



JDF format



NMR*ProcFlow*

Daniel Jacob

Feb. 2018

Bordeaux Metabolome Facility



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



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

Load

Processing

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

<https://nmrprocflow.org>

Instrument/Vendor/Format:

Jeol JDF format

Spectra type:

FID

Parameters

ZIP file

Browse...

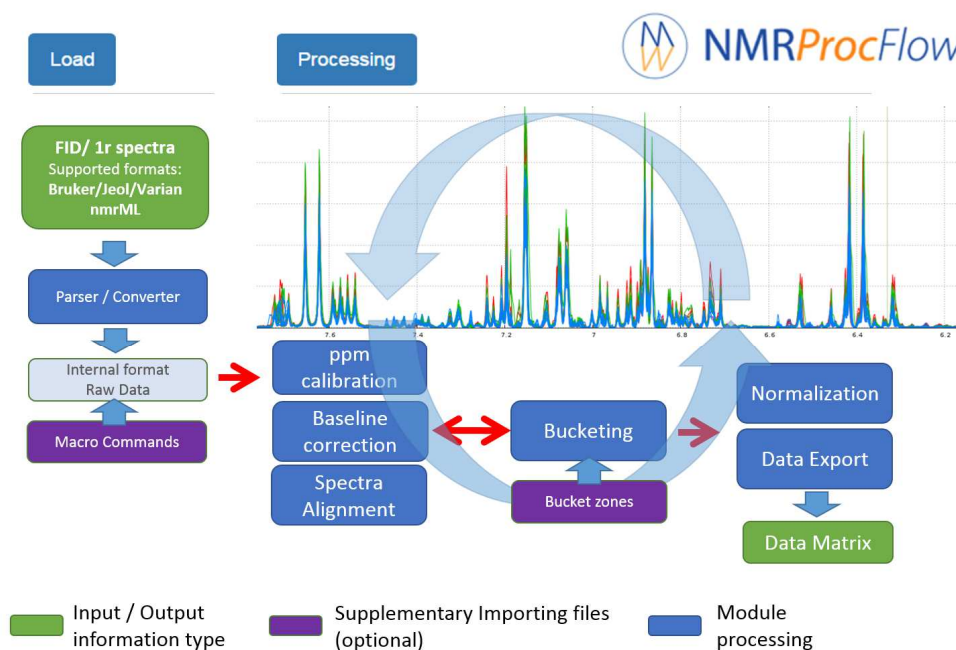
No file selected

Samples file (Tabular format)

Browse...

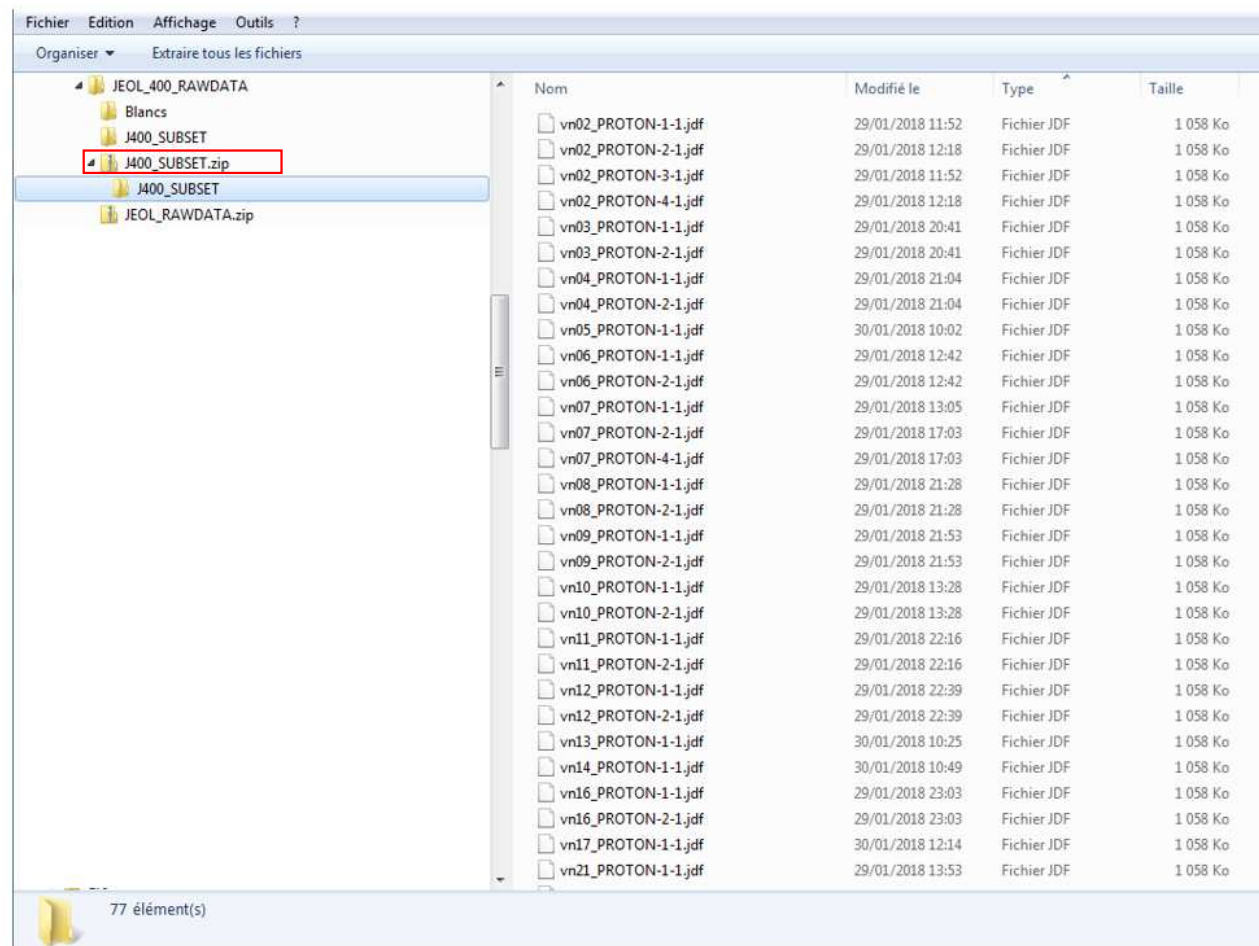
No file selected

[Get more information on input data format](#)





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





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ZIP file
Browse... No file selected

Samples file (Tabular format)
Browse... No file selected

Get more information on input data format

Organiser Nouveau dossier

Favoris

- Bureau
- Emplacements récents
- SkyDrive
- Téléchargements

Bibliothèques

- DATA
- Documents
- Images
- Musique
- Vidéos
- Workdir

Bibliothèque DATA

JEOL_400_RAWDATA

Nom

- J400_SUBSET
- Blancs
- J400_SUBSET.zip
- JEOL_RAWDATA.zip



Load

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FID

Parameters

ZIP file

Browse...

J400_SUBSET.zip

Upload complete

Samples file (Tabular format)

Browse...

No file selected

☐ Advanced User

Launch

Get more information on input data format

Pre-processing Parameters

Exp. Line Broadening:

0.3

Gauss. Line Broadening:

0

- ☐ Intensity offset correction
- ☐ Zero filling
- ☐ first order phase setting
- ☐ Zeroing of Negative Values
- ☒ TSP/TMS/DSS

Close



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J400_SUBSET.zip

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Samples file (Tabular format)

Browse...

No file selected

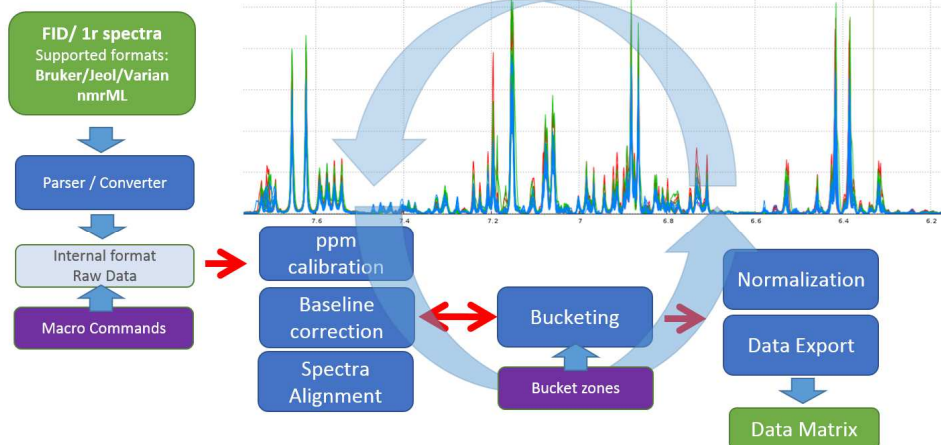
☐ Advanced User

Launch

Get more information on input data format

Load

Processing

Input / Output
information typeSupplementary Importing files
(optional)Module
processing



NMRProcFlow

Preprocessing step

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

The screenshot shows the NMRProcFlow interface with a 'Log Watcher' window open. The window displays the following log entries:

```
Job running since 10.26 secs

Preprocessing ...
  Exp. Line Broadening (LB=0.300000)
  TD = 65536
  SI = 65536
  Applied GRPDLY ...OK
  FFT ...OK
OK
Optimizing the zero order phase ...OK
Initialization of the PPM scale ... OK

[9/76]: vn05_PROTON-1-1.fdf expno=0 - procno=0
-----

Read the FID ...OK
Preprocessing ...
  Exp. Line Broadening (LB=0.300000)
  TD = 65536
  SI = 65536
  Applied GRPDLY ...OK
  FFT ...OK
OK
Optimizing the zero order phase ...OK
Initialization of the PPM scale ... OK
```

At the bottom of the log, there is a progress bar labeled 'current process' which is at 21% completion.

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

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

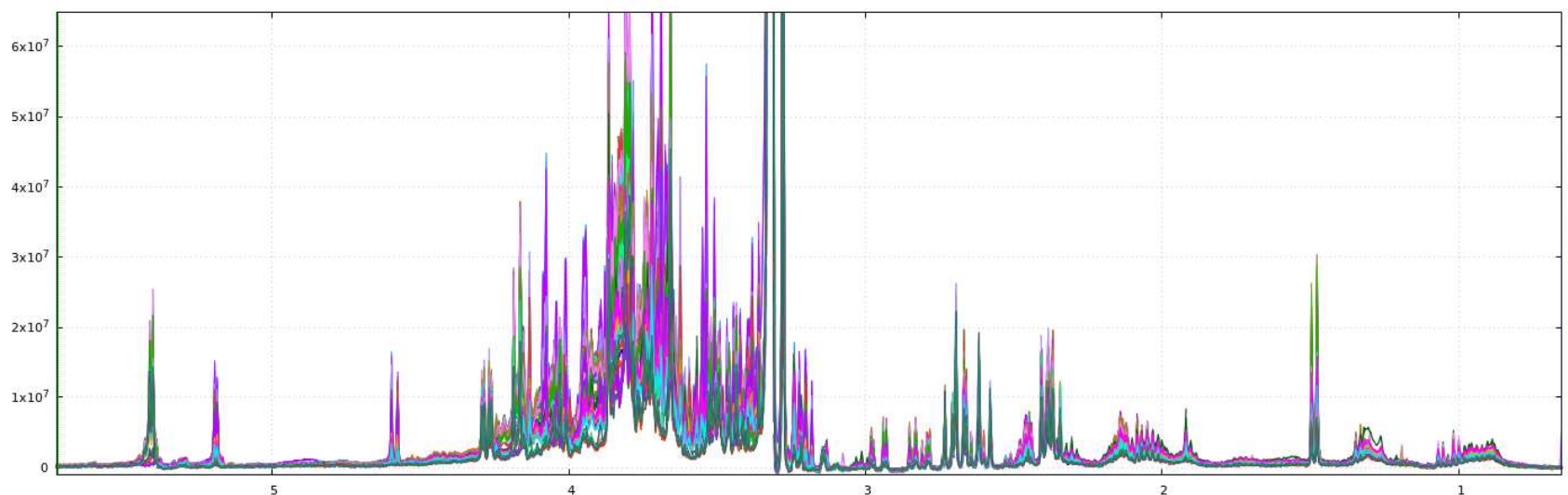
Spectrum	PULSE	NUC	SOLVENT	PHC0	PHC1	SW	SF	SI
vn02_PROTON-1-1.jdf	proton.jxp	1H	METHANOL-D4	3.063094	0	17.52636	399782198	65536
vn02_PROTON-2-1.jdf	proton.jxp	1H	METHANOL-D4	2.914672	0	17.52636	399782198	65536
vn02_PROTON-3-1.jdf	proton.jxp	1H	METHANOL-D4	3.063094	0	17.52636	399782198	65536
vn02_PROTON-4-1.jdf	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



Search:

Load

Processing



zoom out

previous

Samplecode

-- all levels --

10

Stacked spectra

ppm = 5.723

+

+

Processing

Bucketing

Data Export

Processing Type:

- ☐ PPM calibration
- ☐ Normalisation
- ☒ Baseline correction
- ☐ Alignment
- ☐ Zeroing

Type of Correction

Global Correction

Level of Correction

Soft correction

noisy PPM range:

10.5 10.2

+

Launch

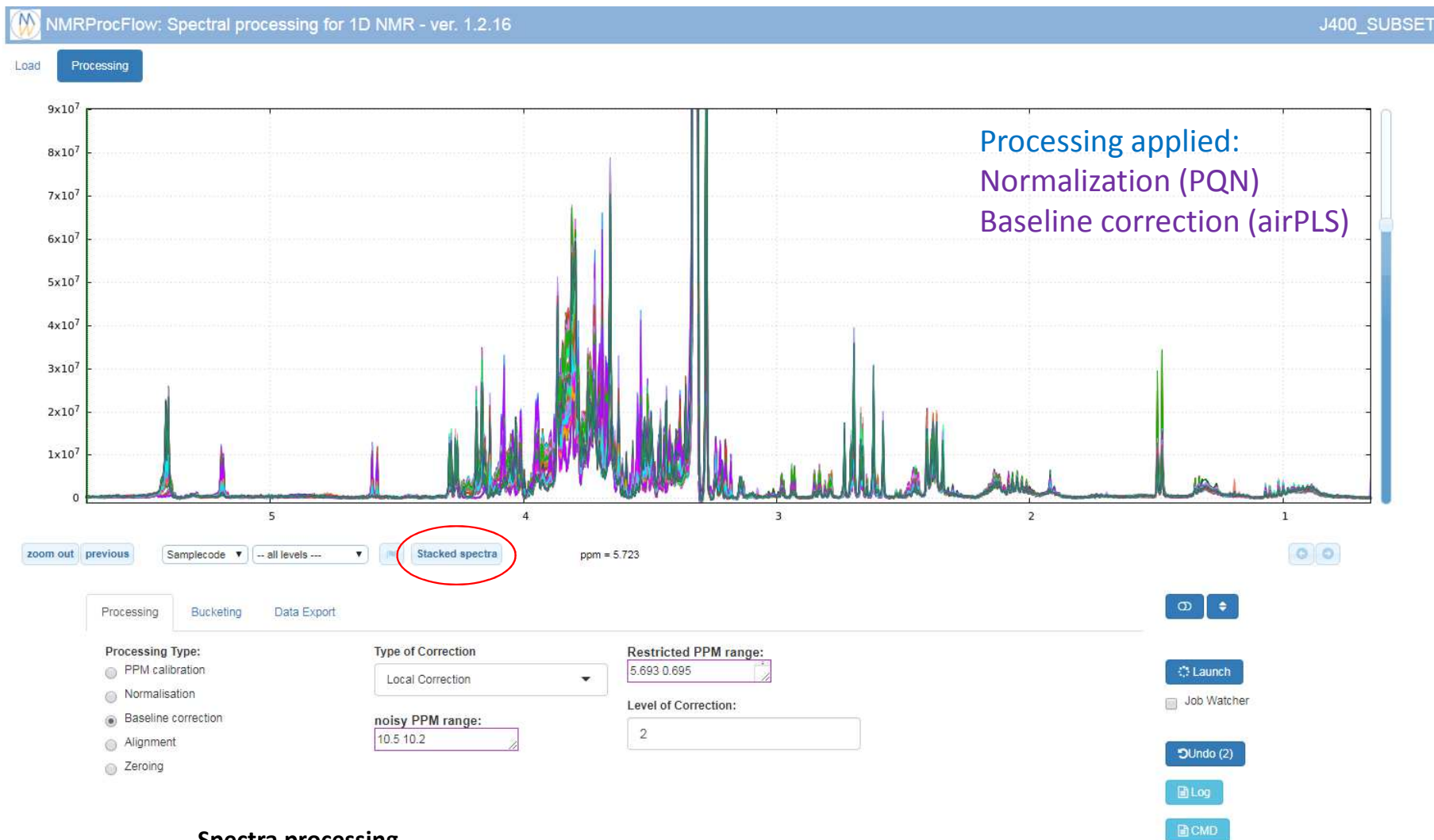
☒ Job Watcher

Undo

Log

CMD

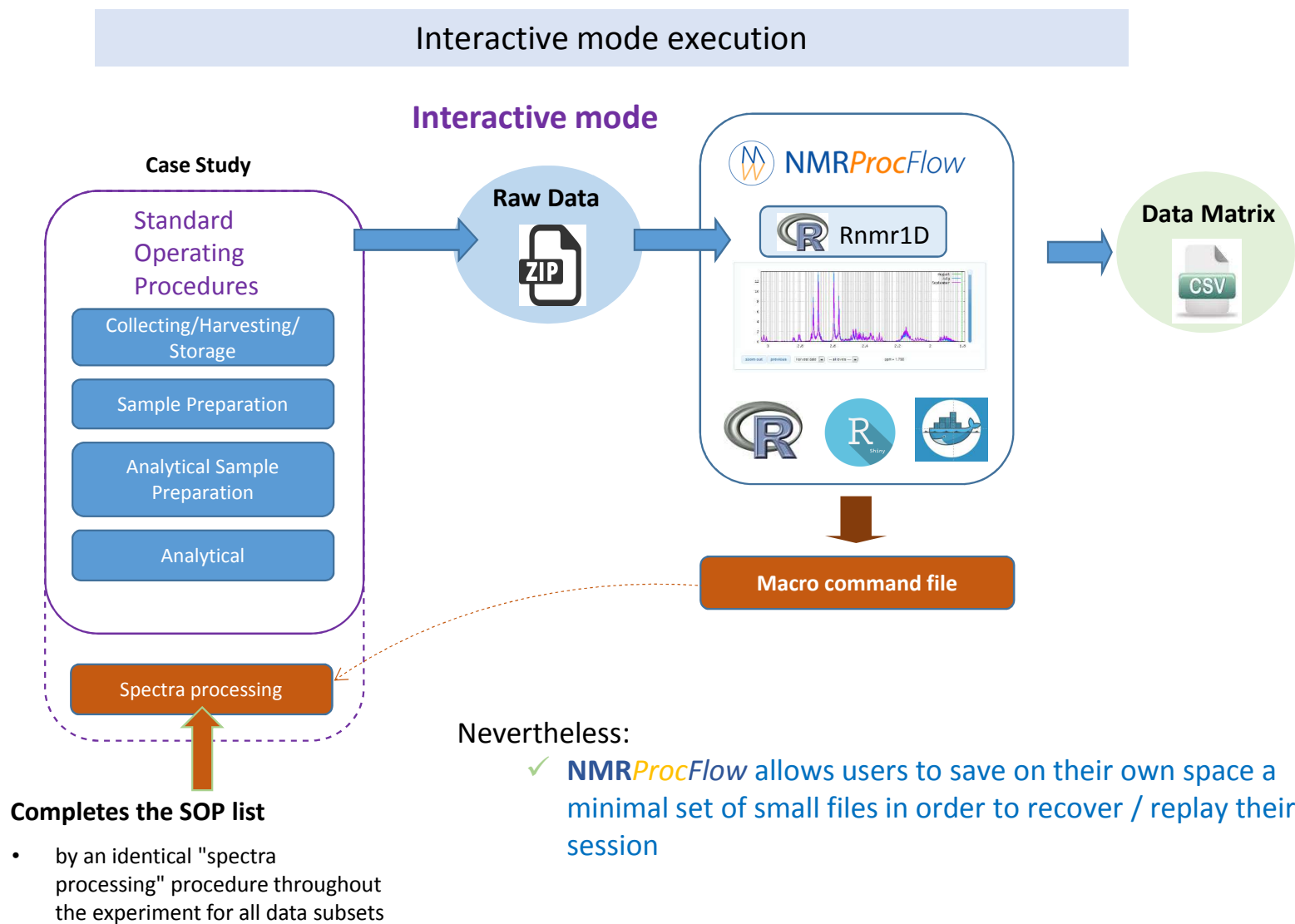
Interactive data processing
<https://nmrprocflow.org/c3>

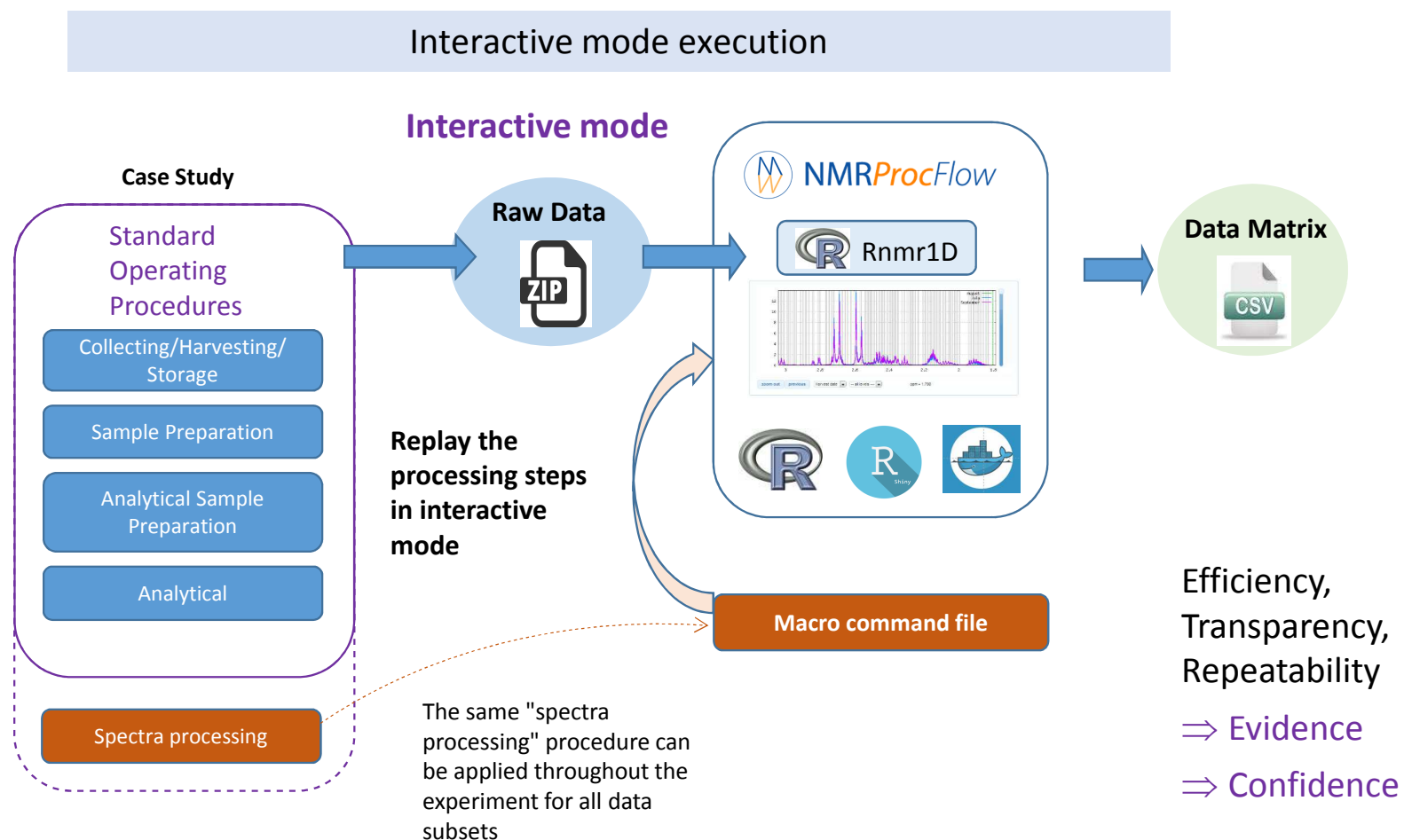


Spectra processing
<https://nmrprocflow.org/c31>




Spectra processing
<https://nmrprocflow.org/c31>





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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Instrument/Vendor/Format:

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FID

Parameters

ZIP file

Browse...

JEOL_500_RAWDATA.zip

Upload complete

2

Samples file (Tabular format)

Browse...

JEOL_500_RAWDATA.txt

Upload complete

☒ Advanced User

1


Macro-commands for processing (Text file)

Browse...

NP_macro_cmd_JEOL_500_RA

Upload complete

Launch


Get more information on input data format

Pre-processing Parameters

Exp. Line Broadening:

0.5

Gauss. Line Broadening:

0

☐ Intensity offset correction

☒ Zero filling

Max factor for Zero Filling:

x4

☐ first order phase setting

☐ Zeroing of Negative Values

☒ TSP/TMS/DSS

Close

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

```
#
# 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

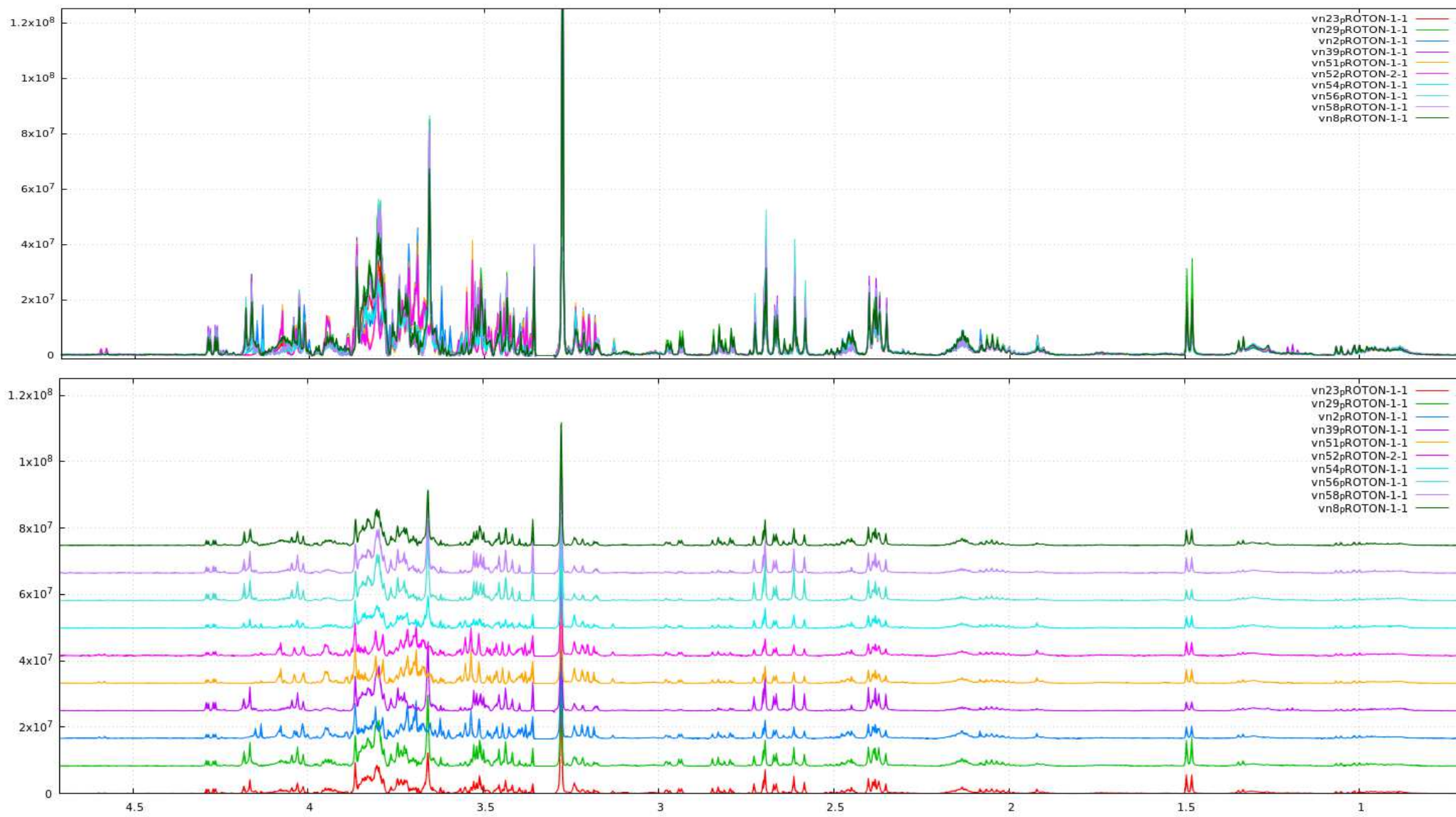
#
# Zeroing the selected zones...
#
zero
3.3 3.355
EOL

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

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

Jeol 500 dataset



Jeol 500 dataset

2 JEOL_500_RAWDATA.txt

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.

	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

