Mestrelab Research

chemistry software solutions

Mnova meets NMReData: automation workflows and new opportunities

NMReData Symposium

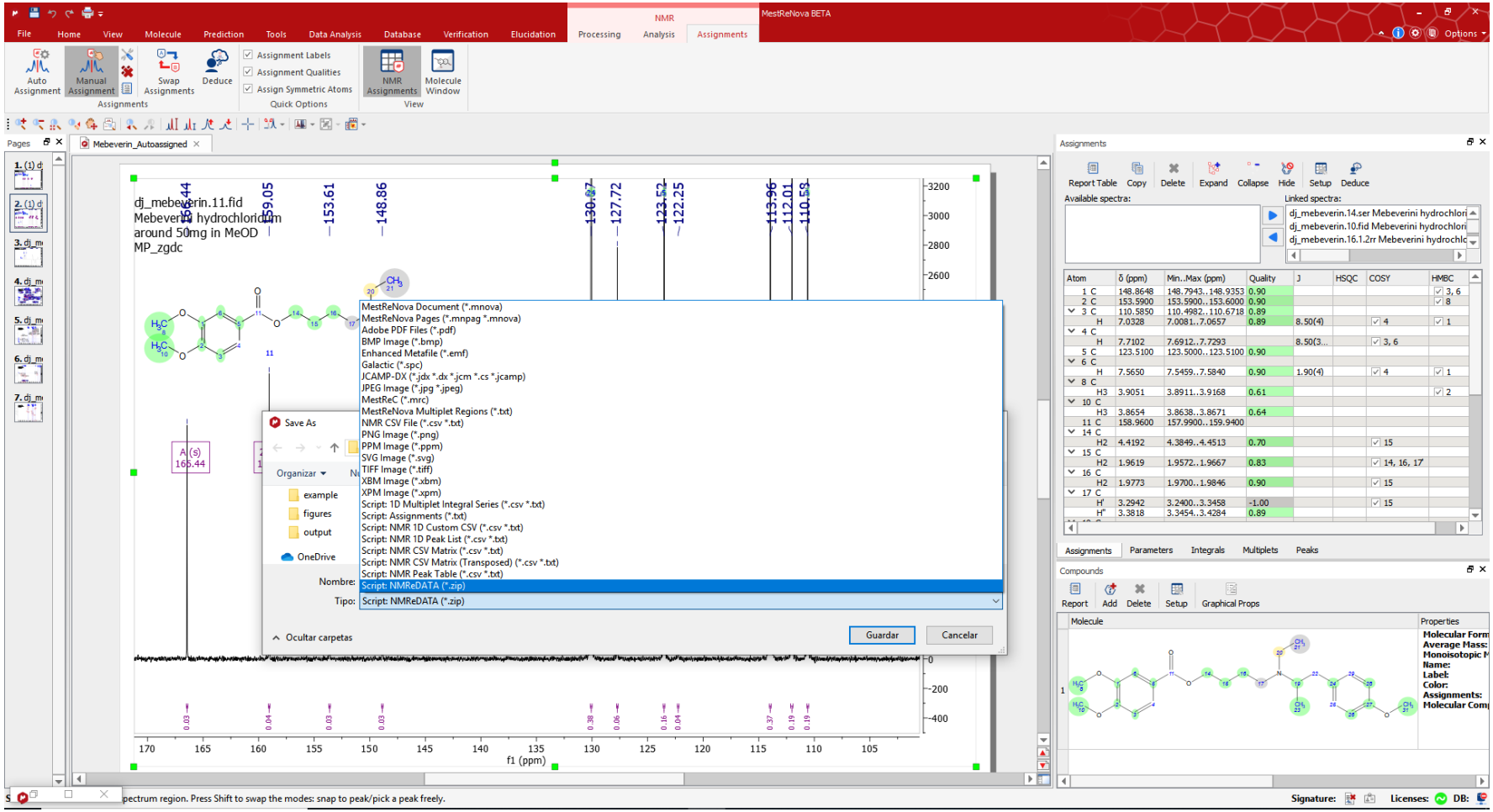
Porto, Portugal, 26 September 2019

Outline

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

NMReData Export from Mnova

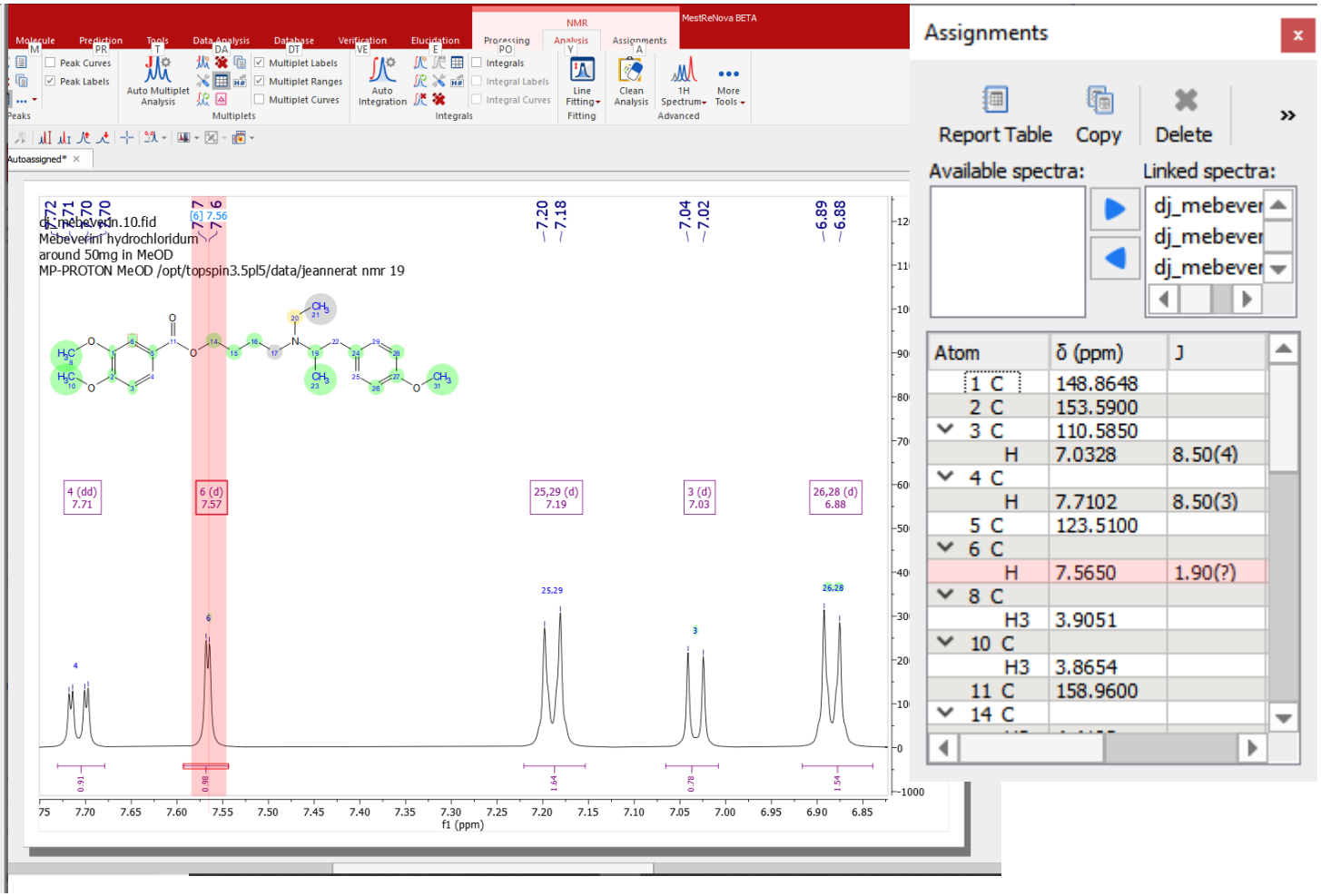
- Standard in Mnova 14.1 when a Mnova file has a molecule
- Save As -> Script: NMReData (*.zip)



NMReData Export from Mnova
Assignment and J Tags

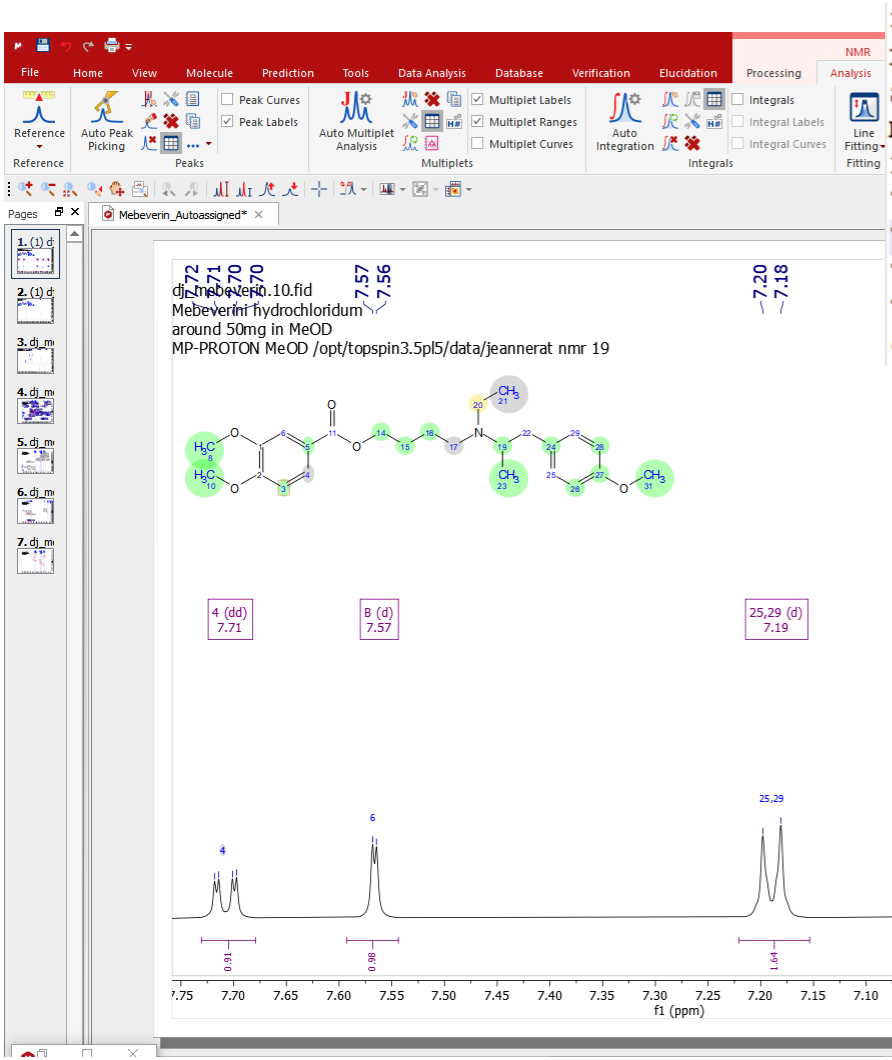
- Assignments and J-Couplings will be exported as in assignment table
- Unassigned J-couplings will not be exported in J-Tag

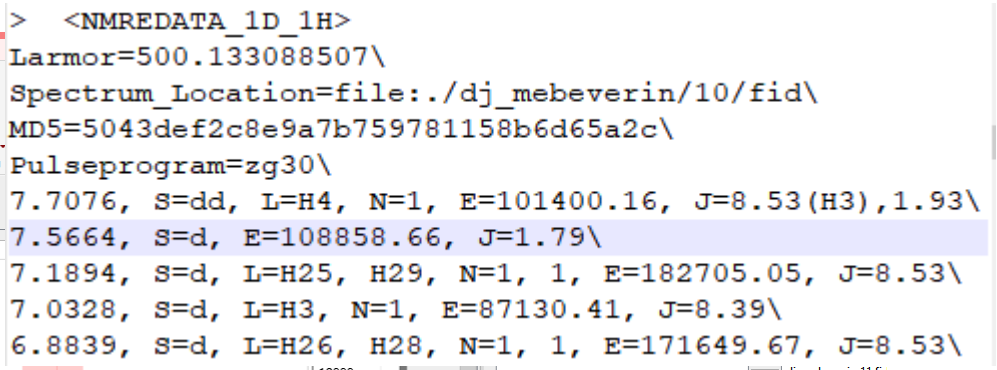
```
>  <NMREDATA_ASSIGNMENT>
1, 148.8648, 1\
2, 153.5900, 2\
3, 110.5850, 3\
H3, 7.0328, H3\
H4, 7.7102, H4\
5, 123.5100, 5\
H6, 7.5650, H6\
H8, 3.9051, H8\
H10, 3.8654, H10\
11, 158.9600, 11\
H14, 4.4192, H14\
H15, 1.9619, H15\
H16, 1.9773, H16\
H17', 3.2942, H17\
H17'', 3.3818, H17\
H19, 3.7040, H19\
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>
```

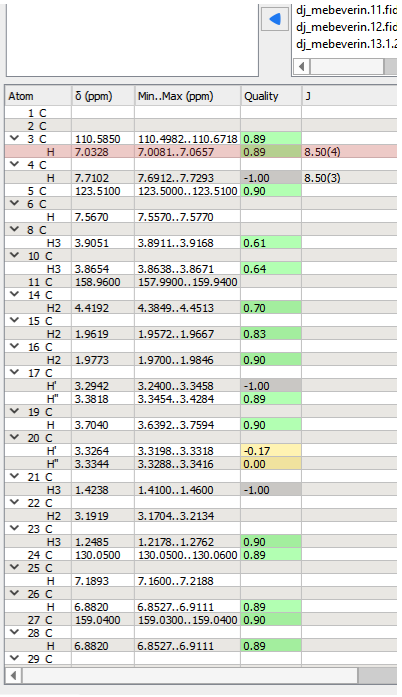


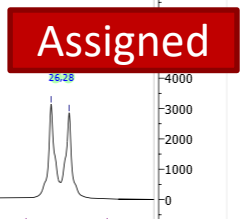
Export of NMReData Spectra TAGs

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





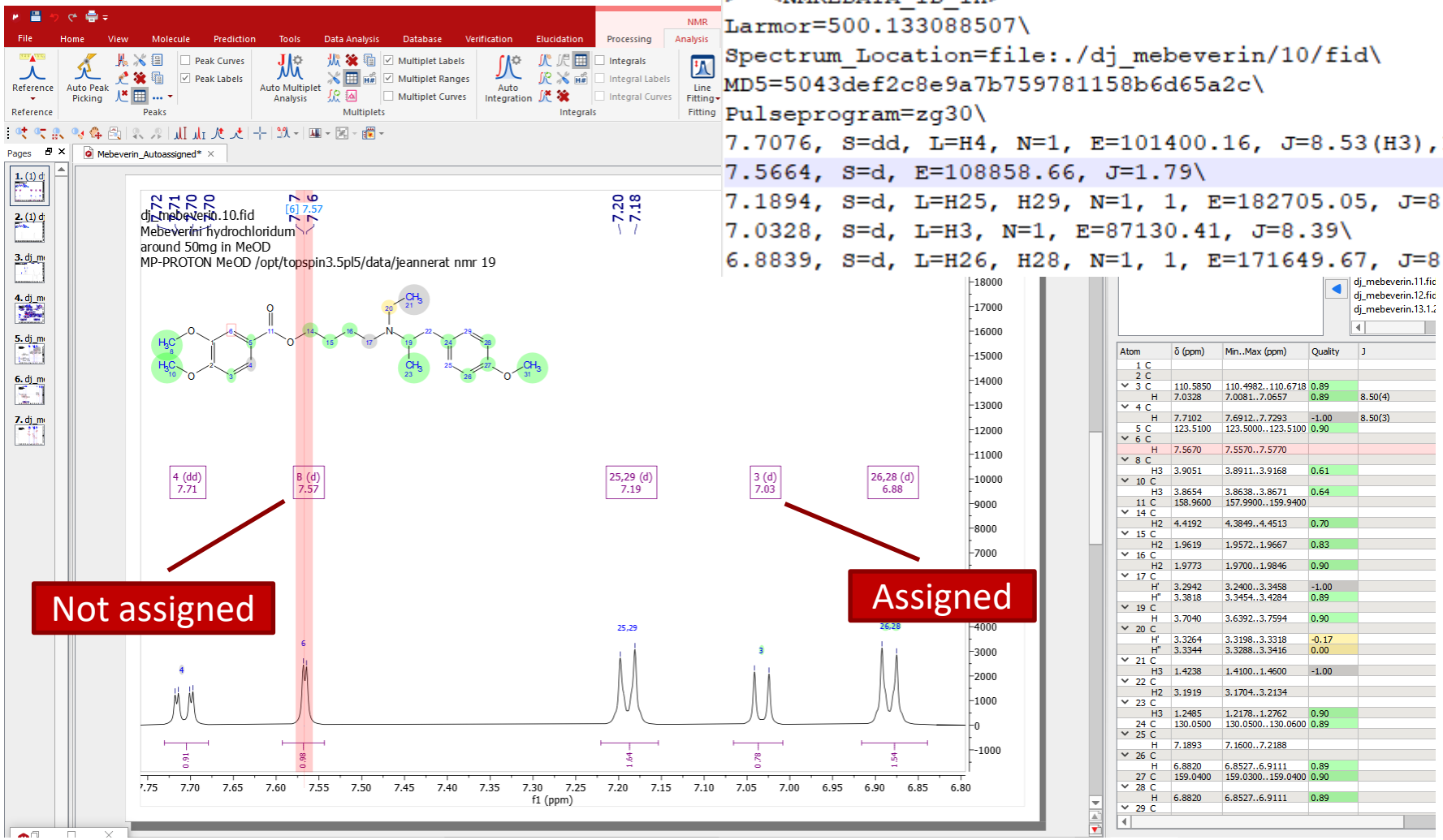




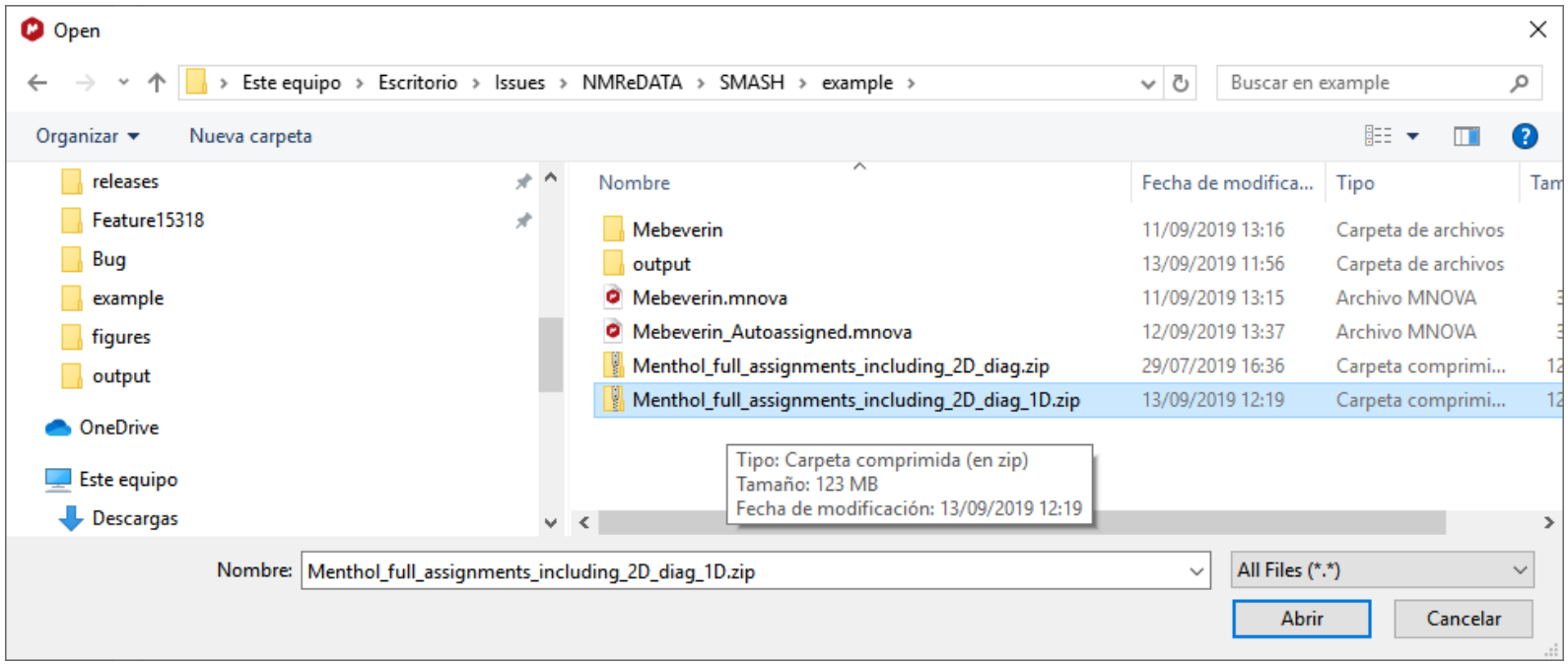
Export of NMReData Spectra TAGs

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

```
>  <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\
```

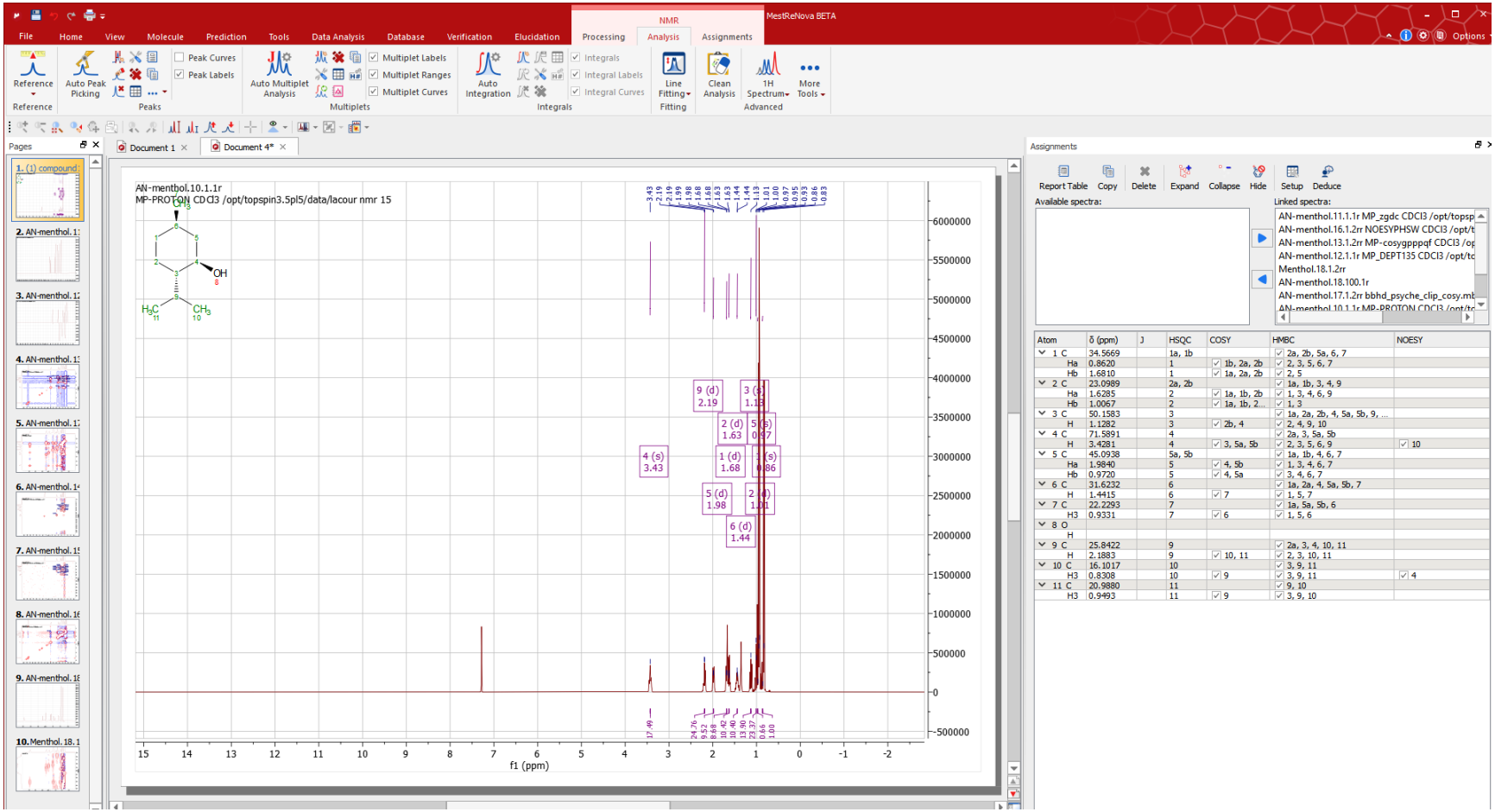


- Standard input in Mnova 14.1 from **.zip** File or **Folder**
- Following operations will import NMReData:
  - File Open
  - Drag & Drop
  - serialization.open(aPath)

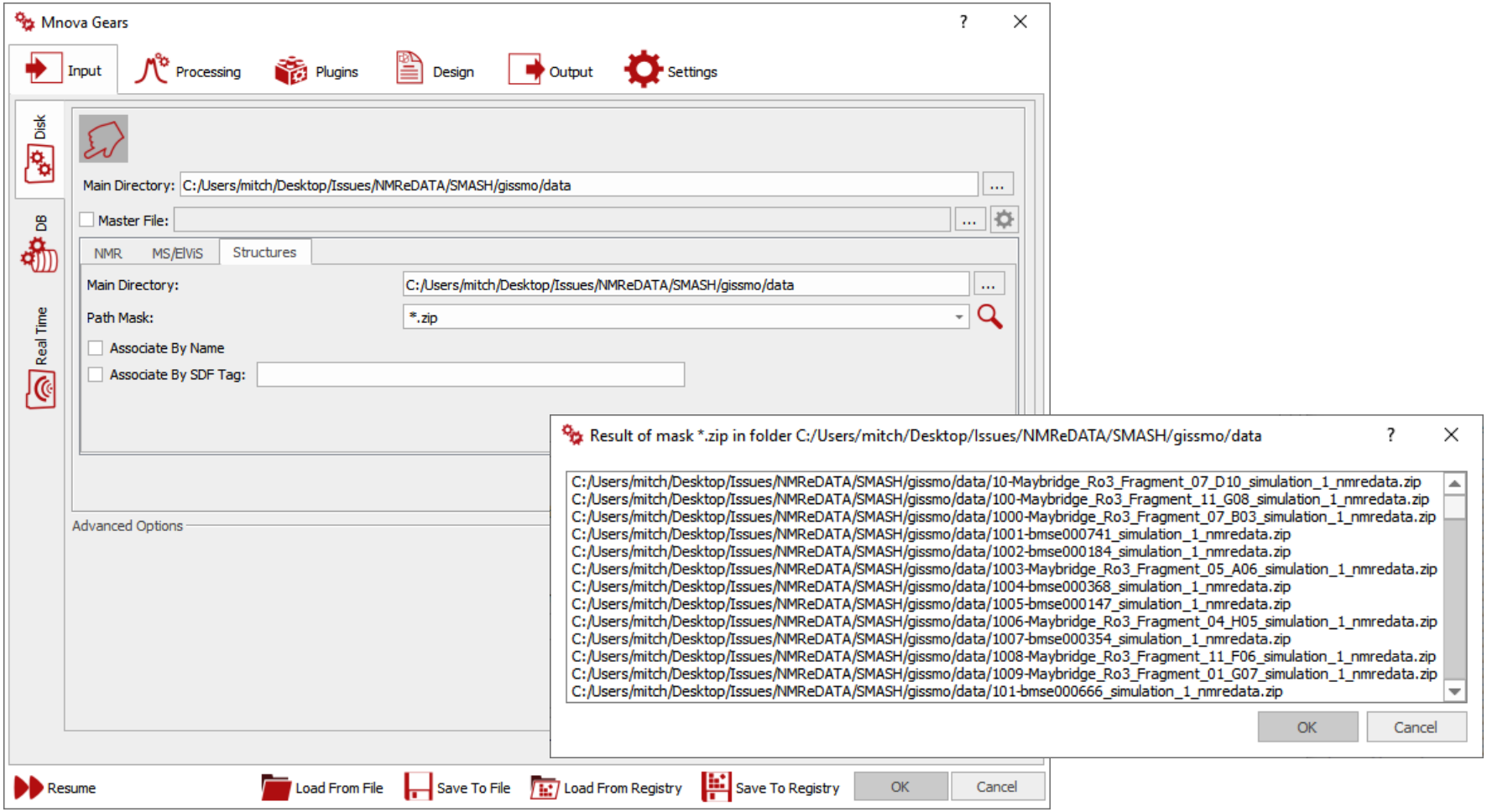


Import of NMReData

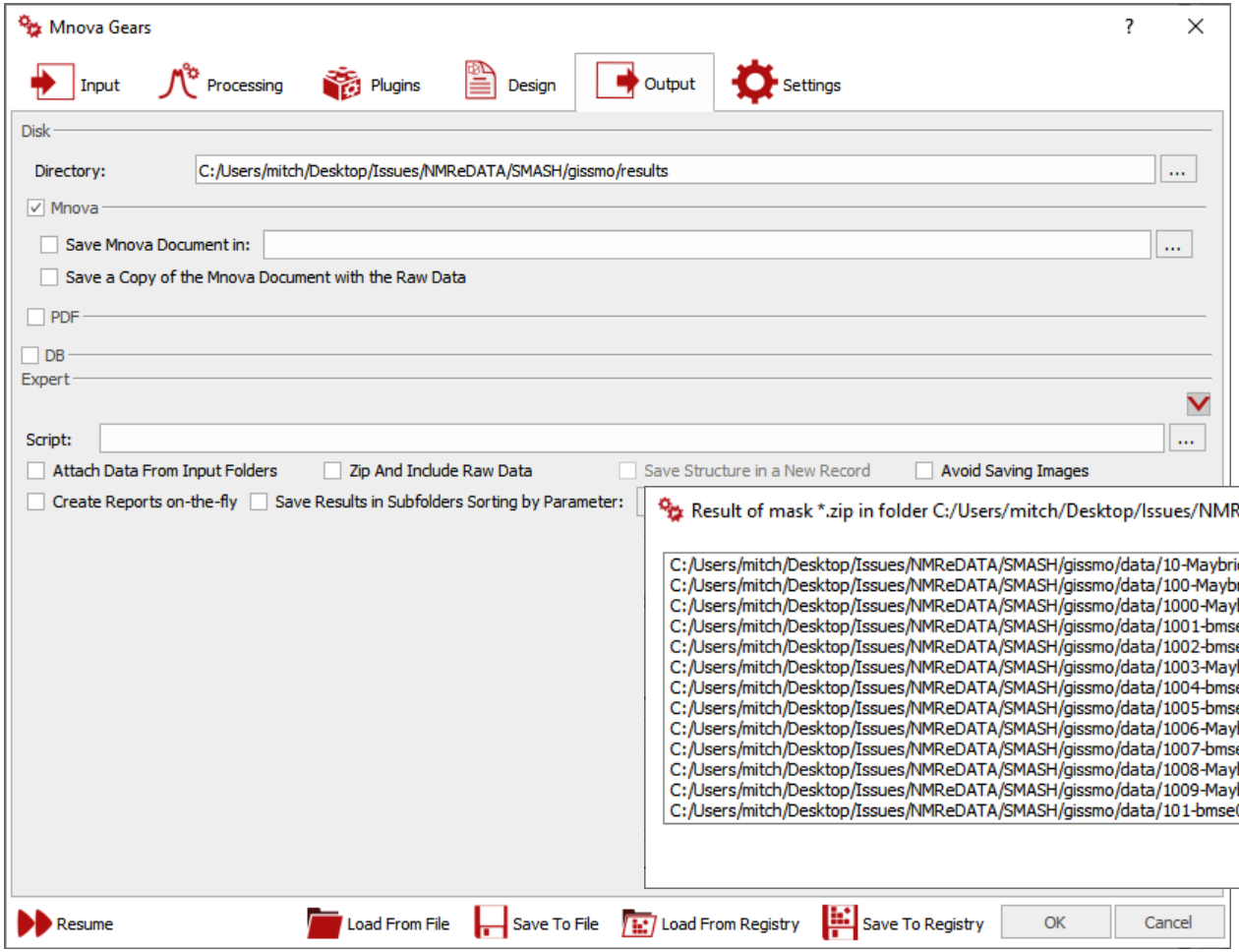
- A new Mnova Document is created, with molecule, spectra, and all imported information, e.g. Assignments, Couplings, Multiplets , Peaks, 2D- Correlations



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

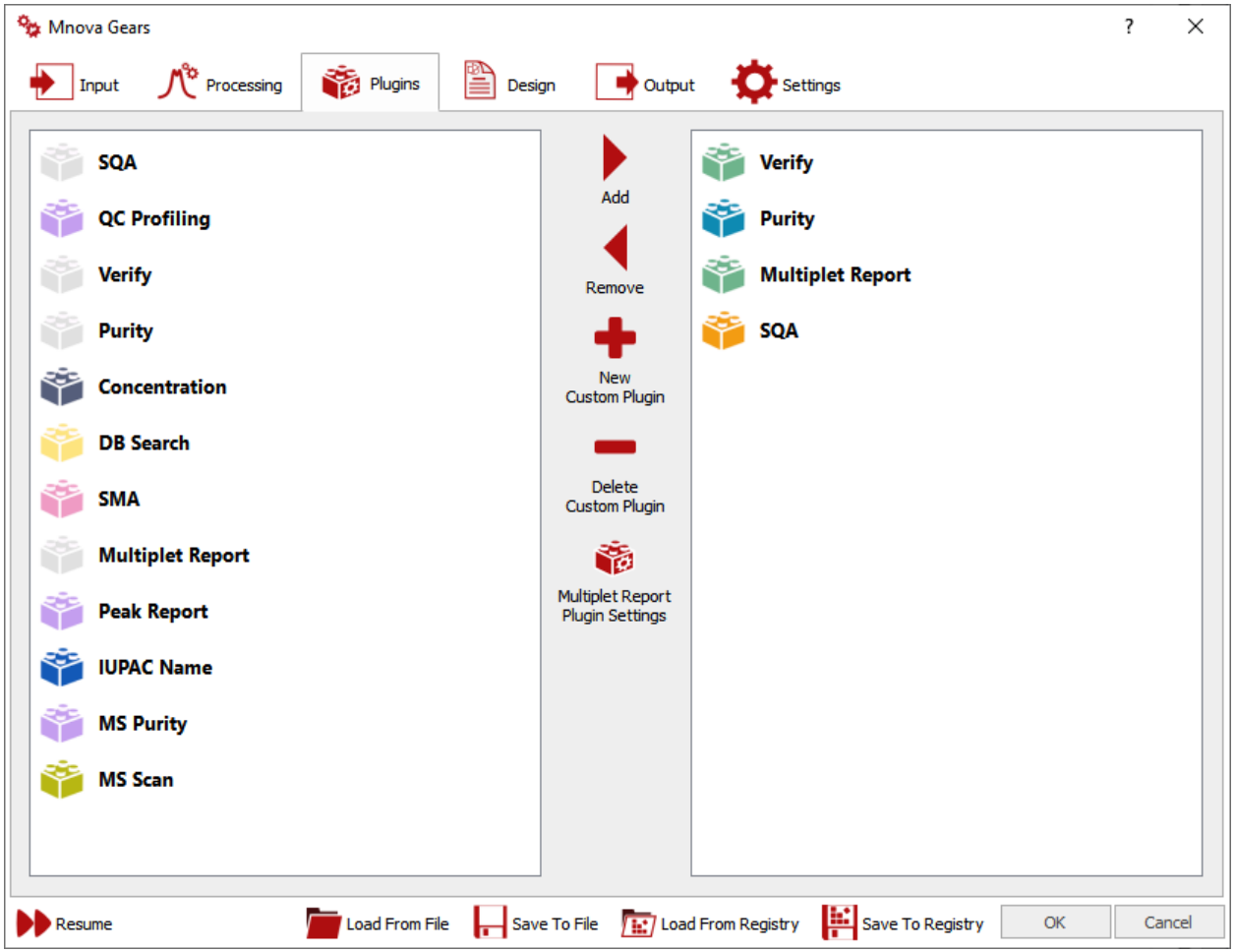


- NMReData is a standard input/output option, it can be used for all Mnova automations, e.g. Mgears:



Converts all NMReData files in a folder in Mnova documents

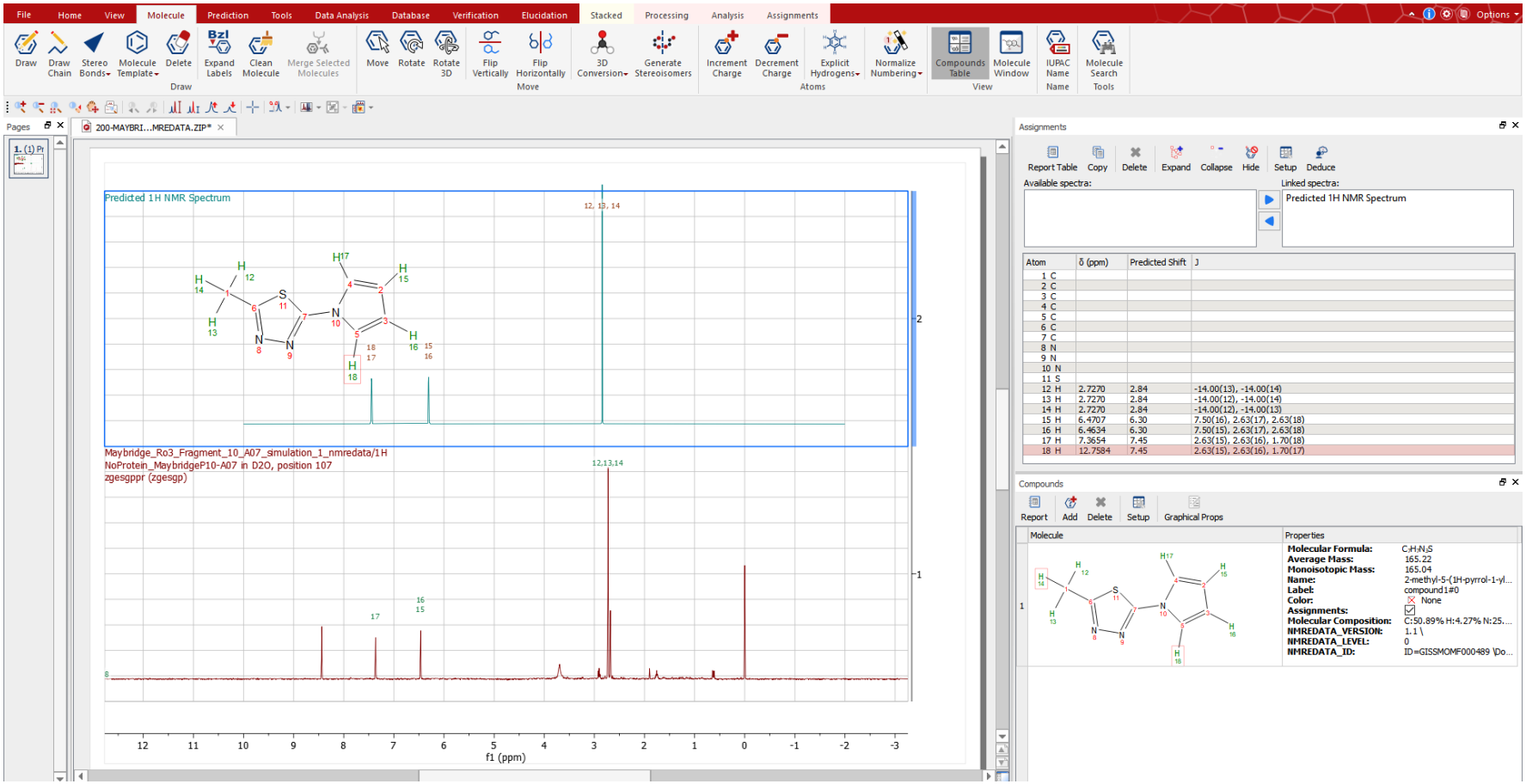
Mgears would allow to perform a great number of analysis using NMReData as Input or Output



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

NMReData in Mnova Automations
Assignments Check in a Database

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



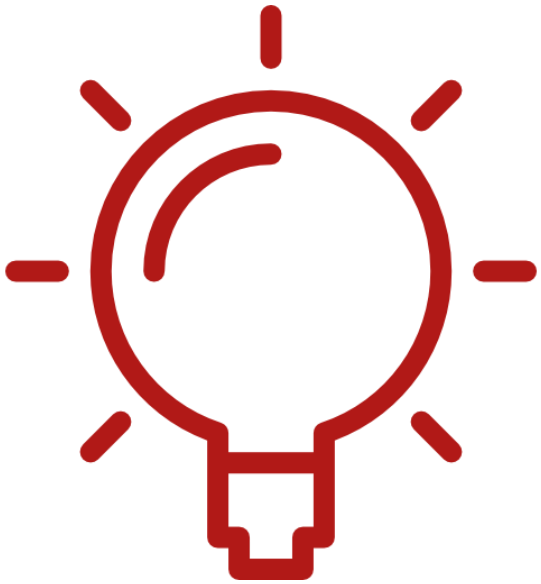
Comparison with Mnova predicted shifts helps with the detection of errors in assignments (or predictions)

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