




Multiplet Analysis

MestReNova: NMRPredict plugin

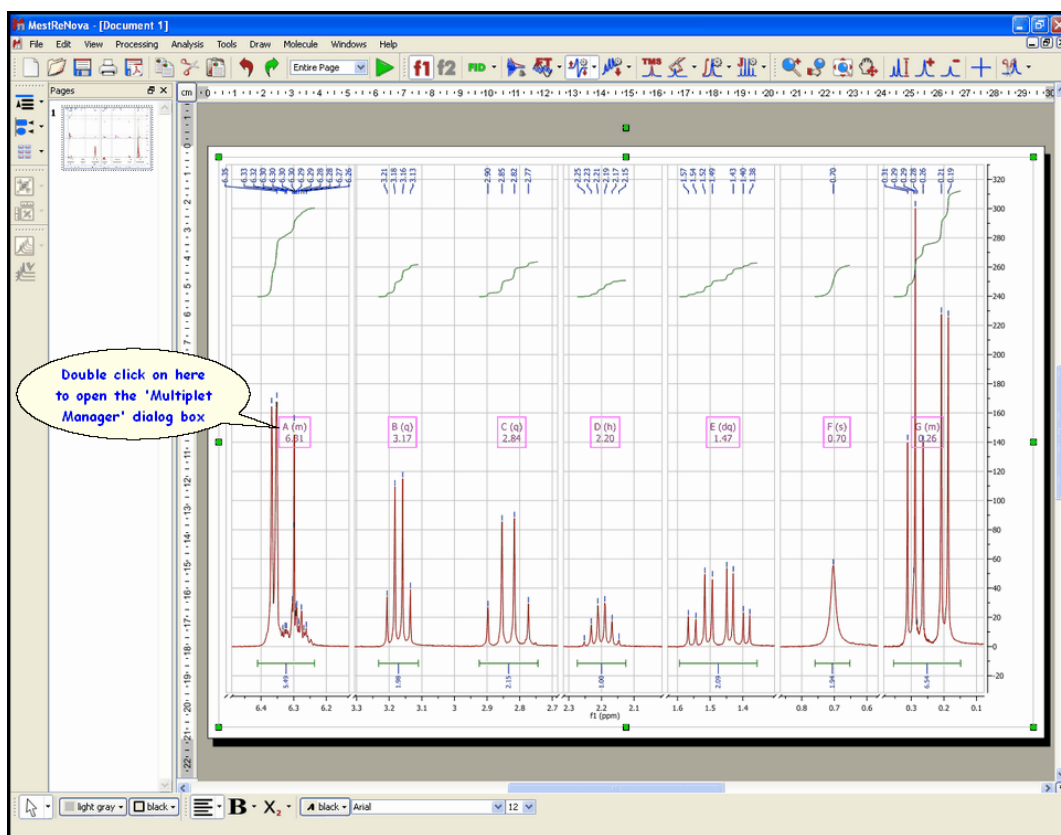
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Mnova incorporates an intuitive and powerful multiplet analyzer. The user will carry out an automatic multiplet analysis by clicking on its respective icon, placed on the analysis

toolbar menu , or by following the menu 'Analysis/Multiplets Analysis/Automatic'. Bear in mind that when you select an automatic multiplet analysis, Mnova will also apply automatic peak picking and integration, so you may need to set the sensitivity in both cases (or even the merging distance of the integrals) to obtain good results.

If you select a 'Manual Multiplet Analysis', please check also the sensitivity used for peak picking, or apply a 'Manual Peak Picking' to obtain a good result. You can also select the peaks by using the 'Peak by Peak' feature. Note that, by default, Mnova will find the peak top by using parabolic interpolation. To pick a peak at an arbitrary position (e.g. not at a local extreme or a shoulder), hold down <Shift> and click.


The user can also apply a manual integration followed by an automatic multiplet analysis. In the capture below, you will see the result of applying an automatic multiplet analysis:

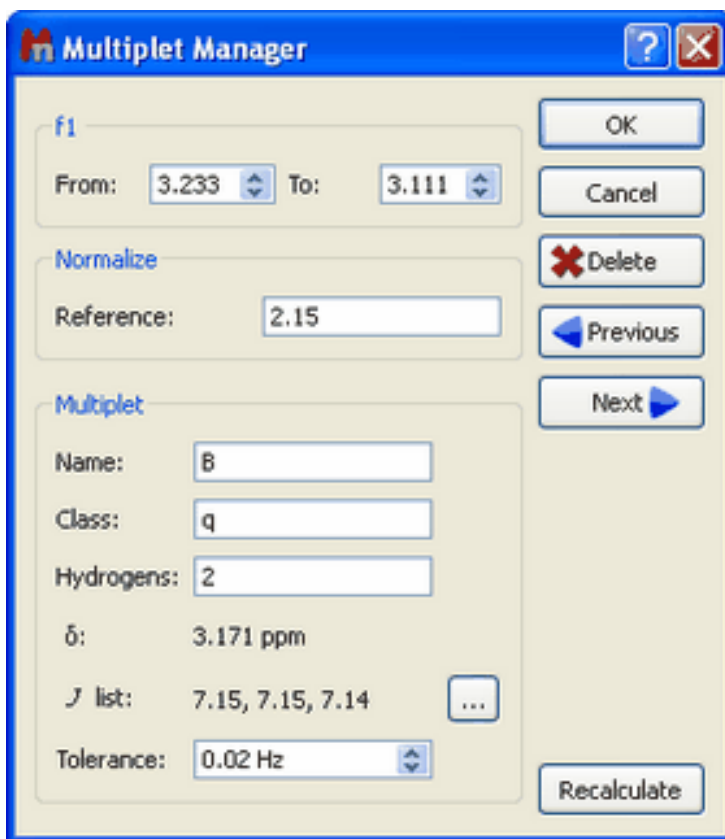


The user will also be able to set the multiplet parameters by double clicking on the magenta square containing the multiplet information. This will display the 'Multiplet




Manager' dialog box, where you will be able to modify the integral limits as well as to normalize its value. In this dialog box, you will also be able to change the multiplet parameters (name, class, number of hydrogens and the coupling constant tolerance limit). The number of hydrogens will be rounded (up or down) by default with respect to the integral value. Bear in mind that, if you change the integral value, the number of hydrogens of the multiplet will be altered, but this will not happen in the opposite way, that is, changes in the number of hydrogens of the multiplet will not affect the integral value.

As you see in the capture below, you can also delete a multiplet by clicking on the 'Delete' button  or navigate through multiplets by using the 'Previous' or 'Next' buttons.

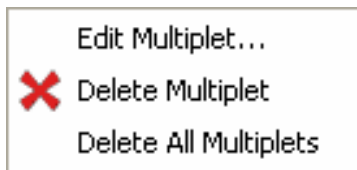


The 'Recalculate' button is used to obtain the new result after having made changes in the spectrum (as a 'refresh' button), or to recover the initial values (useful if you made changes in the 'Multiplet Manager' edit box but you do not remember them).

The user will also be able to add or delete a coupling constant by clicking on . After that, the 'J's Editor' dialog box will be displayed:



Likewise, if you press the right mouse button on a multiplet box, you will get a pop-up menu with the following options:

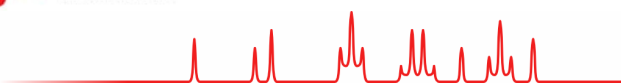


Edit Multiplet: displays the Multiplet Manager dialog box.

Delete Multiplet: deletes the current multiplet.

Delete All Multiplets: deletes all multiplets.

The user will be able to obtain the 'Multiplets' table by following the menu 'View/Tables'. The 'Multiplets' table includes information about the name (by default Mnova will have named the multiplets in alphabetical order, but the user is able to change this order in the 'Multiplet Manager'), the chemical shift (ppm), the range (ppm), number of hydrogens, integral value, type of multiplet and coupling constant values (Hz).






Multiplets ✖

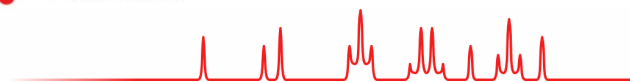
Report Copy Report Special Delete Setup

¹H NMR (500 MHz, CDCl₃) δ 7.70 (s, 1H), 6.56 (s, 1H), 5.77 (s, 1H), 4.20 – 3.50 (m, 13H), 3.12 – 2.90 (m, 3H), 2.71 (ddd, 1H), 2.63 – 2.48 (m, 2H), 2.23 (dt, 1H), 1.82 – 1.64 (m, 2H), 1.33 (d, 1H), 1.13 (dt, 1H).

	Name	Shift	Range	H's	Integral	Class	J's
1	A (s)	7.6975	7.76 .. 7.65	1	1.00	s	
2	B (s)	6.5637	6.62 .. 6.51	1	1.02	s	
3	C (s)	5.7654	5.83 .. 5.71	1	1.02	s	
4	D (m)	3.9183	4.20 .. 3.50	13	12.64	m	
5	E (m)	3.0073	3.12 .. 2.90	3	3.39	m	
6	F (ddd)	2.7134	2.76 .. 2.66	1	1.02	ddd	6.4423, 10.0493, 12.2939
7	G (m)	2.5504	2.63 .. 2.48	2	2.04	m	
8	H (dt)	2.2252	2.28 .. 2.18	1	0.99	dt	4.3184, 4.3184, 14.2714
9	I (m)	1.7355	1.82 .. 1.64	2	2.01	m	
10	J (d)	1.3299	1.41 .. 1.28	1	0.98	d	14.3154
11	K (dt)	1.1313	1.20 .. 1.09	1	1.02	dt	3.1299, 3.1299, 10.4290

The user can paste the 'Multiplets' table on the spectrum by clicking on the **'Report'** icon  and also can delete a multiplet from this table by using the **'Delete'** icon  when the undesired multiplet is highlighted.

Finally, the user will be able to obtain the multiplet report list by clicking on the **'Report Special'** icon . This will display the 'Multiplet Report' dialog box, which will allow the user to select the desired template (JACS, Royal Society of Chemistry and Angewandte).



1st: Click on the 'Report Special' icon

2nd: Select the desired 'Multiplet Report Template' and click on OK

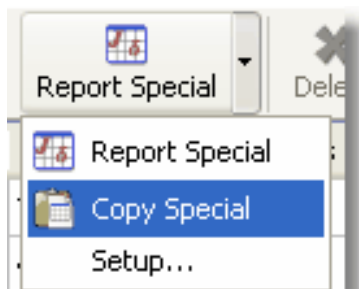
Parameter	Value
1 Title	j17pmquin
2 Origin	hova
3 Solvent	CDCl3
4 Pulse Sequence	h2prul
5 Acquisition Date	2007-10-22
6 Temperature	25.0
7 Number of Scans	200
8 Spectrometer Frequency	399.97
9 Spectral Width	8599.5
10 Lowest Frequency	5799.9
11 Nucleus	1H
12 Acquired Size	8959
13 Spectral Size	32768

Range	Normalized	Absolute
1 8.77 - 8.43	1.00	312539.10
2 8.07 - 7.83	1.02	317788.87
3 7.48 - 7.45	1.10	339626.84
4 7.28 - 7.13	2.72	899103.66
5 5.85 - 5.59	1.02	312535.66
6 5.51 - 5.46	1.14	353557.21
7 4.98 - 4.87	2.10	699443.84
8 3.91 - 3.82	3.39	1048807.84
9 3.43 - 3.30	2.16	665558.61
10 3.21 - 2.93	2.34	724253.91
11 2.69 - 2.58	2.29	706440.23
12 2.35 - 2.09	1.12	347817.41
13 1.98 - 1.85	2.08	645003.41
14 1.85 - 1.35	5.92	1827616.80

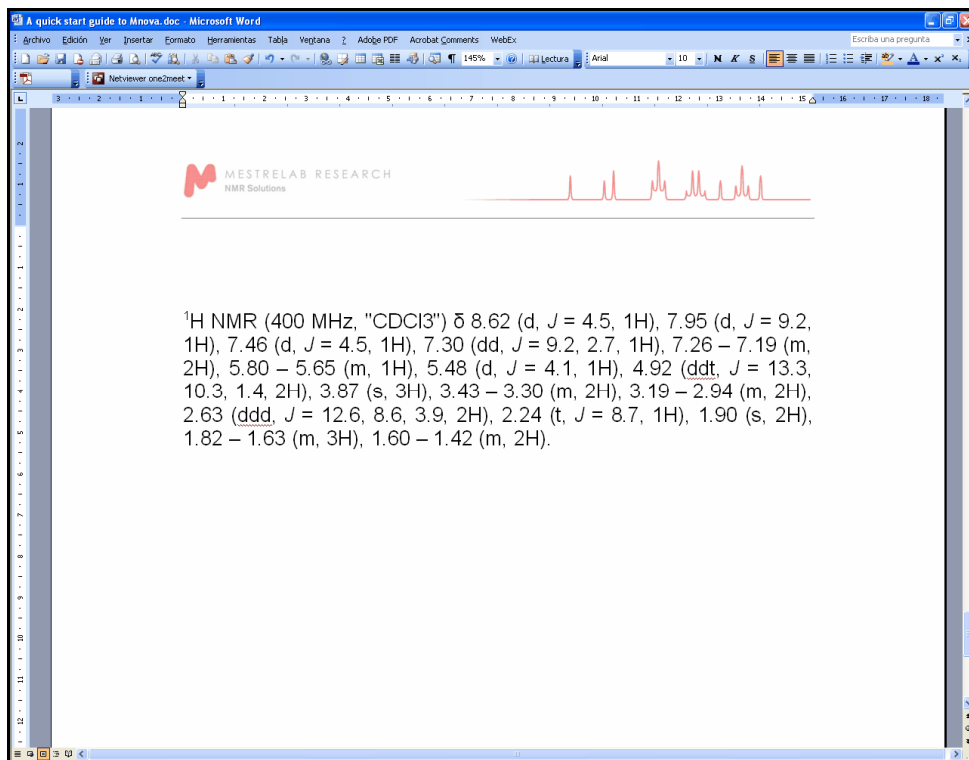
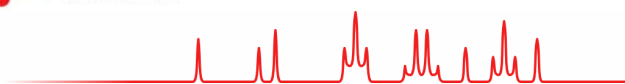
¹H NMR (400 MHz, CDCl₃) δ 8.62 (d, J = 4.5, 1H), 7.95 (d, J = 9.2, 1H), 7.46 (d, J = 4.5, 1H), 7.38 - 7.13 (m, 3H), 5.85 - 5.59 (m, 1H), 5.48 (d, J = 4.1, 1H), 4.92 (ddt, J = 13.3, 10.3, 1.4, 2H), 3.87 (s, 3H), 3.43 - 3.30 (m, 2H), 3.21 - 2.93 (m, 2H), 2.63 (ddd, J = 12.6, 8.6, 3.9, 2H), 2.35 - 2.09 (m, 1H), 1.90 (s, 2H), 1.85 - 1.35 (m, 6H).

After that, you will obtain in your spectrum the multiplet report as it is shown in the picture above.

The user will be able to copy the multiplet report to the clipboard by selecting 'Copy Special' on the 'Report Special' scroll bar menu:



And then paste the multiplet report on another document just by using Ctrl+V or Cmd+V.



The user will be able to change the multiplet report templates; by following the menu 'File/Edit Script' and opening the corresponding script file ('MultipletReporter.qs' in this case). Once the changes has been made, please save the new script and follow the menu 'View/Tables/Multiplets and select 'Setup' in the 'Report Special' scroll down menu to choose your new multiplet script.

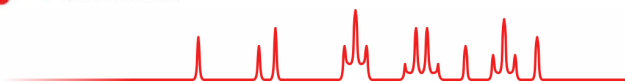
You will find below one of the most relevant parts of the multiplet script:

```
// This function defines JACS-like multiplet report.
// To customize report, edit this class or implement another one.
function JACSMultipletReporter()
{
    MultipletReporter.call(this);

    this.onlyElementName=false;
    // Define font size and font family
    this.font = "<font style=\"font-size: 10pt; font-family: Times New Roman\">";

    this.nucleusTemplate="%1";
    // Report header. %1 will be replaced with nucleusString, %2 with frequency, %3 with
    solvent
    this.header = "%1 NMR (%2 MHz, %3) &delta; ";

    // Multiplet templates. %1 - delta, %2 - category, %3 - nH
    this.reportRange = true; // set to true to get multiplet range instead of delta.
    this.withoutJsTemplate = "%1 (%2, %3H)"; // multiplet template without J's
```



```

this.withJsTemplate = " %1 (%2, %4, %3H)"; // multiplet template with J's
this.rangeTemplate = "%1 &ndash; %2";

// J's list template. %1 - list of J's
this.jListTemplate = "<i>J</i> = %1";

this.jPrecision = 1; // J's precision
this.deltaPrecision = 2; // delta precision
this.mSeparator = ", "; // multiplet separator
this.jSeparator = ", "; // J's separator

this.start = this.font;
this.end = "</font>";
}

JACSMultipletReporter.prototype = new MultipletReporter();
JACSMultipletReporter.prototype.toString = function() { return
"JACSMultipletReporter()"; }

(...)

```

The user will be able to change the multiplet report template to obtain the desired multiplet report; for example:

this.onlyElementName=false; changing false with true, we will obtain only the element name without the atomic mass (For example: H, C instead of ¹H, ¹³C).

The function: **this.font = "**"; will define the font size and the font family of the multiplet report.

The line: **this.header = "%1 NMR (%2 MHz, %3) δ "**; is used to print the header of the report, where %1 will be the nucleus (H or C), %2 the frequency of the spectrometer (in MHz), and %3 the solvent, followed by a delta symbol (δ). For example: "¹H NMR (500 MHz, CDCl₃) δ ".

The sentence: **this.reportRange = true** is used to obtain the multiplet range instead of the chemical shift.

The functions: **this.withoutJsTemplate = " %1 (%2, %3H)"** and **this.withJsTemplate = " %1 (%2, %4, %3H)"** are used to customize the appearance of the multiplet report by changing the positions of %1, %2, %3H, or %4 (where, %1 means: chemical shift; %2 means: type of multiplet (s, d, t, etc); %3H means: number of hydrogens and %4 means the coupling constant value). As you can see, the first line shows a multiplet without coupling constants, (while the last line shows a multiplet with coupling constants).

So, if you need to obtain something like this (japanese format):

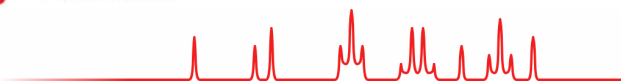
1H NMR (300 MHz, Solvent) δ ppm 6.43-6.22 (1 H, m), 3.17 (1 H, q, J = 7.15 Hz) etc...

You should modify both lines, as you can see below:

```

this.withoutJsTemplate = "%1 (%3H, %2)";
this.withJsTemplate = "%1 (%3H, %2, %4)";

```



If you prefer to obtain something like this:

1H NMR (300 MHz, Solvent) δ ppm 1.23 (d, $J = 1.2$ Hz, 3 H), etc...

Just replace the original lines with:

```
this.withoutJsTemplate = "%1 (%2, %3H)";  
this.withJsTemplate = "%1 (%2, %4, %3H)";
```

To obtain the coupling constant symbol in normal instead of *italic*, just modify the script by removing the italic format (`<i>J</i>`). If you prefer to obtain it in **"bold"** just type:

```
this.jListTemplate = "<b>J</b> = %1";
```

The following paragraph will be used to customize the appearance of the coupling constants list:

```
this.jPrecision = 1; // J's precision  
this.deltaPrecision = 2; // delta precision  
this.mSeparator = ", "; // multiplet  
separator  
this.jSeparator = ", "; // J's separator
```

The first line is used for the precision of the coupling constants values, the second will be used for the precision of the chemical shift and the remaining two lines will print the separation between the multiplets and the coupling constants values.

If you need to obtain the coupling constants in descending order, replace **'true'** with **'false'** in the following line:

```
var jList = new JList(multiplet.jList());  
jList.sort(true);
```

If you want to obtain the multiplet chemical shifts in ascending order, just replace the **'false'** with **'true'** in the script:

```
var multiplets = new Multiplets(spectrum.multiplets()); // get  
multiplets from spectrum  
jList.sort(true);
```

To obtain the multiplet range in ascending order, just replace the rangeMin with rangeMax in the below line of the script:

```
shiftStr = this.rangeTemplate.argDec(multiplet.rangeMax, 0, 'f',  
this.deltaPrecision).argDec(multiplet.rangeMin, 0, 'f', this.deltaPrecision);
```

Please make sure that, once the changes has been made, you save the new script and follow the menu 'View/Tables/Multiplets and select 'Setup' in the 'Report Special' scroll down menu to choose your new multiplet script.