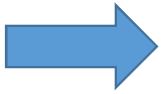
JDF format



Daniel Jacob
Feb. 2018

Bordeaux Metabolome Facility

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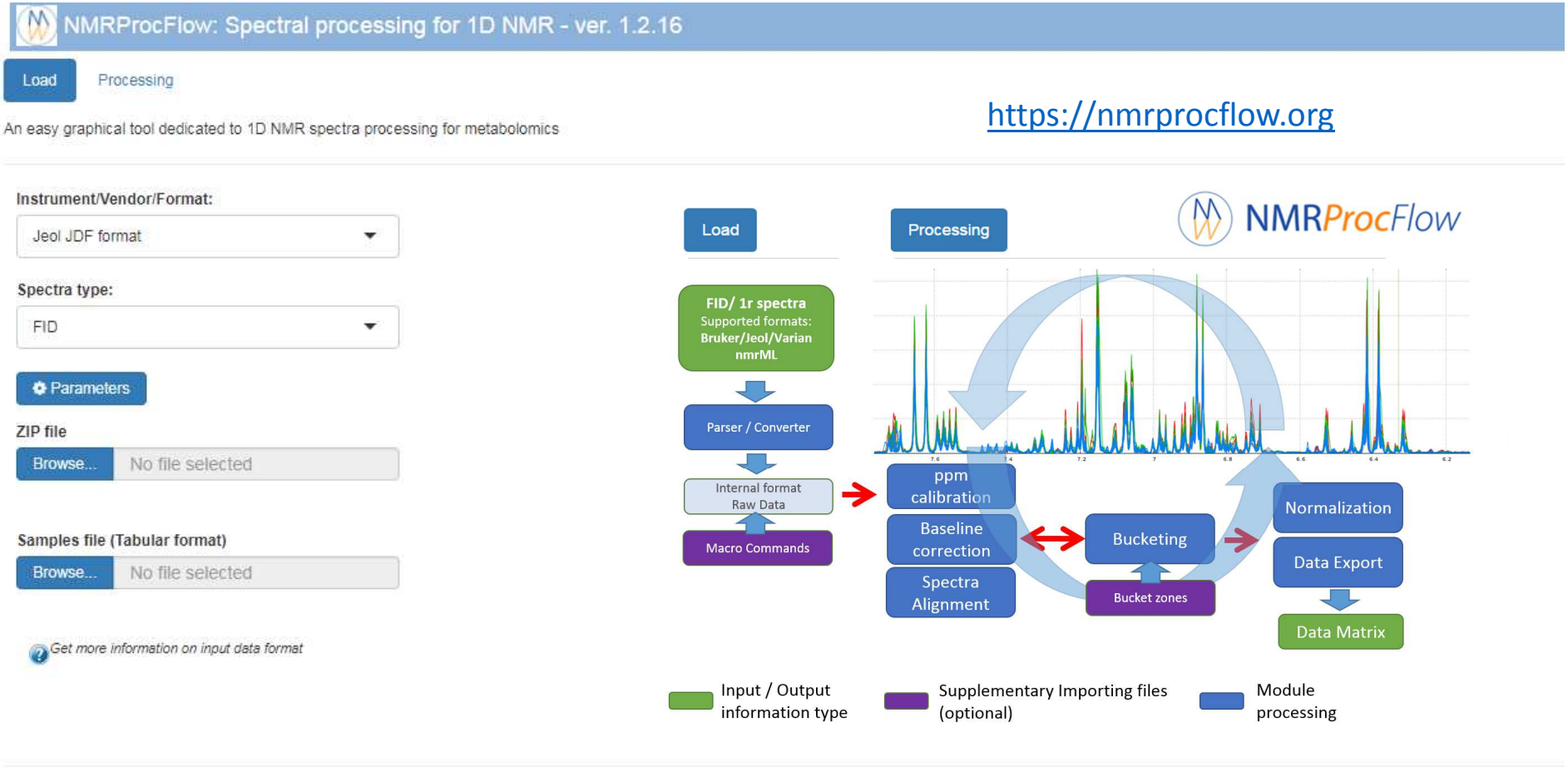
Data preparation step

An easy GUI tool dedicated to 1D NMR spectra processing (1H & 13C) for metabolomics



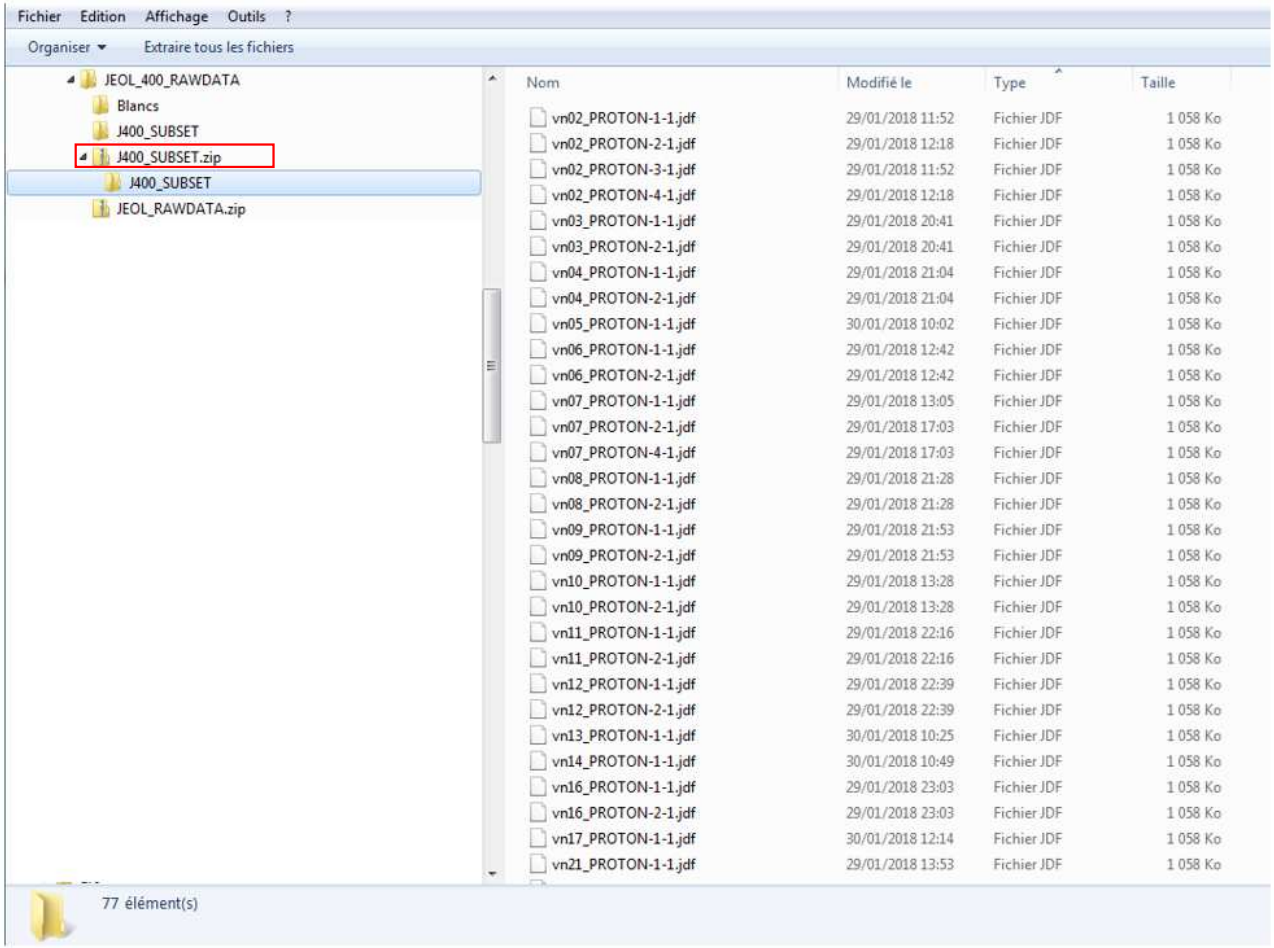
https://nmrprocflow.org

NMRProcFlow -(C) INRA UMR 1332 BFP, Metabolomics Facility - 2016-2018

NMRProcFlow

Data preparation step

Simply zip the entire directory including all spectra of the experiment in JDF format



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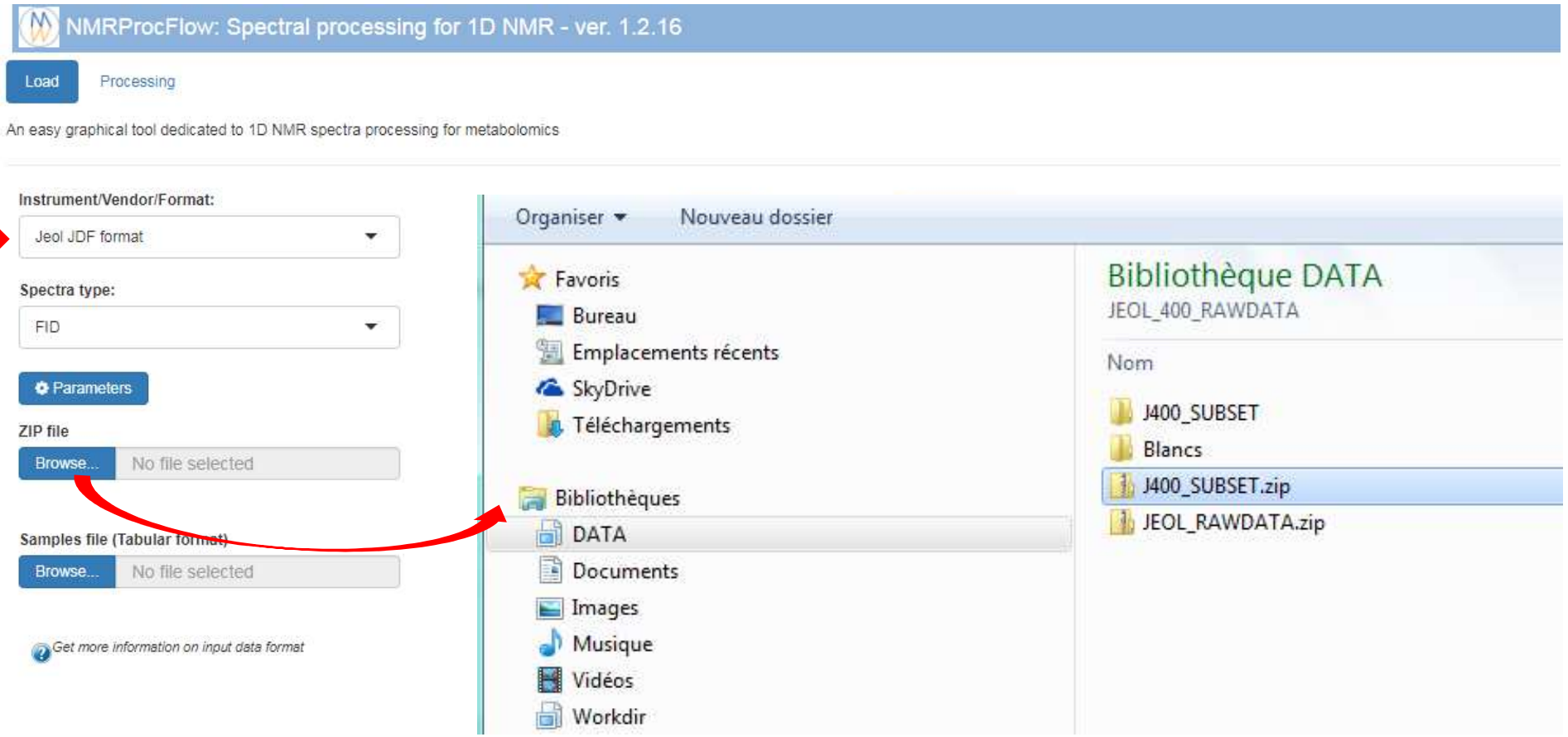
NMRProcFlow

Preprocessing step



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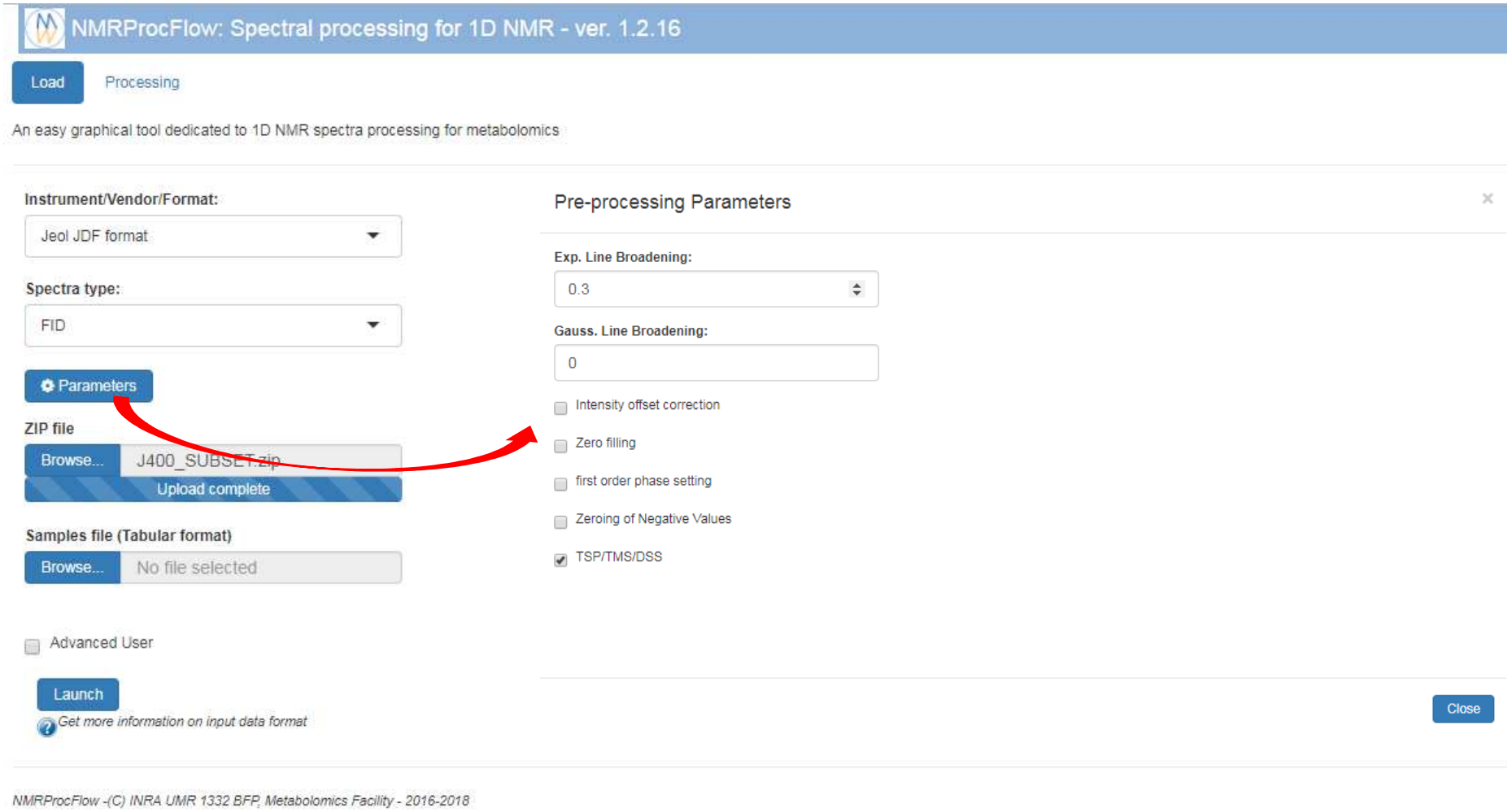
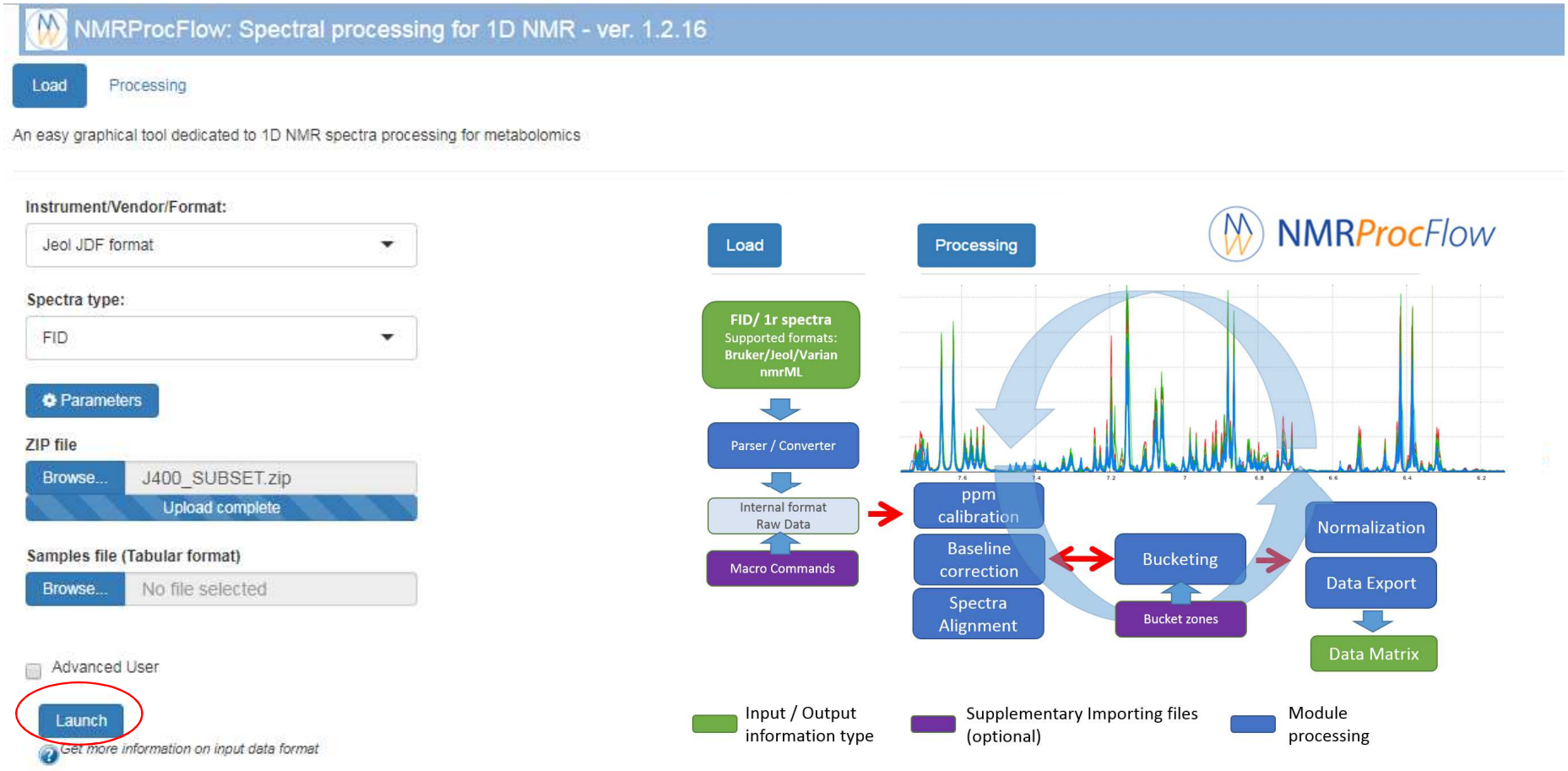
NMRProcFlow Preprocessing step



NMRProcFlow Preprocessing step



https://nmrprocflow.org/np/

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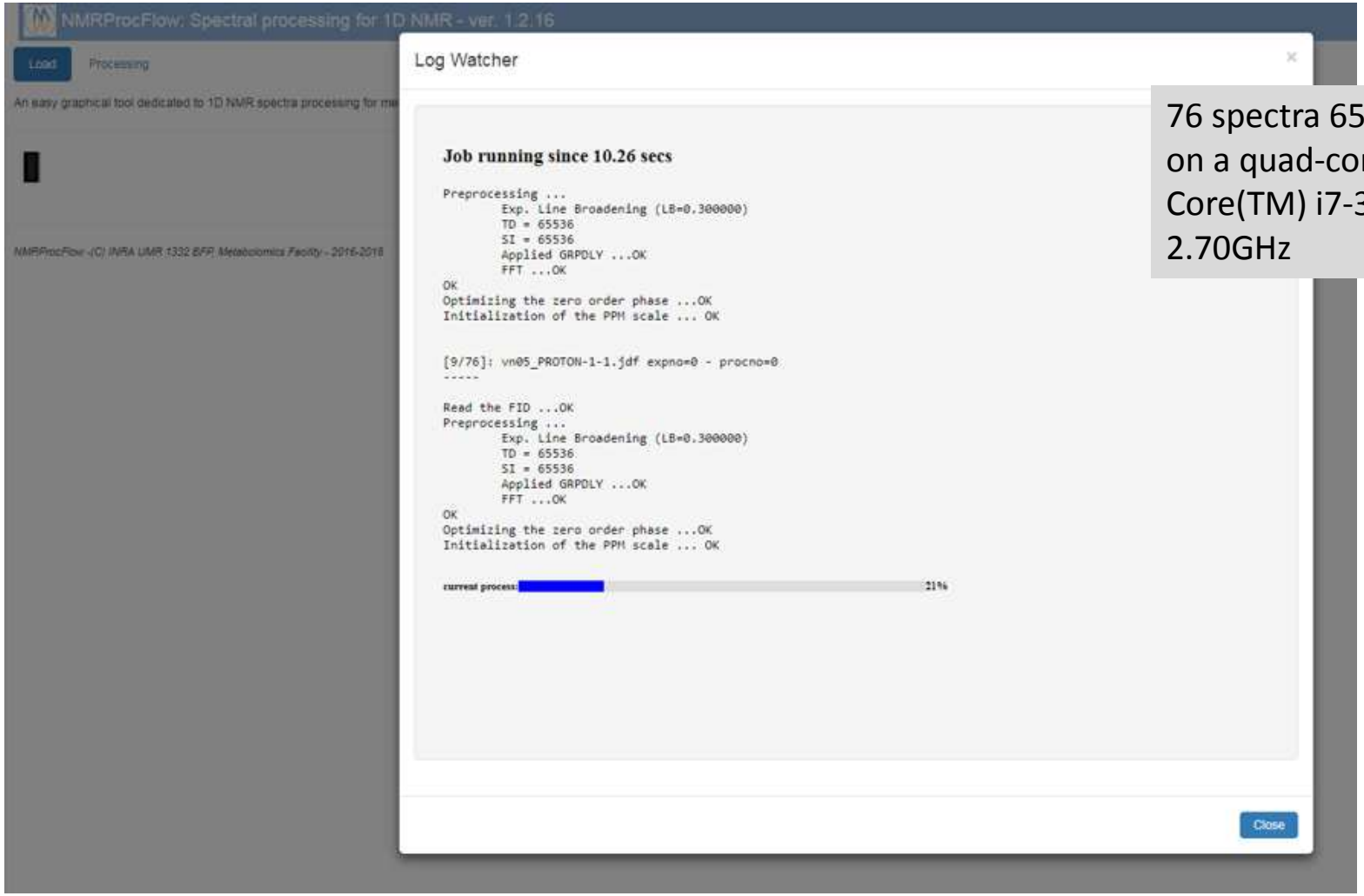
NMRProcFlow

Preprocessing step

The preprocessing is the most time consuming step.
(especially the Zero & first order phasing)



76 spectra 65K => 30 sec
on a quad-core Intel(R) Core(TM) i7-3740QM CPU @ 2.70GHz

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NMRProcFlow

NMRProcFlow: Spectral processing for 1D NMR - ver. 1.2.16 J400_SUBSET

Load Processing

An easy graphical tool dedicated to 1D NMR spectra processing for metabolomics

```
Shiny Server version 1.5.7.886
----
Session Identifier = _f7a82c6ddbc86cf2d74dbc63fc59ee
Instrument/Vendor/Format = jeol
Spectra type = fid
The original name of the Zip file = J400_SUBSET.zip
The original name of the Samples file = NA
The macro-command file for processing =
The number of Spectra = 76
The number of Factors = 0
----
```

Reset Log Export Parameters

Show 10 entries Search:

Spectrum	PULSE	NUC	SOLVENT	PHC0	PHC1	SW	SF	SI
vn02_PROTON-1-1.jdf	proton.jxp	1H	METHANOL-D4	3.063094	0	17.52636	399782198	65536
vn02_PROTON-2-1.jdf	proton.jxp	1H	METHANOL-D4	2.914672	0	17.52636	399782198	65536
vn02_PROTON-3-1.jdf	proton.jxp	1H	METHANOL-D4	3.063094	0	17.52636	399782198	65536
vn02_PROTON-4-1.jdf	proton.jxp	1H	METHANOL-D4	2.914672	0	17.52636	399782198	65536
vn03_PROTON-1-1.jdf	proton.jxp	1H	METHANOL-D4	3.067867	0	17.52636	399782198	65536
vn03_PROTON-2-1.jdf	proton.jxp	1H	METHANOL-D4	3.067867	0	17.52636	399782198	65536
vn04_PROTON-1-1.jdf	proton.jxp	1H	METHANOL-D4	3.062744	0	17.52636	399782198	65536
vn04_PROTON-2-1.jdf	proton.jxp	1H	METHANOL-D4	3.062744	0	17.52636	399782198	65536
vn05_PROTON-1-1.jdf	proton.jxp	1H	METHANOL-D4	2.810931	0	17.52636	399782198	65536
vn06_PROTON-1-1.jdf	proton.jxp	1H	METHANOL-D4	2.829285	0	17.52636	399782198	65536

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NMRProcFlow

Interactive data processing
https://nmrprocflow.org/c3

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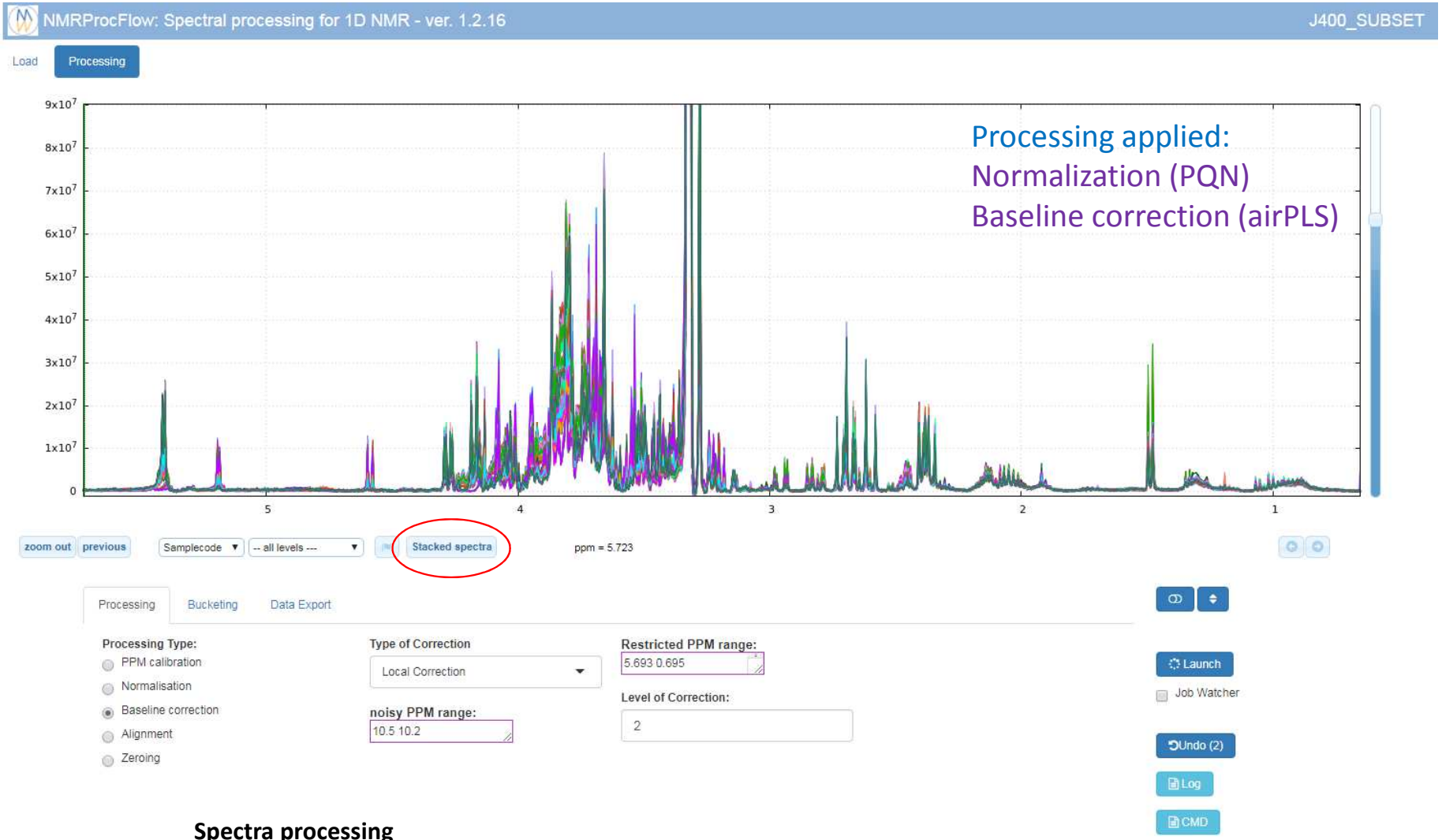
NMRProcFlow

… after some processing …



Spectra processing
https://nmrprocflow.org/c31

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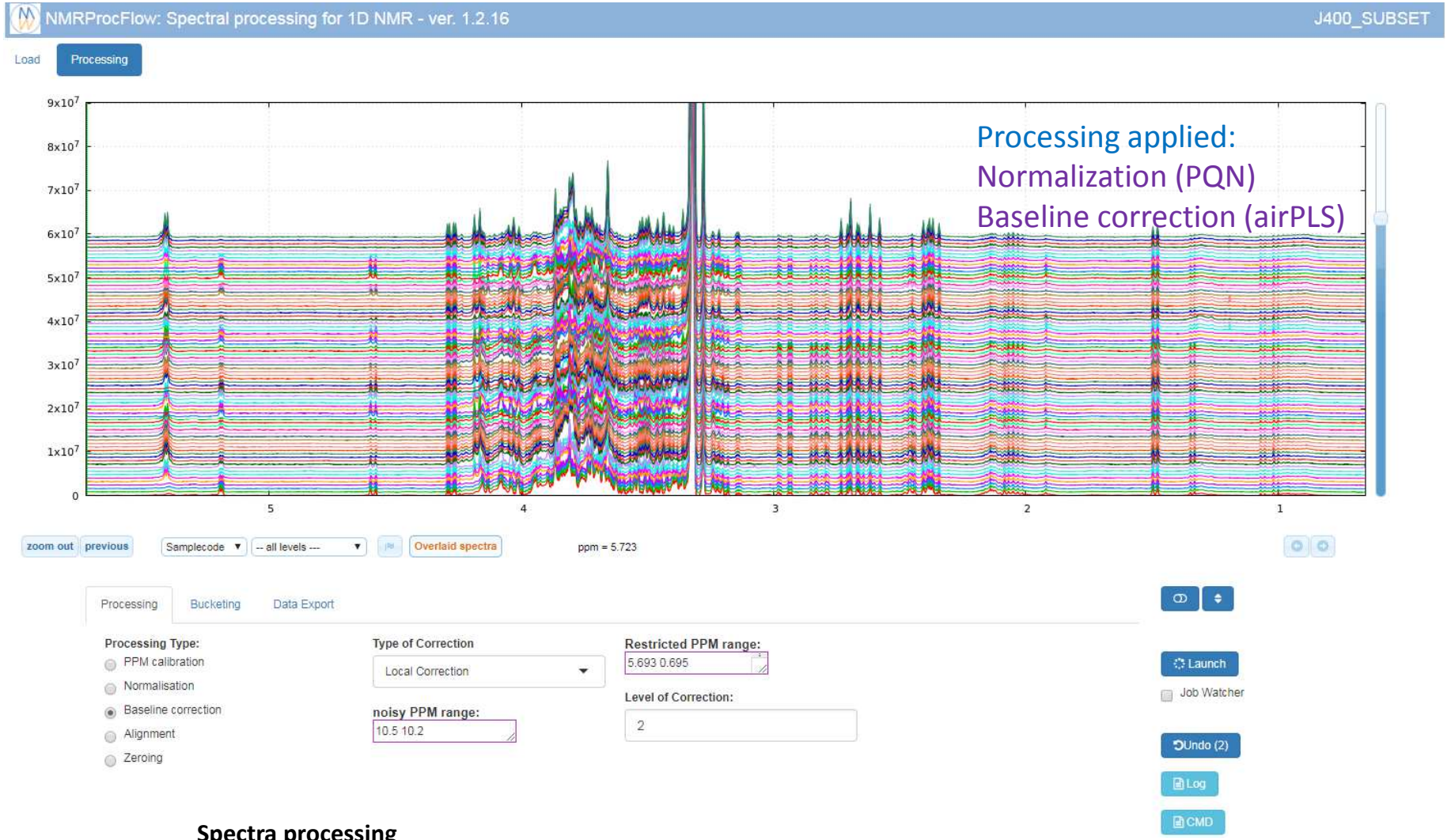
NMRProcFlow

… after some processing …



Spectra processing
https://nmrprocflow.org/c31

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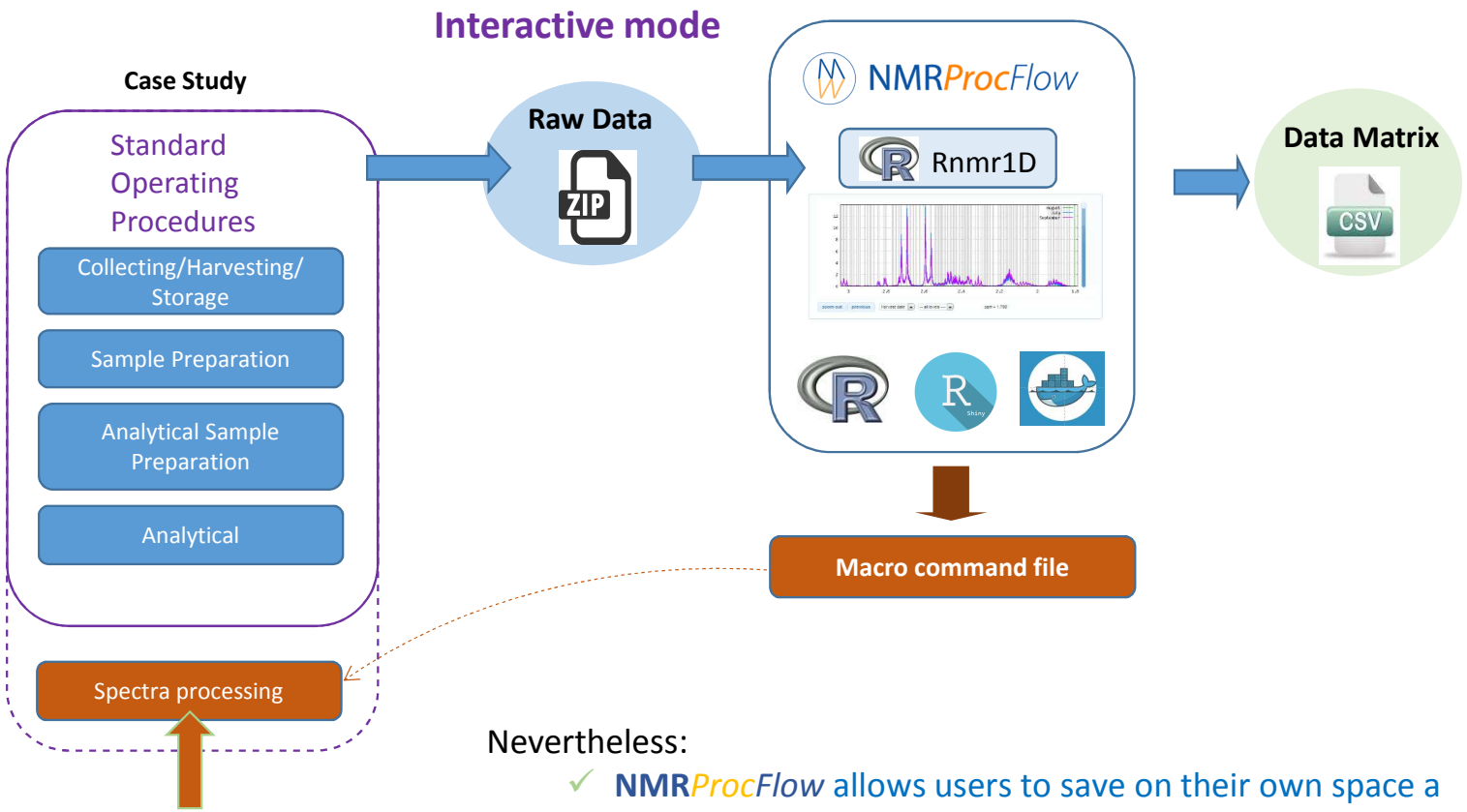
NMRProcFlow

Interactive mode execution



Completes the SOP list

- by an identical "spectra processing" procedure throughout the experiment for all data subsets

Nevertheless:

- ✓ **NMR***ProcFlow* allows users to save on their own space a minimal set of small files in order to recover / replay their session

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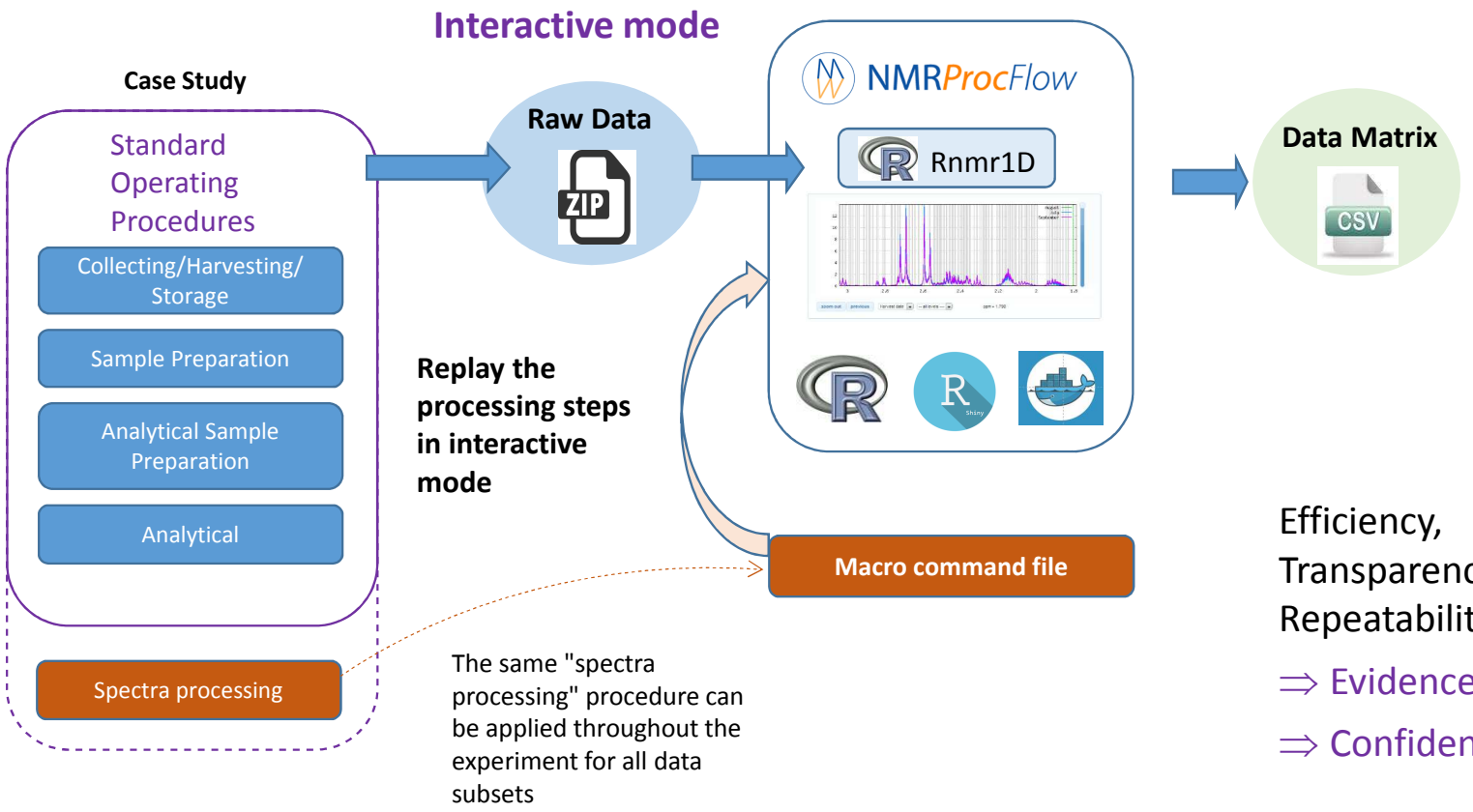
NMRProcFlow

Interactive mode execution



Efficiency,
Transparency,
Repeatability

⇒ Evidence

⇒ Confidence

Fulfilling the need of traceability, of repeatability allows to consolidate the spectra processing step within a set of SOP, and thus satisfy requirements for an open science

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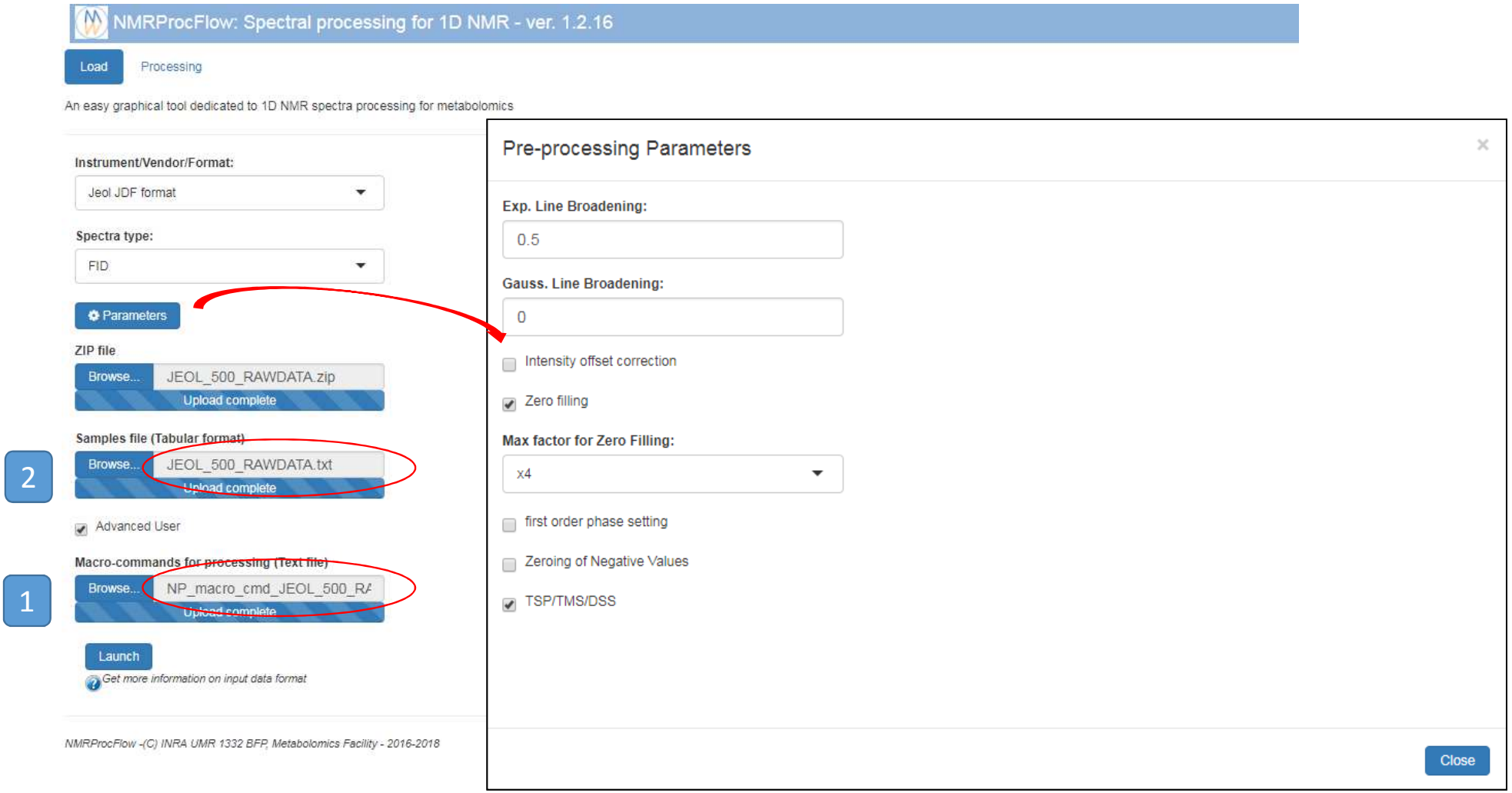
NMRProcFlow

Jeol 500 dataset



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NMRProcFlow

Jeol 500 dataset

1 NP_macro_cmd_JEOL_500_RAWDATA.txt

```
#
# Normalisation ( PQN ) of the Intensities based on the selected PPM ranges...
#
normalisation PQN
0.623 4.841
EOL

#
# Baseline Correction: PPM Range = ( 0.731 , 3.296 )
#
airpls 0.731 3.296 2

#
# Baseline Correction: PPM Range = ( 3.297 , 5.275 )
#
airpls 3.297 5.275 3

#
# Zeroing the selected zones ...
#
zero
3.3 3.355
EOL

#
# Alignment of the selected zones ( 0.776 , 3.322 )
#
clupa 10.2 10.5 0.776 3.322 0.01 5 0
```

Job Watcher

```
[9/10]: vn58_PROTON-1-1.jdf expno=0 - procno=0
-----

Read the FID ...OK
Preprocessing ...
        Exp. Line Broadening (LB=0.500000)
        TD = 65536
        Zero Filling (x2)
        SI = 131072
        Applied GRPDLY ...OK
        FFT ...OK
OK
Optimizing the zero order phase ...OK
Initialization of the PPM scale ... PPM min =-3.952077
OK


Rnmr1D:  Generate the final matrix of spectra...

Rnmr1D:  Write the spec.pack file ...

Rnmr1D:  Write the list_pars.csv file ...

Rnmr1D: -----------------------------------
Rnmr1D: Process the Macro-commands file
Rnmr1D: -----------------------------------
Rnmr1D:
Rnmr1D:  Normalisation of the Intensities based on the selected PPM ranges...
Rnmr1D:     Method =PQN
Rnmr1D:  Baseline Correction: PPM Range = ( 0.731 , 3.296 )
Rnmr1D:     Type=airPLS, lambda= 2
Rnmr1D:  Baseline Correction: PPM Range = ( 3.297 , 5.275 )
Rnmr1D:     Type=airPLS, lambda= 3
Rnmr1D:  Zeroing the selected PPM ranges ...
Rnmr1D:     Zone 1 = ( 3.3 , 3.355 )
Rnmr1D:  Alignment: PPM Range = ( 0.776 , 3.322 )
Rnmr1D:     CluPA - Resolution =0.01 - SNR threshold=5 - Reference=0
Rnmr1D:  Write the spec.pack file ...
```

Close

Apply some processing after preprocessing …

Fulfilling the need of traceability, of repeatability allows to consolidate the spectra processing step within a set of SOP, and thus satisfy requirements for an open science

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NMRProcFlow

Jeol 500 dataset

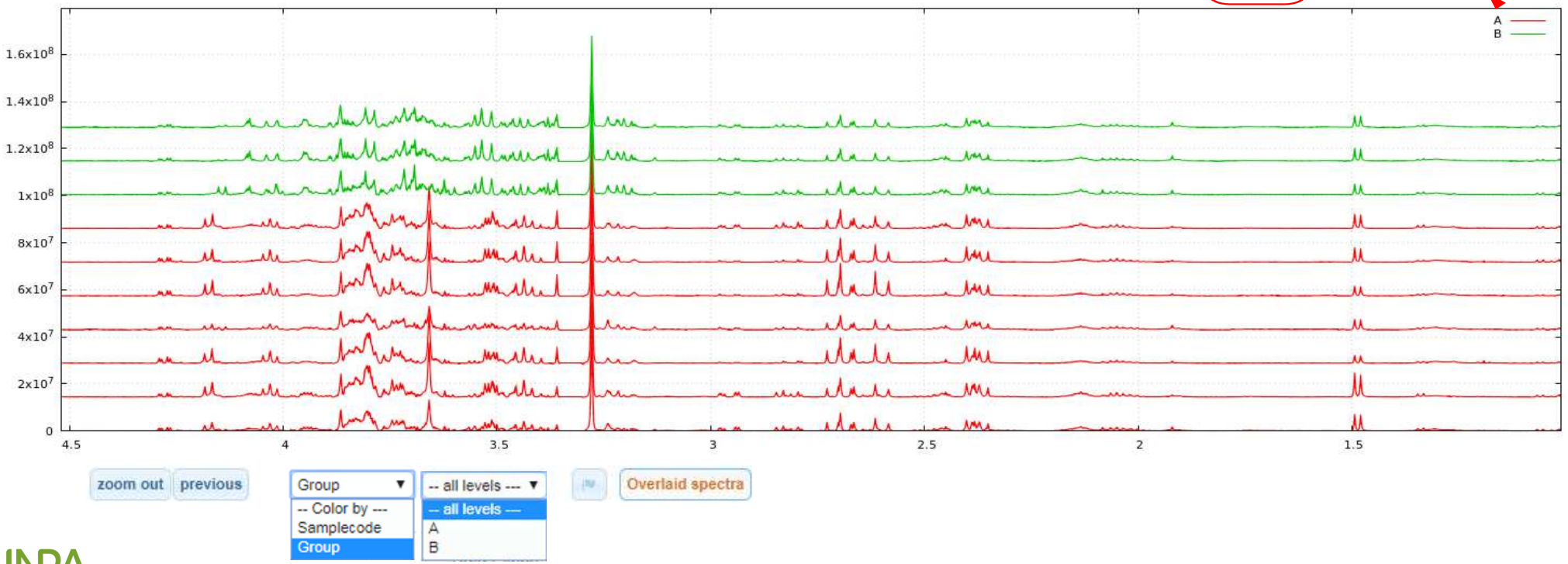
NMRProcFlow

Jeol 500 dataset

2 JEOL_500_RAWDATA.txt

	A	B	C
1	Spectrum	Samplecode	Group
2	vn23_PROTON-1-1.jdf	vn23_PROTON-1-1	A
3	vn29_PROTON-1-1.jdf	vn29_PROTON-1-1	A
4	vn2_PROTON-1-1.jdf	vn2_PROTON-1-1	B
5	vn39_PROTON-1-1.jdf	vn39_PROTON-1-1	A
6	vn51_PROTON-1-1.jdf	vn51_PROTON-1-1	B
7	vn52_PROTON-2-1.jdf	vn52_PROTON-2-1	B
8	vn54_PROTON-1-1.jdf	vn54_PROTON-1-1	A
9	vn56_PROTON-1-1.jdf	vn56_PROTON-1-1	A
10	vn58_PROTON-1-1.jdf	vn58_PROTON-1-1	A
11	vn8_PROTON-1-1.jdf	vn8_PROTON-1-1	A

Interaction between Biologists and NMR spectroscopists by visualizing the NMR spectra along with their corresponding experimental-factor levels, thus setting a bridge between experimental design and subsequent statistical analyses.



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