



Mestrelab Research

chemistry software solutions

**Mnova meets NMReData: automation
workflows and new opportunities**

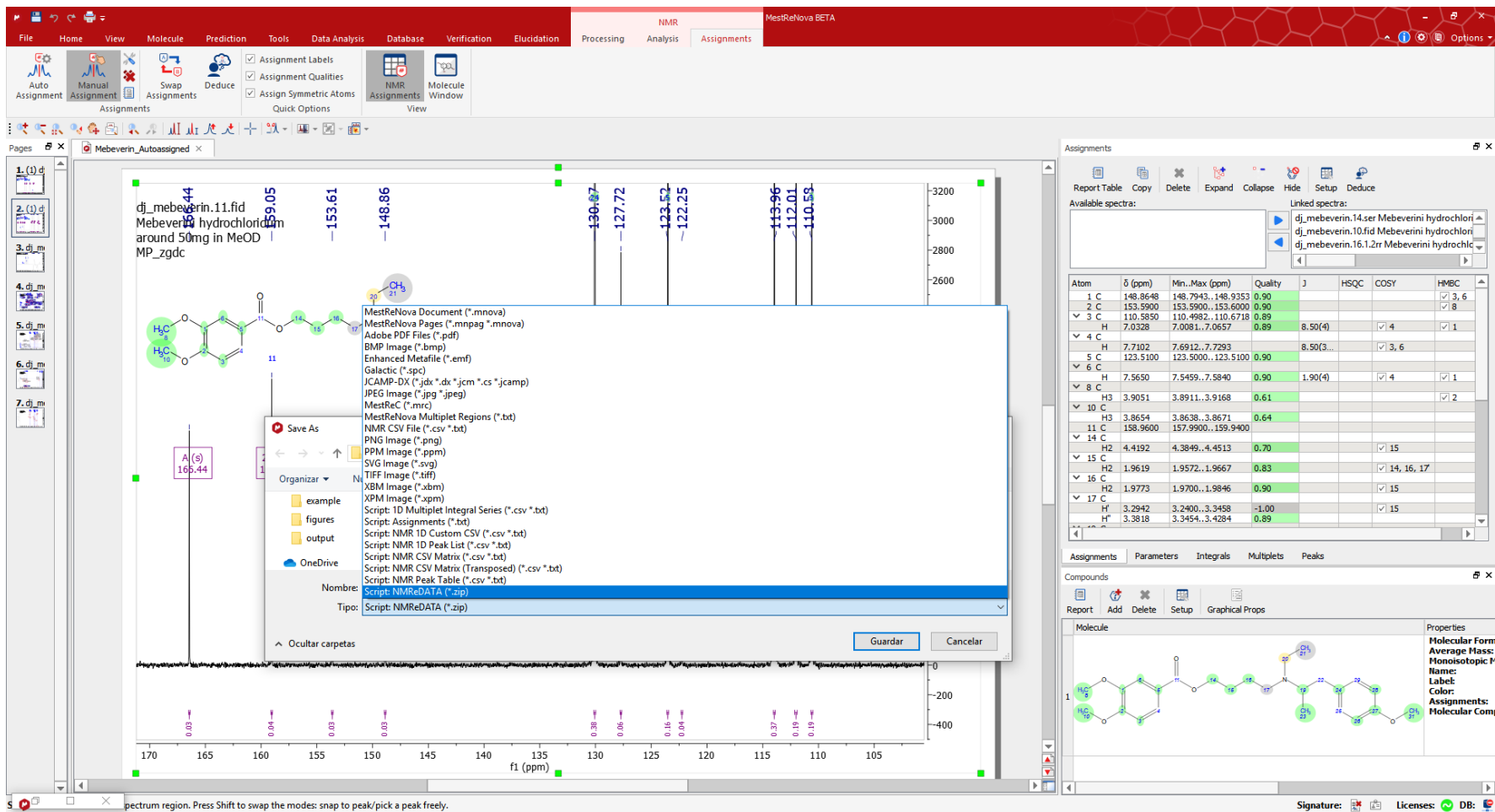
NMReData Symposium

Porto, Portugal, 26 September 2019

Outline

- NMReData implementation in Mnova
 - Export
 - Import
- NMReData in Mnova Automations

- Standard in Mnova 14.1 when a Mnova file has a molecule
- Save As -> Script: NMReData (*.zip)



The screenshot displays the Mnova 14.1 software interface. The main window shows an NMR spectrum with several peaks labeled with their chemical shifts: 165.44, 159.05, 153.61, 148.86, 136.87, 127.72, 123.52, 122.25, 113.96, 112.01, and 110.58. A chemical structure of Mebeverin hydrochloride is visible on the left. A 'Save As' dialog box is open, showing a list of file types. The 'Script: NMReData (*.zip)' option is selected. The 'Assignments' panel on the right shows a table of peak assignments.

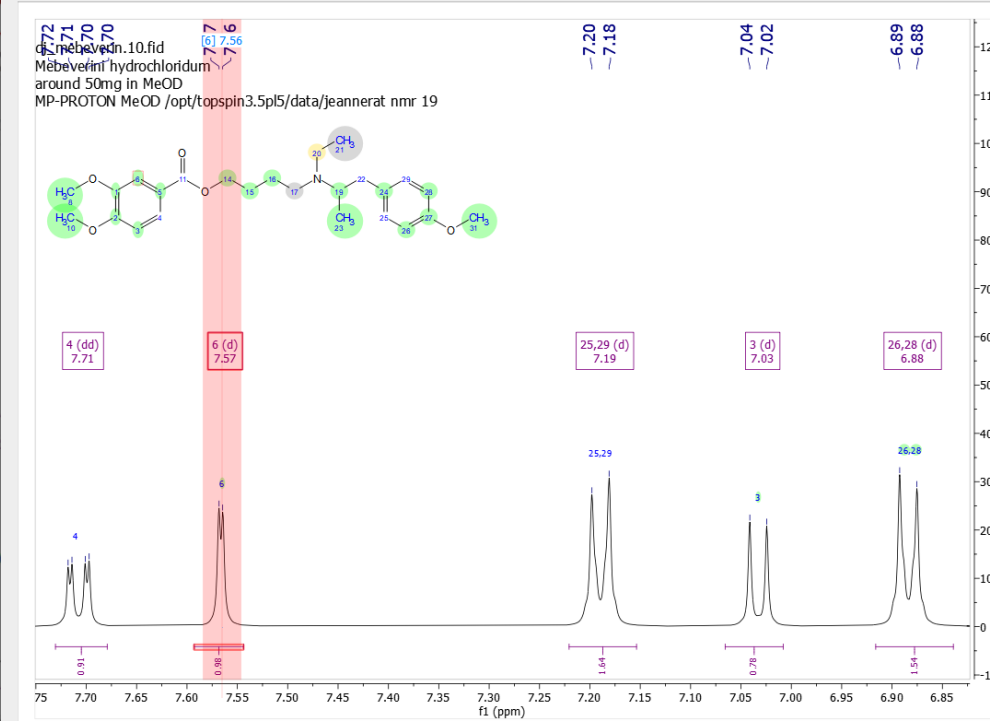
Atom	δ (ppm)	Min..Max (ppm)	Quality	J	HSQC	COSY	HMBC
1 C	148.8648	148.7943..148.9353	0.90				✓ 3, 6
2 C	153.5900	153.5900..153.6000	0.90				✓ 8
3 C	110.5850	110.4982..110.6718	0.89				
H	7.0328	7.0081..7.0657	0.89	8.50(4)	✓ 4		✓ 1
4 C							
H	7.7102	7.6912..7.7293	0.90	8.50(3...)	✓ 3, 6		
5 C	123.5100	123.5000..123.5100	0.90				
6 C							
H	7.5650	7.5459..7.5840	0.90	1.90(4)	✓ 4		✓ 1
8 C							
H3	3.9051	3.8911..3.9168	0.61				✓ 2
10 C							
H3	3.8654	3.8638..3.8671	0.64				
11 C	158.9600	157.9900..159.9400					
14 C							
H2	4.4192	4.3849..4.4513	0.70		✓ 15		
15 C							
H2	1.9619	1.9572..1.9667	0.83		✓ 14, 16, 17		
16 C							
H2	1.9773	1.9700..1.9846	0.90		✓ 15		
17 C							
H	3.2942	3.2400..3.3458	-1.00		✓ 15		
H'	3.3818	3.3454..3.4284	0.89				

- Assignments and J-Couplings will be exported as in assignment table
- Unassigned J-couplings will not be exported in J-Tag

```
> <NMREDATA_ASSIGNMENT>
1, 148.8648, 1\
2, 153.5900, 2\
3, 110.5850, 3\
H3, 7.0328, H3\
H4, 7.7102, H4\
5, 123.5100, 5\
H6, 7.5650, H6\
H8, 3.9051, H8\
H10, 3.8654, H10\
11, 158.9600, 11\
H14, 4.4192, H14\
H15, 1.9619, H15\
H16, 1.9773, H16\
H17', 3.2942, H17\
H17'', 3.3818, H17\
H19, 3.7040, H19\
H20', 3.3264, H20\
H20'', 3.3344, H20\
H21, 1.4238, H21\
H22, 3.1919, H22\
H23, 1.2485, H23\
24, 130.0500, 24\
H25, 7.1893, H25\
H26, 6.8820, H26\
27, 159.0400, 27\
H28, 6.8820, H28\
H29, 7.1893, H29\
H31, 3.7829, H31\

> <NMREDATA_J>
H3, H4, 8.50, nb=3\

> <NMREDATA_1D_1H>
```



Mebeverin hydrochloride
around 50mg in MeOD
MP-PROTON MeOD /opt/topspin3.5pl5/data/jeannerat nmr 19

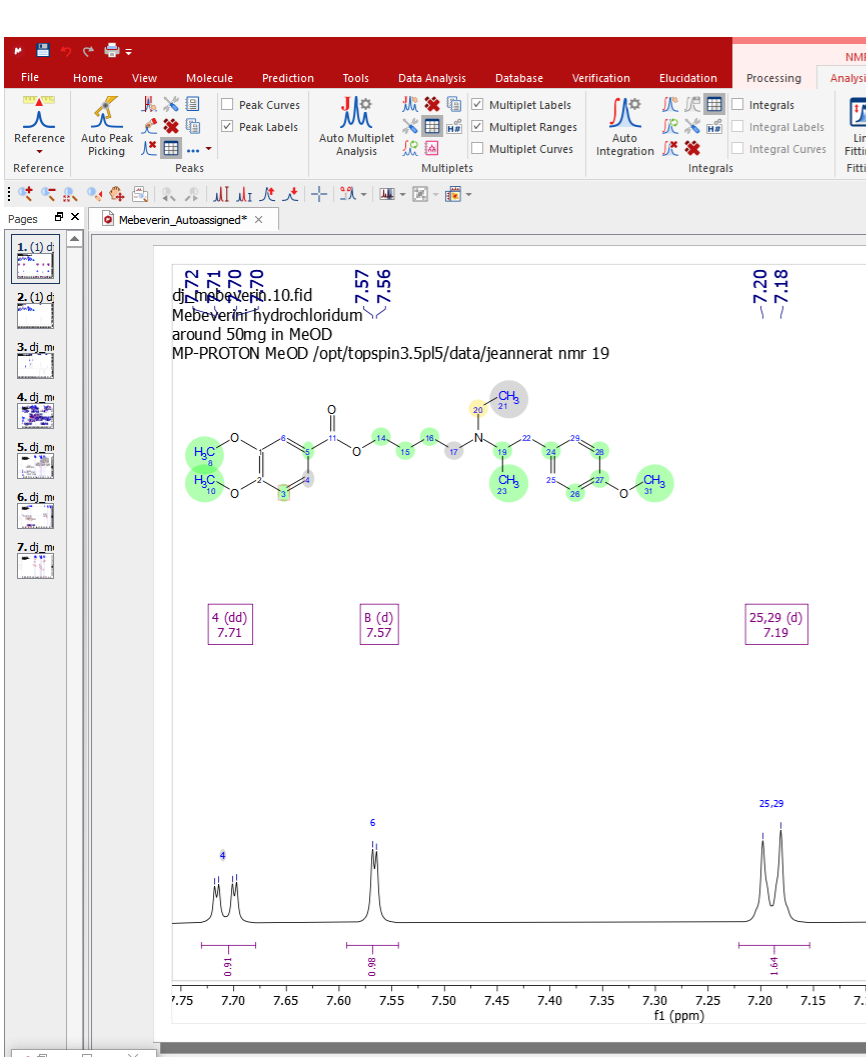
Assignments

Report Table Copy Delete

Available spectra: Linked spectra:

Atom	δ (ppm)	J
1 C	148.8648	
2 C	153.5900	
3 C	110.5850	
H	7.0328	8.50(4)
4 C		
H	7.7102	8.50(3)
5 C	123.5100	
6 C		
H	7.5650	1.90(?)
8 C		
H3	3.9051	
H3	3.8654	
11 C	158.9600	
14 C		

- Multiplets or Peaks must be assigned to be exported as such in Spectrum Tags

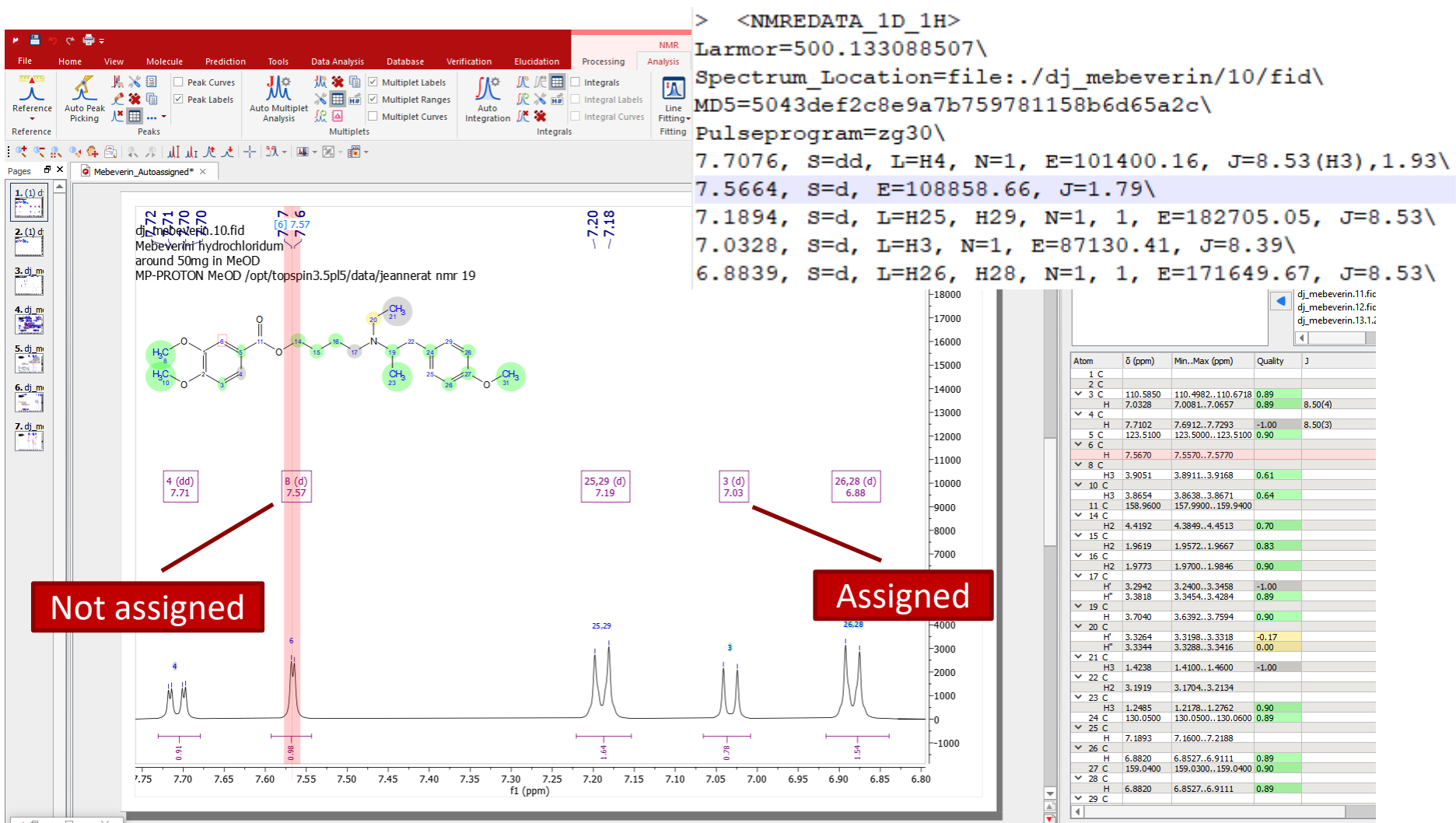


Mebeverin hydrochloride
around 50mg in MeOD
MP-PROTON MeOD /opt/topspin3.5pl5/data/jeannerat nmr 19

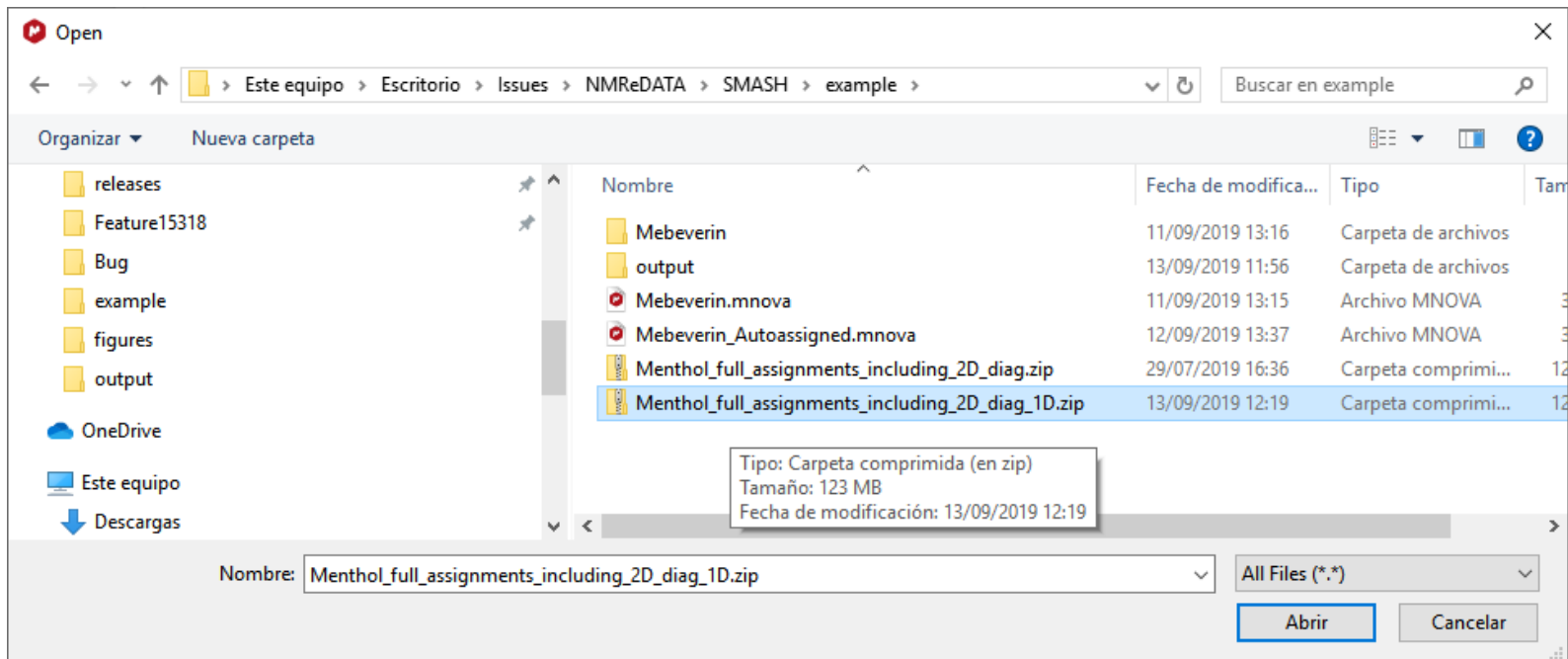
```
> <NMREDATA_1D_1H>
Larmor=500.133088507\
Spectrum_Location=file:./dj_mebeverin/10/fid\
MD5=5043def2c8e9a7b759781158b6d65a2c\
Pulseprogram=zg30\
7.7076, s=dd, L=H4, N=1, E=101400.16, J=8.53(H3),1.93\
7.5664, s=d, E=108858.66, J=1.79\
7.1894, s=d, L=H25, H29, N=1, 1, E=182705.05, J=8.53\
7.0328, s=d, L=H3, N=1, E=87130.41, J=8.39\
6.8839, s=d, L=H26, H28, N=1, 1, E=171649.67, J=8.53\
```

Atom	δ (ppm)	Min..Max (ppm)	Quality	J
1 C				
2 C				
3 C	110.5850	110.4982..110.6718	0.89	
H	7.0328	7.0081..7.0657	0.89	8.50(4)
4 C				
H	7.7102	7.6912..7.7293	-1.00	8.50(3)
5 C	123.5100	123.5000..123.5100	0.90	
6 C				
H	7.5670	7.5570..7.5770		
8 C				
H3	3.9051	3.8911..3.9168	0.61	
10 C				
H3	3.8654	3.8638..3.8671	0.64	
11 C	158.9600	157.9900..159.9400		
14 C				
H2	4.4192	4.3849..4.4513	0.70	
15 C				
H2	1.9619	1.9572..1.9667	0.83	
16 C				
H2	1.9773	1.9700..1.9846	0.90	
17 C				
H	3.2942	3.2400..3.3458	-1.00	
H	3.3818	3.3454..3.4284	0.89	
19 C				
H	3.7040	3.6392..3.7594	0.90	
20 C				
H	3.3264	3.3198..3.3318	-0.17	
H	3.3344	3.3288..3.3416	0.00	
21 C				
H3	1.4238	1.4100..1.4600	-1.00	
22 C				
H2	3.1919	3.1704..3.2134		
23 C				
H3	1.2485	1.2178..1.2762	0.90	
24 C	130.0500	130.0500..130.0600	0.89	
25 C				
H	7.1893	7.1600..7.2188		
26 C				
H	6.8820	6.8527..6.9111	0.89	
27 C	159.0400	159.0300..159.0400	0.90	
28 C				
H	6.8820	6.8527..6.9111	0.89	
29 C				

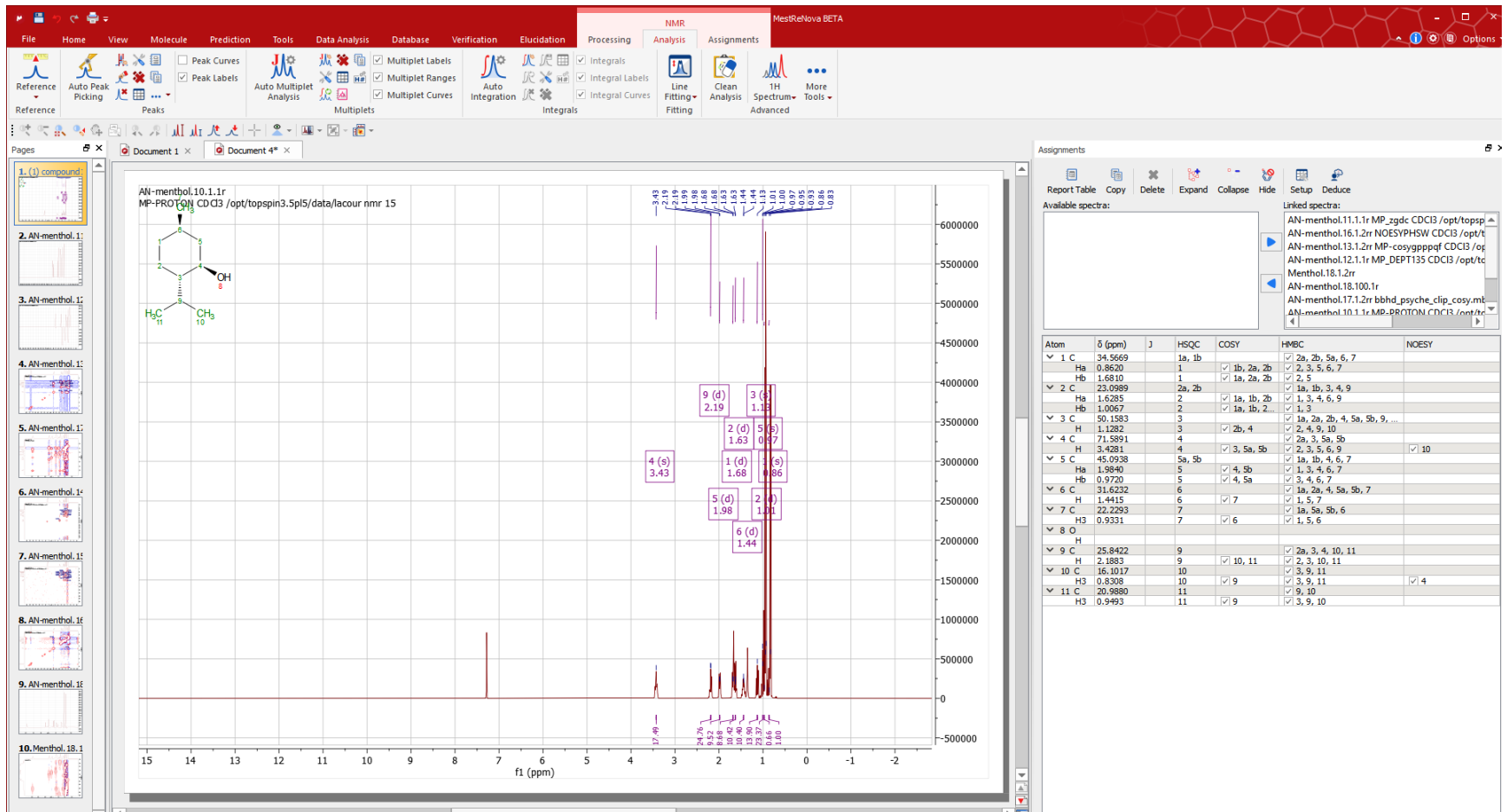
- Multiplets or Peaks must be assigned to be exported as such in Spectrum Tags



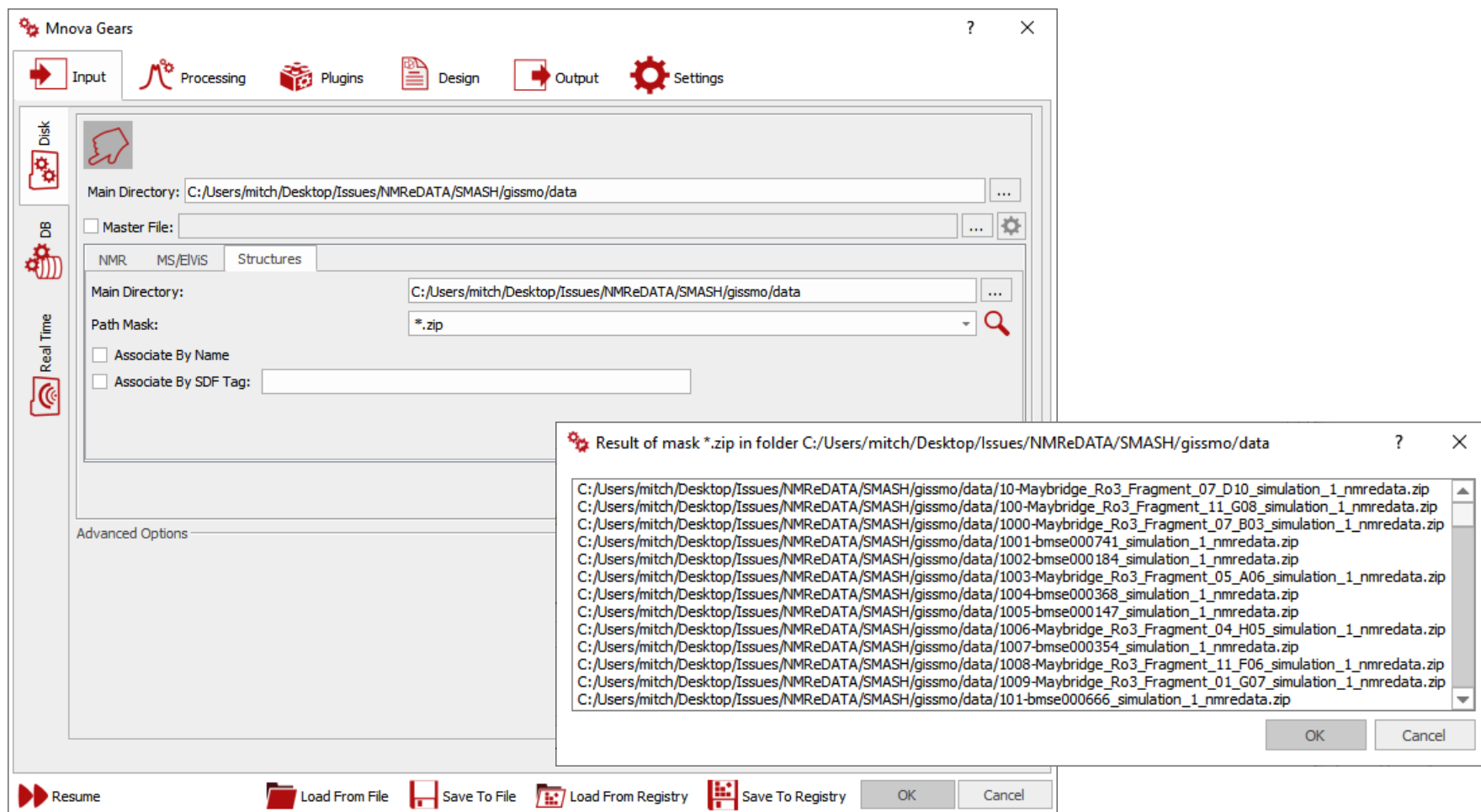
- Standard input in Mnova 14.1 from **.zip** File or **Folder**
- Following operations will import NMReData:
 - File Open
 - Drag & Drop
 - `serialization.open(aPath)`



- A new Mnova Document is created, with molecule, spectra, and all imported information, e.g. Assignments, Couplings, Multiplets, Peaks, 2D- Correlations

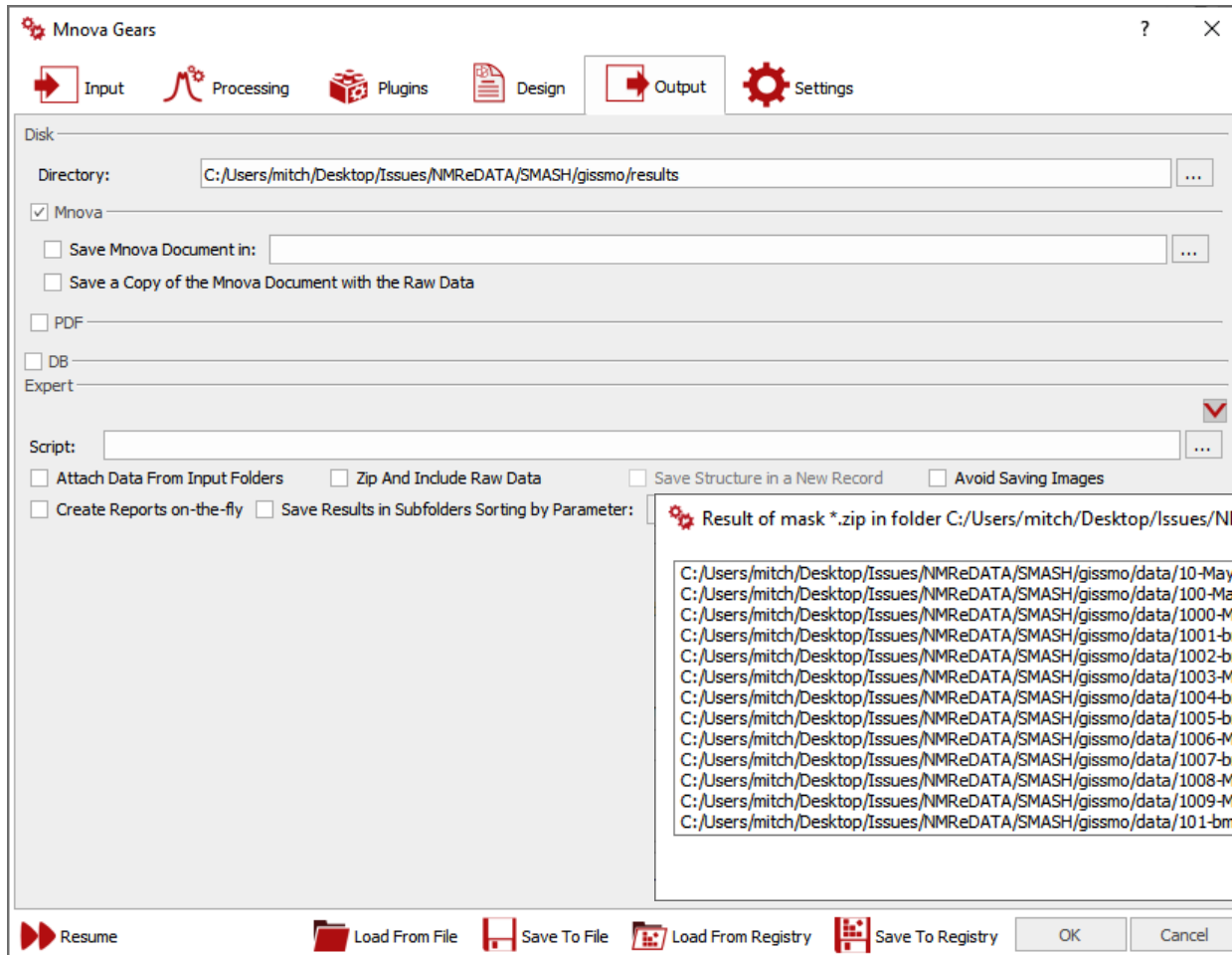


- NMReData is a standard input/output option, it can be used for all Mnova automations, e.g. Mgears:



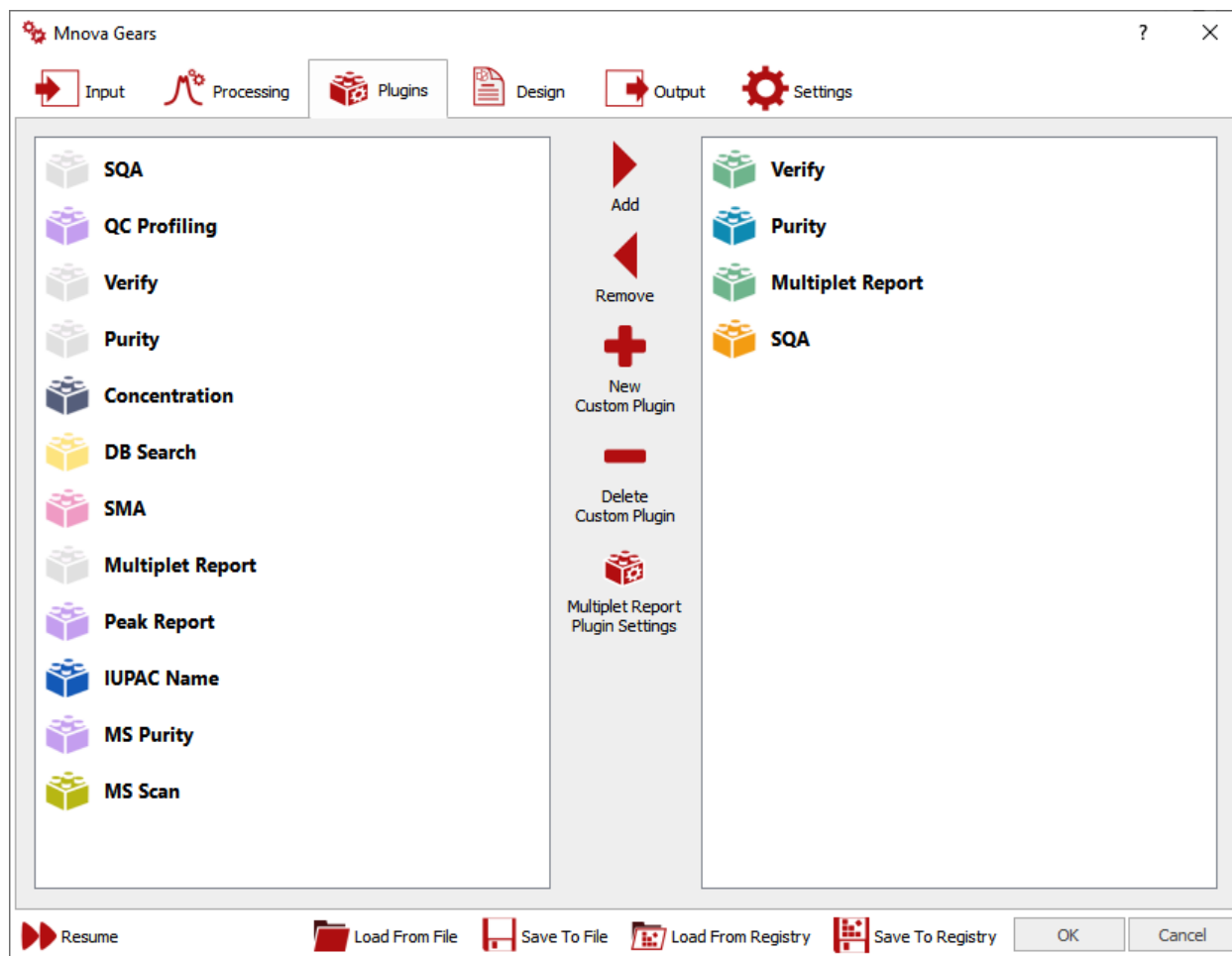
The screenshot displays the Mnova Gears application window. The main interface is divided into several sections: a top toolbar with 'Input', 'Processing', 'Plugins', 'Design', 'Output', and 'Settings'; a left sidebar with 'Disk', 'DB', and 'Real Time' icons; and a central workspace. The 'Disk' section is active, showing a 'Main Directory' field with the path `C:/Users/mitch/Desktop/Issues/NMReDATA/SMASH/gissmo/data`. Below this, there are tabs for 'NMR', 'MS/EIVIS', and 'Structures'. The 'NMR' tab is selected, and it shows a 'Main Directory' field with the same path, a 'Path Mask' field with the value `*.zip`, and checkboxes for 'Associate By Name' and 'Associate By SDF Tag'. A search icon is visible next to the 'Path Mask' field. A modal window titled 'Result of mask *.zip in folder C:/Users/mitch/Desktop/Issues/NMReDATA/SMASH/gissmo/data' is open in the foreground, displaying a list of 15 file paths that match the mask. The paths are all zip files located in the same directory as the main window. The modal window has 'OK' and 'Cancel' buttons at the bottom. At the bottom of the Mnova Gears window, there is a toolbar with 'Resume', 'Load From File', 'Save To File', 'Load From Registry', 'Save To Registry', 'OK', and 'Cancel' buttons.

- NMReData is a standard input/output option, it can be used for all Mnova automations, e.g. Mgears:



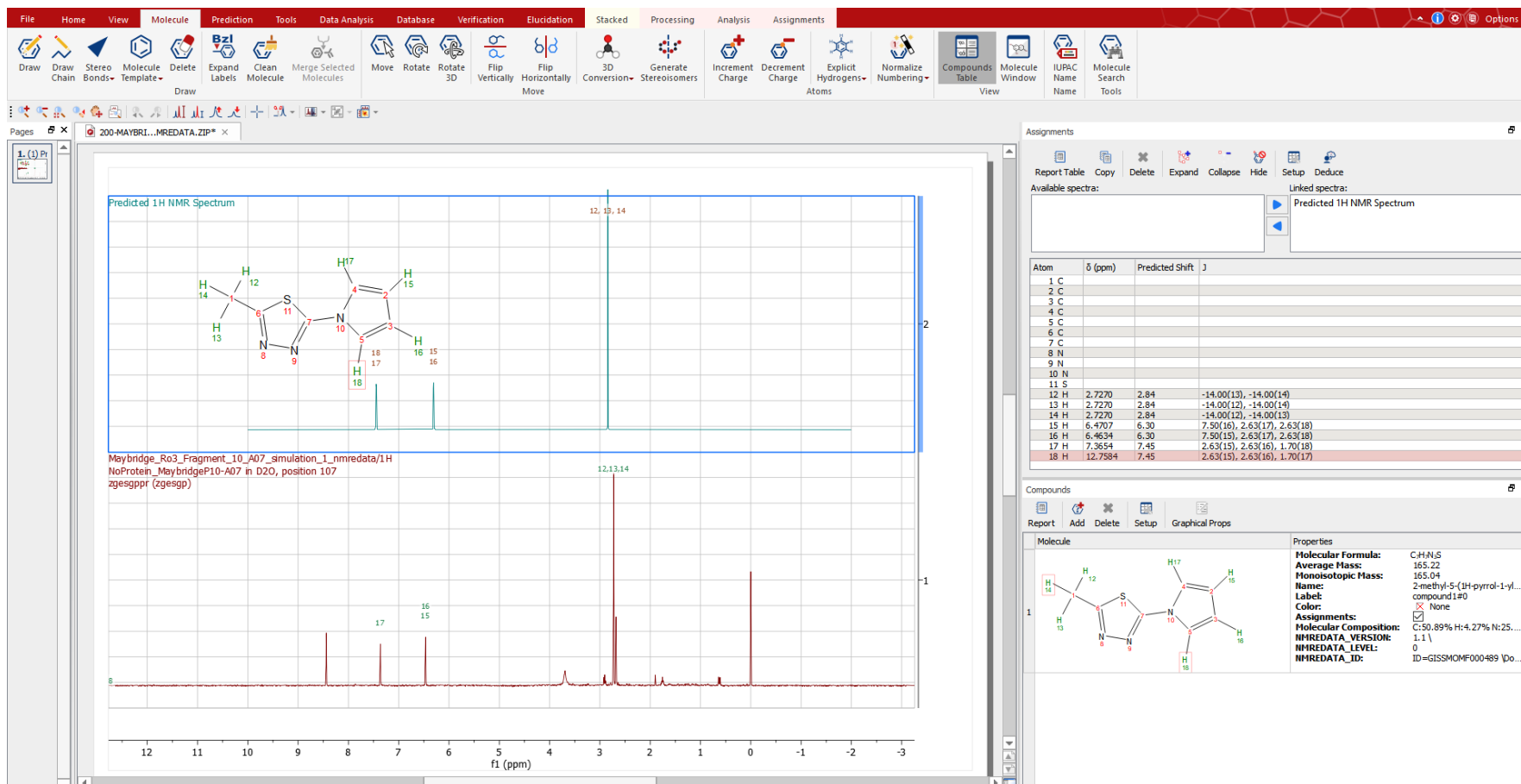
Converts all NMReData files in a folder in Mnova documents

Mgears would allow to perform a great number of analysis using NMReData as Input or Output



- Data Quality Assessments
- Structure verification
- Quantitation
- **Any evaluation that can use NMReData as input/output**

- GISSMO database: <http://gissmo.nmrfam.wisc.edu/>



The screenshot displays the Mnova software interface. The main window shows a predicted 1H NMR spectrum with a chemical structure of a pyrazole derivative. The spectrum has peaks at 12.13, 13.14, 16, 15, and 17 ppm. The assignment table on the right provides the following data:

Atom	δ (ppm)	Predicted Shift	J
1 C			
2 C			
3 C			
4 C			
5 C			
6 C			
7 C			
8 N			
9 N			
10 N			
11 S			
12 H	2.7270	2.84	-14.00(13), -14.00(14)
13 H	2.7270	2.84	-14.00(12), -14.00(14)
14 H	2.7270	2.84	-14.00(12), -14.00(13)
15 H	6.4707	6.30	7.50(16), 2.63(17), 2.63(18)
16 H	6.4634	6.30	7.50(15), 2.63(17), 2.63(18)
17 H	7.3654	7.45	2.63(15), 2.63(16), 1.70(18)
18 H	12.7584	7.45	2.63(15), 2.63(16), 1.70(17)

The bottom right panel shows the compound's properties:

- Molecular Formula:** C₄H₄N₂S
- Average Mass:** 165.22
- Monoisotopic Mass:** 165.04
- Name:** 2-methyl-5-(1H-pyrazol-1-yl)pyrazole
- Label:** compound1#0
- Color:** None
- Assignments:** None
- Molecular Composition:** C:50.89% H:4.27% N:25.11%
- NMReDATA_VERSION:** 1-1 \
- NMReDATA_LEVEL:** 0
- NMReDATA_ID:** ID=GISSMOMF000489 | Do...

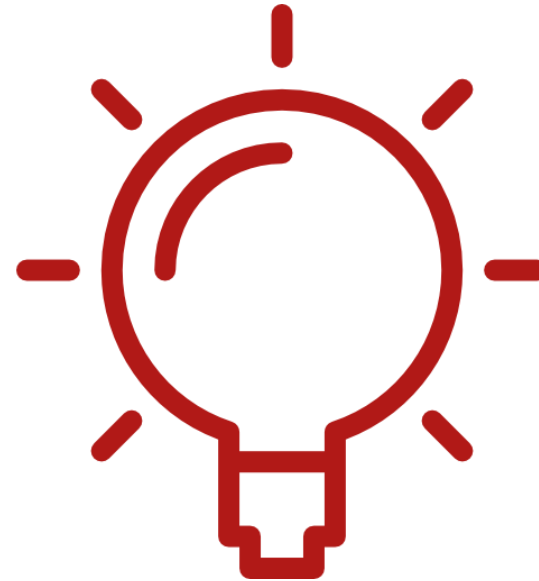
Comparison with Mnova predicted shifts helps with the detection of errors in assignments (or predictions)

Conclusions

- Mnova 14.1 supports NMReData as input and output
- Great potential for automated solutions

Acknowledgments

- Mnova Team in Santiago de Compostela
 - Maruxa Sordo, Isaac Iglesias, Carlos Cobas
 - Eva Muñoz, Gustavo Prado



Questions Time!

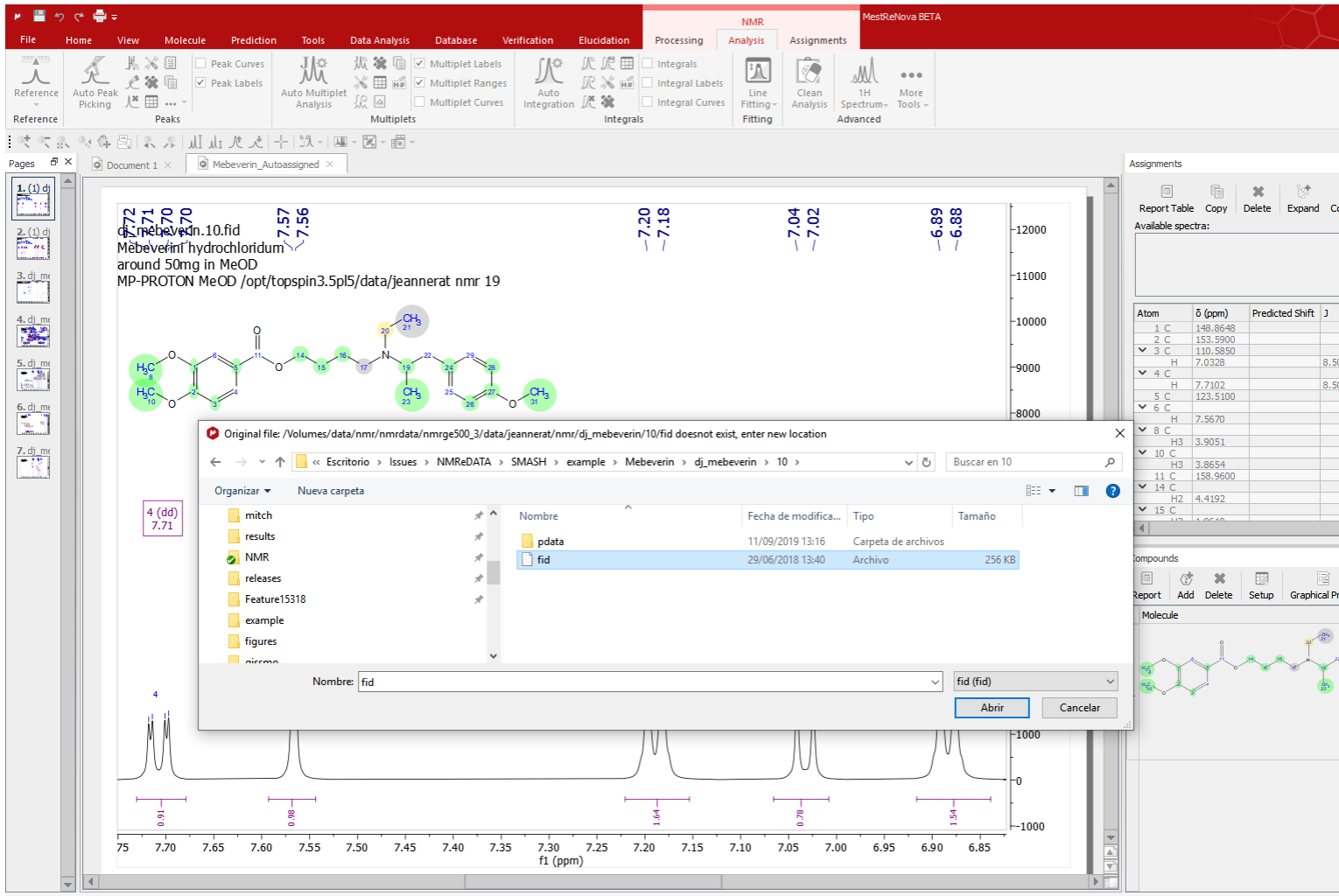


Mestrelab Research

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*thank
you*

If original data files are “Not found”, Mnova will ask for their location



The screenshot shows the Mnova software interface. The main window displays an NMR spectrum with a chemical structure of Mebeverin hydrochloride overlaid. The spectrum shows several peaks with chemical shifts labeled: 7.72, 7.71, 7.70, 7.57, 7.56, 7.20, 7.18, 7.04, 7.02, 6.89, and 6.88 ppm. The x-axis is labeled 'f1 (ppm)' and ranges from 7.5 to 6.85. The y-axis represents intensity, ranging from -1000 to 12000.

A dialog box is open in the foreground, titled "Original file: /Volumes/data/nmr/nmrdata/nmrge500_3/data/jeannerat/nmr/dj_mebeverin/10/fid doesnot exist, enter new location". The dialog shows a file explorer view of the directory: `Escritorio > Issues > NMRdata > SMASH > example > Mebeverin > dj_mebeverin > 10 >`. The file list shows a folder named 'fid' with a size of 256 KB. The 'Nombre:' field contains 'fid' and the 'Nombre:' dropdown menu is set to 'fid (fid)'. The 'Abrir' (Open) button is highlighted.

On the right side of the interface, there is an 'Assignments' panel with a table of atom data:

Atom	δ (ppm)	Predicted Shift	J
1 C	148.8648		
2 C	153.5900		
3 C	110.5850		
4 C	7.0328	8.50	
H	7.7102	8.50	
5 C	123.5100		
6 C			
H	7.5670		
8 C			
H3	3.9051		
10 C			
H3	3.8654		
11 C	158.9600		
14 C			
H2	4.4192		
15 C			
H3	1.0616		