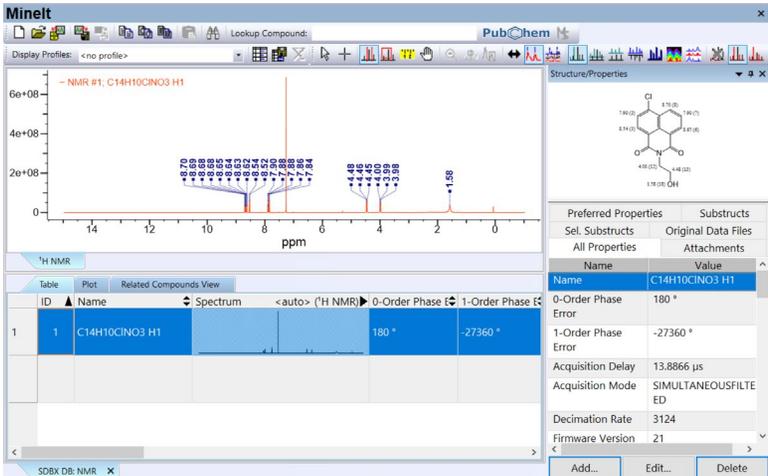
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3	Click Save to add the structure to the Minelt record.	<p>The structure is attached to the Minelt record:</p>  <p>The screenshot shows the Minelt software window with the following data table:</p> <table border="1"> <thead> <tr> <th>ID</th> <th>Name</th> <th>Spectrum</th> <th><auto> ('H NMR)</th> <th>0-Order Phase</th> <th>1-Order Phase</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>C14H10ClNO3 H1</td> <td></td> <td></td> <td>180 °</td> <td>-27360 °</td> </tr> </tbody> </table> <p>Additional parameters shown in the interface include: Acquisition Delay (13.8866 µs), Acquisition Mode (SIMULTANEOUSFILTERED), Decimation Rate (3124), and Firmware Version (21).</p>	ID	Name	Spectrum	<auto> ('H NMR)	0-Order Phase	1-Order Phase	1	C14H10ClNO3 H1			180 °	-27360 °																																				
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4	Choose NMR Tools > Assign Structure .	<p>The Assign Structure dialog is launched:</p>  <p>The screenshot shows the Assign Structure dialog with the following data table:</p> <table border="1"> <thead> <tr> <th>Atom ID</th> <th># Hs</th> <th>δ (ppm)</th> <th>Peaks (ppm)</th> <th>Pattern</th> <th>J [Hz]</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>1</td> <td>1.5781</td> <td>1.5781</td> <td>t</td> <td>5.28</td> </tr> <tr> <td>2</td> <td>3</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>4</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>7</td> <td>7.8676</td> <td>7.8281, 7.8579, 7.8762, 7.87</td> <td>multiplet</td> <td></td> </tr> <tr> <td>5</td> <td>8</td> <td>8.5280</td> <td>8.5180, 8.5380</td> <td>d</td> <td>8.01</td> </tr> <tr> <td>6</td> <td>8</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>8</td> <td>8.6868</td> <td>8.6762, 8.6792, 8.6945, 8.69</td> <td>dd</td> <td>1.17, 7.29</td> </tr> </tbody> </table> <p>The dialog also features an NMR spectrum at the bottom and buttons for 'Save', 'Save And Edit Multiplets...', and 'Cancel'.</p> <p>The multiplet information from the Define Multiplets dialog is prepopulated.</p>	Atom ID	# Hs	δ (ppm)	Peaks (ppm)	Pattern	J [Hz]	1	1	1.5781	1.5781	t	5.28	2	3	3.9900	3.9768, 3.9897, 4.0032	t	5.28	3	4	4.4619	4.4487, 4.4622, 4.4751	t	5.28	4	7	7.8676	7.8281, 7.8579, 7.8762, 7.87	multiplet		5	8	8.5280	8.5180, 8.5380	d	8.01	6	8	8.6346	8.6225, 8.6254, 8.6438, 8.64	dd	1.17, 8.52	7	8	8.6868	8.6762, 8.6792, 8.6945, 8.69	dd	1.17, 7.29
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	Action	Result
5	Verify the Assign Structure dialog settings under View tab. Group atom IDs for equivalent atoms should have a checkmark. Assign atom IDs to all atoms should be unchecked.	 <p>Group atom IDs for equivalent atoms is used to add/remove equivalent numeration for symmetrical structures.</p> <p>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	<p>Click on the row with δ equal 8.6868 ppm. Use the dropdown menus 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> <p>Note: More than one proton can be selected for assignment using this menu.</p> <p>Note: 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.</p> <p>Note: 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> 

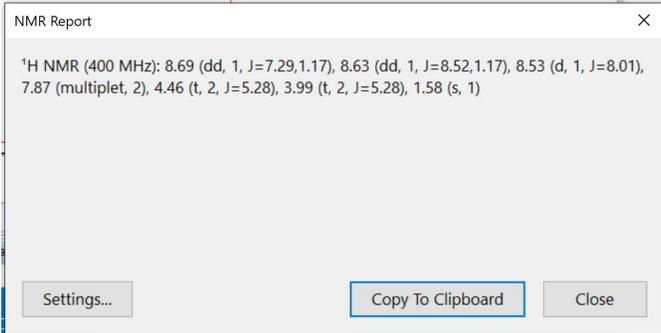
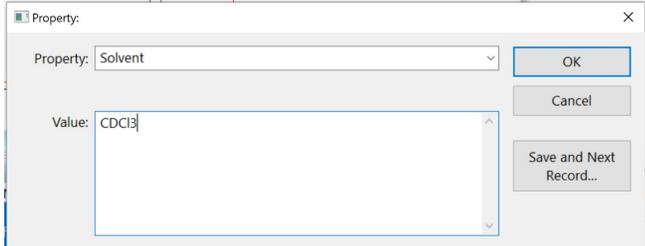
	Action	Result
7	<p>In the lower table within the Assign Structure dialog, use the Atom ID 2 column and the dropdown menus within the cells to assign the small J-value (~1.17 Hz) to proton #4 and the large J-value (~7.29 Hz) to proton #5.</p>	<p>The Atom ID 2 column in the lower table becomes populated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

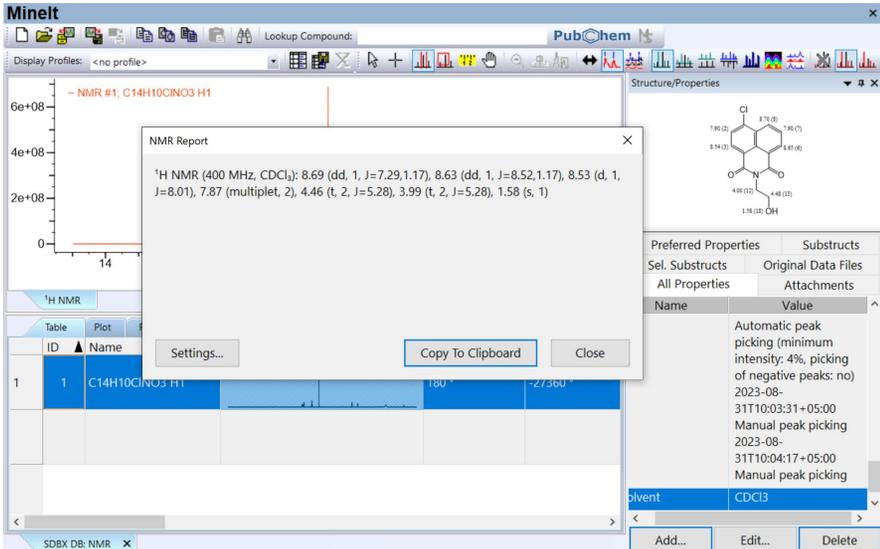
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8	<p>Repeat steps 6 and 7 for each proton in the structure. Assign the following pairs:</p> <table border="1"> <thead> <tr> <th>Atom ID</th> <th>δ</th> <th>Atom ID 2</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>1.5781</td> <td>N/A</td> </tr> <tr> <td>3</td> <td>3.9900</td> <td>2</td> </tr> <tr> <td>2</td> <td>4.4619</td> <td>3</td> </tr> <tr> <td>5, 7</td> <td>7.8676</td> <td>N/A</td> </tr> <tr> <td>8</td> <td>8.5280</td> <td>7</td> </tr> <tr> <td>4</td> <td>8.6346</td> <td>6 (1.17) 5 (8.52)</td> </tr> </tbody> </table>	Atom ID	δ	Atom ID 2	1	1.5781	N/A	3	3.9900	2	2	4.4619	3	5, 7	7.8676	N/A	8	8.5280	7	4	8.6346	6 (1.17) 5 (8.52)	<p>The Atom ID column for the Assign Structure dialog is filled:</p>
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3	3.9900	2																					
2	4.4619	3																					
5, 7	7.8676	N/A																					
8	8.5280	7																					
4	8.6346	6 (1.17) 5 (8.52)																					
9	<p>Click Save to commit the changes to the record.</p> <p>Note: Clicking Save And Edit Multiplets allows for fast interchanging between Define Multiplets and Assign Structure dialogs.</p>	<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 interface with an NMR spectrum on the left and the Structure/Properties window on the right. The spectrum is titled "NMR #1, C14H10ClNO3 H1" and shows a peak at approximately 1.8 ppm. The Structure/Properties window displays the chemical structure of C14H10ClNO3 with atom IDs (1-13) assigned to various atoms. A table in the window lists properties for the selected atom (ID 1, Name C14H10ClNO3 H1):</p> <table border="1" data-bbox="1207 641 1417 852"> <thead> <tr> <th>Name</th> <th>Value</th> </tr> </thead> <tbody> <tr> <td>0-Order Phase</td> <td>180 °</td> </tr> <tr> <td>1-Order Phase</td> <td>-27360 °</td> </tr> <tr> <td>Acquisition Delay</td> <td>13.8866 µs</td> </tr> <tr> <td>Acquisition Mode</td> <td>SIMULTANEOUSFILTERED</td> </tr> <tr> <td>Decimation Rate</td> <td>3124</td> </tr> <tr> <td>Firmware Version</td> <td>21</td> </tr> </tbody> </table>	Name	Value	0-Order Phase	180 °	1-Order Phase	-27360 °	Acquisition Delay	13.8866 µs	Acquisition Mode	SIMULTANEOUSFILTERED	Decimation Rate	3124	Firmware Version	21										
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11	To view the cross-coupling information, choose View > Windows/Tables > Coupling Data Table.	 <p>The screenshot shows the Minelt interface with the NMR spectrum and the Coupling Data Table window. The table lists coupling constants (J) in Hz between atoms:</p> <table border="1" data-bbox="829 982 1060 1128"> <thead> <tr> <th>Atom #</th> <th>Atom #</th> <th>J (Hz)</th> </tr> </thead> <tbody> <tr> <td>12</td> <td>13</td> <td>5.28</td> </tr> <tr> <td>13</td> <td>12</td> <td>5.28</td> </tr> <tr> <td>3</td> <td>2</td> <td>8.01</td> </tr> <tr> <td>6</td> <td>8</td> <td>1.17</td> </tr> <tr> <td>6</td> <td>7</td> <td>8.52</td> </tr> <tr> <td>8</td> <td>6</td> <td>1.17</td> </tr> <tr> <td>8</td> <td>7</td> <td>7.29</td> </tr> </tbody> </table>	Atom #	Atom #	J (Hz)	12	13	5.28	13	12	5.28	3	2	8.01	6	8	1.17	6	7	8.52	8	6	1.17	8	7	7.29
Atom #	Atom #	J (Hz)																								
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3	2	8.01																								
6	8	1.17																								
6	7	8.52																								
8	6	1.17																								
8	7	7.29																								

	Action	Result																												
12	Click X to close the Coupling Data Table .	<p>The coupling data table is hidden:</p>  <p>The screenshot displays the Minelt software interface. At the top, there is a title bar with 'Minelt' and 'Pubchem'. Below the title bar, there is a toolbar with various icons. The main window is divided into several sections. On the left, there is a plot of the ¹H NMR spectrum, showing intensity versus chemical shift (ppm) from 14 to 0. The spectrum shows several peaks, with the most prominent one at approximately 8.5 ppm. On the right, there is a 'Structure/Properties' panel showing the chemical structure of the compound, C14H10ClNO3, and its properties. Below the structure, there is a table with columns for 'Name' and 'Value'. The table contains the following data:</p> <table border="1"> <thead> <tr> <th>Name</th> <th>Value</th> </tr> </thead> <tbody> <tr> <td>C14H10ClNO3 H1</td> <td></td> </tr> <tr> <td>0-Order Phase</td> <td>180 °</td> </tr> <tr> <td>1-Order Phase</td> <td>-27360 °</td> </tr> <tr> <td>Acquisition Delay</td> <td>13.8866 μs</td> </tr> <tr> <td>Acquisition Mode</td> <td>SIMULTANEOUSFILTE ED</td> </tr> <tr> <td>Decimation Rate</td> <td>3124</td> </tr> <tr> <td>Firmware Version</td> <td>21</td> </tr> </tbody> </table> <p>At the bottom of the window, there is a 'Coupling Data Table' which is currently hidden. The table has columns for 'ID', 'Name', 'Spectrum', '<auto> (¹H NMR)', '0-Order Phase', and '1-Order Phase'. The table contains one entry:</p> <table border="1"> <thead> <tr> <th>ID</th> <th>Name</th> <th>Spectrum</th> <th><auto> (¹H NMR)</th> <th>0-Order Phase</th> <th>1-Order Phase</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>C14H10ClNO3 H1</td> <td></td> <td></td> <td>180 °</td> <td>-27360 °</td> </tr> </tbody> </table>	Name	Value	C14H10ClNO3 H1		0-Order Phase	180 °	1-Order Phase	-27360 °	Acquisition Delay	13.8866 μs	Acquisition Mode	SIMULTANEOUSFILTE ED	Decimation Rate	3124	Firmware Version	21	ID	Name	Spectrum	<auto> (¹ H NMR)	0-Order Phase	1-Order Phase	1	C14H10ClNO3 H1			180 °	-27360 °
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1	C14H10ClNO3 H1			180 °	-27360 °																									

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 ^1H and ^{13}C NMR spectra. 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. A dialog box titled "NMR Report" is open, displaying the following text: ^1H NMR (400 MHz, CDCl_3): 8.69 (dd, 1, $J=7.29, 1.17$), 8.63 (dd, 1, $J=8.52, 1.17$), 8.53 (d, 1, $J=8.01$), 7.87 (multiplet, 2), 4.46 (t, 2, $J=5.28$), 3.99 (t, 2, $J=5.28$), 1.58 (s, 1) The background shows a plot of the NMR spectrum and a table with columns for ID, Name, and chemical shift. The table has one row with ID 1, Name C14H10ClNO3 H1, and chemical shift 1.58. The solvent is listed as CDCl3.</p>

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™

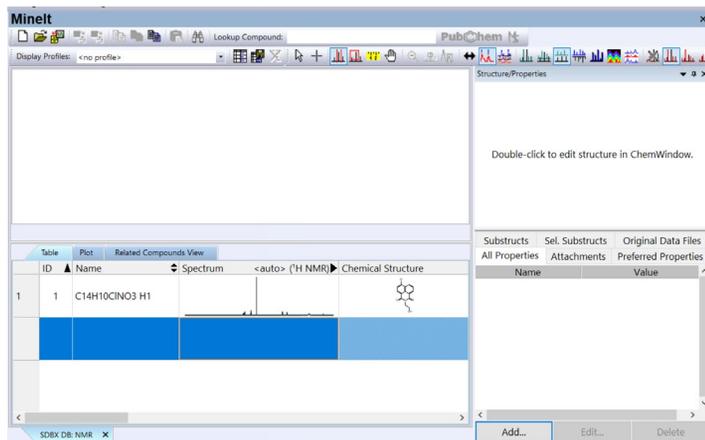
Generating a Database Record from NMR Report or Peak List

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.

Note: In **Minelt**, it is possible to create a database record using peak list information or peak information contained in an NMR report for decoupled data.

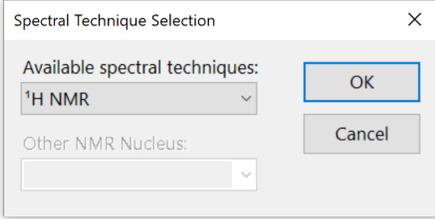
A blank record is displayed:



The screenshot shows the Minelt software interface. At the top, there is a toolbar with various icons and a search bar. Below the toolbar is a large empty area for displaying a structure or spectrum. On the right side, there is a 'Structure/Properties' panel with a 'Double-click to edit structure in ChemWindow.' instruction. Below this panel is a table with columns for 'Name' and 'Value'. At the bottom of the interface, there is a 'Table' section with a grid. The grid has columns for 'ID', 'Name', 'Spectrum', and 'Chemical Structure'. The first row is highlighted in blue and contains the text '1', 'C14H10ClNO3 H1', a spectrum plot, and a chemical structure. Below the grid are 'Add...', 'Edit...', and 'Delete' buttons.

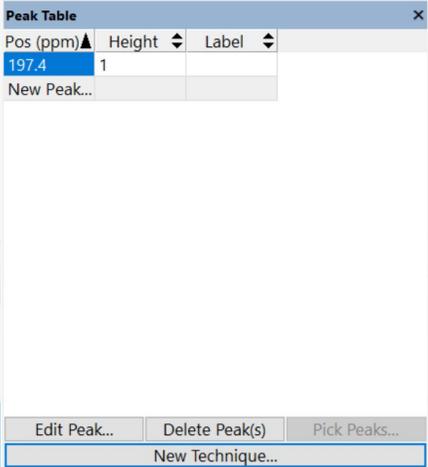
ID	Name	Spectrum	Chemical Structure
1	C14H10ClNO3 H1		

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	Change the Available spectral techniques to ^{13}C NMR using the drop-down menu, then click OK .	The Spectral Technuque Selection dialog is closed and the blank Peak Table remains visible.

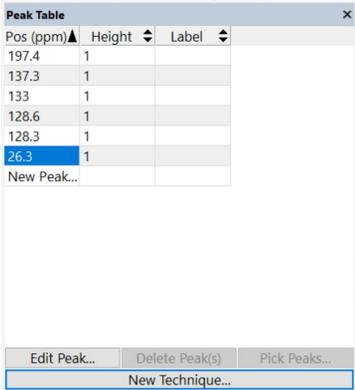
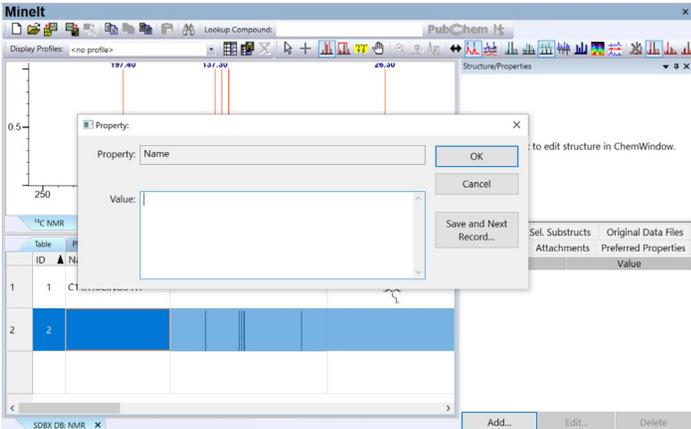
- 5 Double click on the cell that reads "New Peak" in the **Peak Table** and enter the value 197.4. Click on the white space below the filled rows to save the entry.

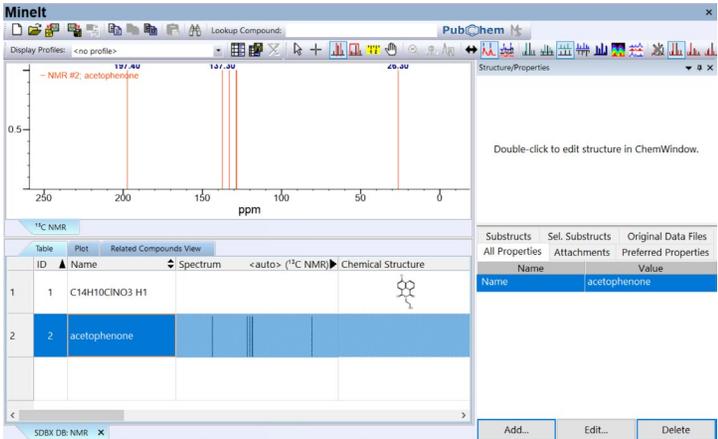
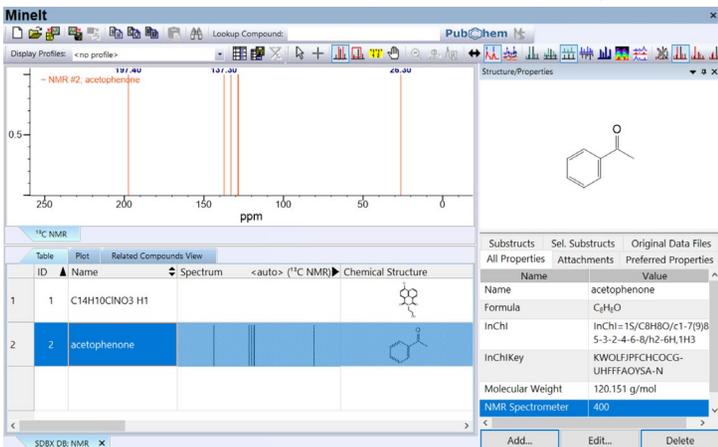
The **Peak Table** displays 197.4 as a peak in the first cell, with a default peak height of 1:

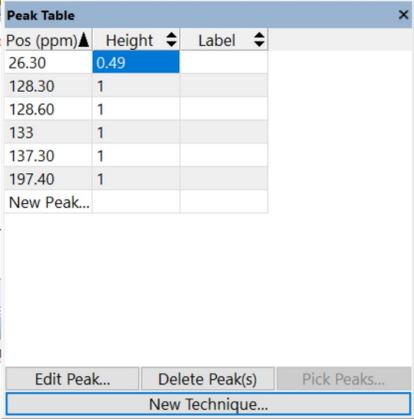
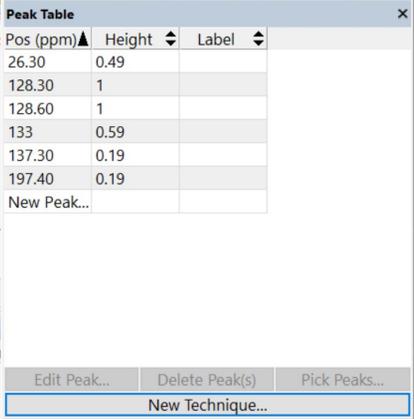


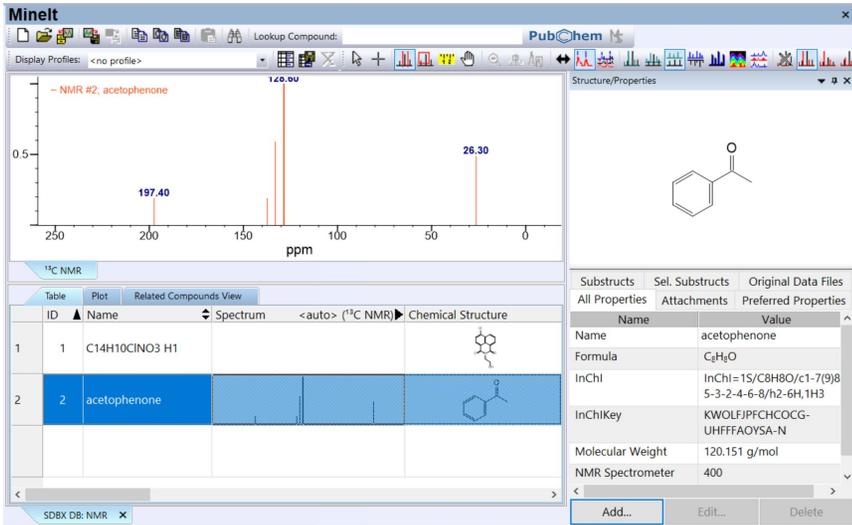
Pos (ppm)	Height	Label
197.4	1	
New Peak...		

Edit Peak... Delete Peak(s) Pick Peaks...
New Technique...

	Action	Result
6	<p>Repeat step 5 for each of the following peaks: 137.3, 133, 128.6, 128.3, 26.3. You can quickly begin a new row by clicking the down arrow on a keyboard between each value.</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 X on the Peak Table dialog to save the changes, then double click on row 2 in the Name column.</p>	<p>The Peak Table closes. Upon clicking the Name cell, Minelt refreshes and the generate 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:</p> 
9	Note: The chemical structure and NMR Spectrometer Frequency can be attached to the record applying skills previously reviewed in this document.	<p>The chemical structure and NMR spectrometer frequency information have been attached to the simulated spectrum:</p> 

	Action	Result																								
10	<p>Peak Height information can also be included in the simulation. Choose View > Windows/Tables > Peak Table. 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" data-bbox="659 386 1073 805"> <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" data-bbox="659 862 1073 1281"> <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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	Action	Result
12	<p>Click X on the Peak Table dialog to save the changes.</p> <p>Note: You may need to refresh the record by clicking on another record then returning to record #2.</p>	<p>The simulated spectrum is updated according to the peak height values:</p>  <p>The screenshot displays the Minelt software interface. At the top, there's a 'Minelt' window with a 'PubChem' logo and a 'Lookup Compound' field. Below this is a plot of the ¹³C NMR spectrum for acetophenone, showing three peaks at 197.40, 146.84, and 26.30 ppm. The x-axis is labeled 'ppm' and ranges from 250 to 0. The y-axis is labeled '0.5'. Below the plot is a table with columns for 'ID', 'Name', 'Spectrum', and 'Chemical Structure'. The table has two rows: row 1 for 'C14H10CINO3 H1' and row 2 for 'acetophenone'. The 'acetophenone' row is selected. To the right of the table is a 'Structure/Properties' panel showing the chemical structure of acetophenone and its properties: Name (acetophenone), Formula (C₈H₈O), InChI, InChIKey, Molecular Weight (120.151 g/mol), and NMR Spectrometer (400).</p>