Spectral preprocessing for 1D NMR (1H & 13C)

A simple application (developed with R Shiny and embedding the Rnmr1D package) which aims to test and validate the spectral preprocessing for 1D NMR (1H & 13C). The term pre-processing designates here the transformation of the NMR spectrum from time domain to frequency domain, including the Fast Fourier Transform (FFT) and the phase correction.

BRUKER

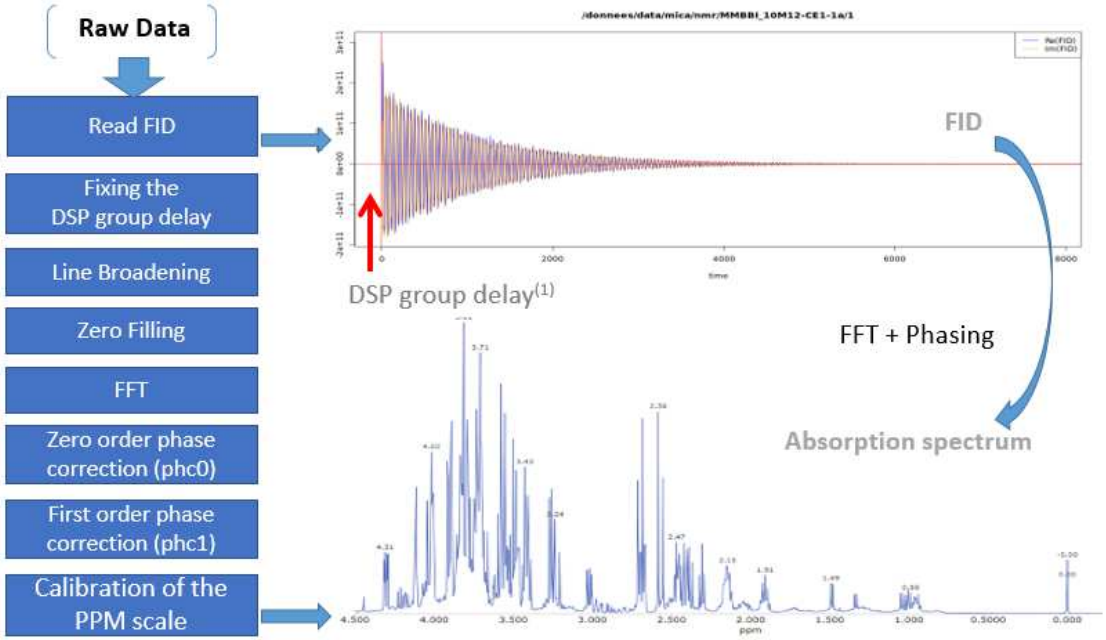
Agilent Technologies

nmrML

JEOL

RS²D

https://pmb-bordeaux.fr/nmrspec/



(1) See http://nmr-analysis.blogspot.fr/2008/02/why-arent-bruker-fids-time-corrected.html

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Spectral preprocessing for 1D NMR (1H & 13C)

Processing | Export | Help

Rnmr1D is a simple application (developed with R Shiny) that allows to perform the preprocessing of any 1D NMR spectrum (1H & 13C)

Instrument/Vendor/Format:

-- Select the input format --

- -- Select the input format --
- nmrML v1.0.rc1
- Bruker (TopSpin/X-winnmr)
- Varian/Agilent (VNMRJ)
- Jeol (JDF/DELTA)
- RS2D (SPINit)

(C) LEGO

BRUKER

Agilent Technologies

JEOL

RS²D

nmrML

This website is optimized for: chrome

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Spectral preprocessing for 1D NMR (1H & 13C)

Processing Export Help

Rnmr1D is a simple application (developed with R Shiny) that allows to perform the preprocessing of any 1D NMR spectrum (1H & 13C)

Instrument/Vendor/Format:

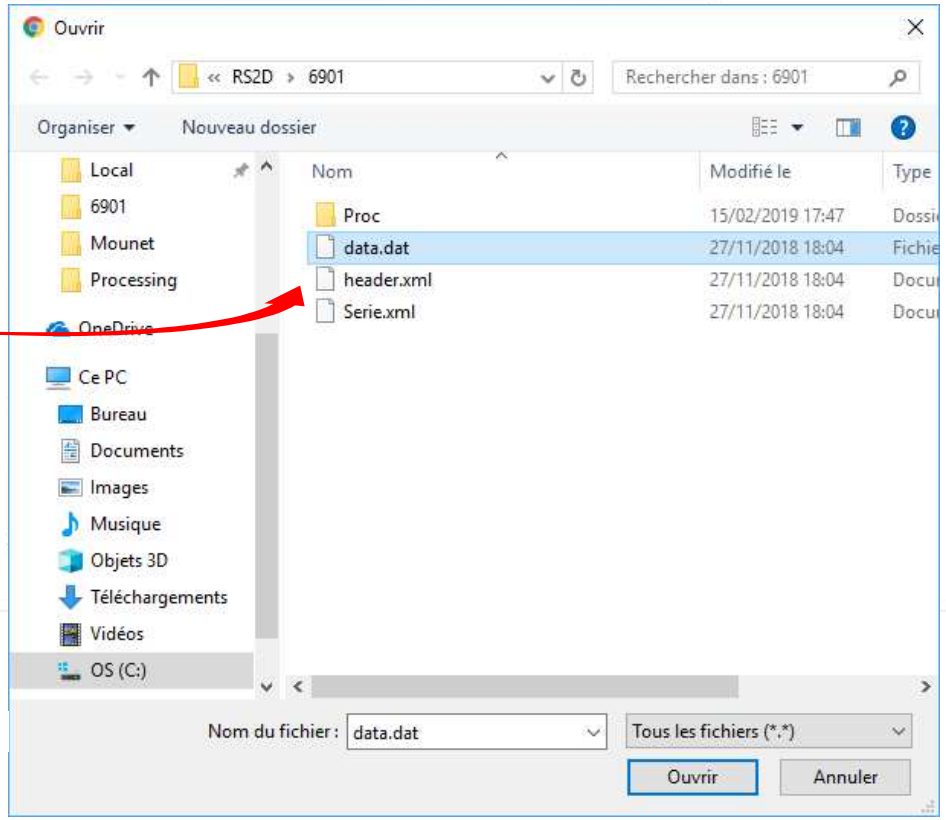
RS2D (SPINit)

FID raw file

Browse... No file selected

Acquisition parameter file

Browse... No file selected



This website is optimized for: chrome

(C) Daniel Jacob - INRA UMR 1332, PMB, MetaboHUB, 2019

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Spectral preprocessing for 1D NMR (1H & 13C)

Processing | Export | Help

Rnmr1D is a simple application (developed with R Shiny) that allows to perform the preprocessing of any 1D NMR spectrum (1H & 13C)

Instrument/Vendor/Format:

RS2D (SPINit)

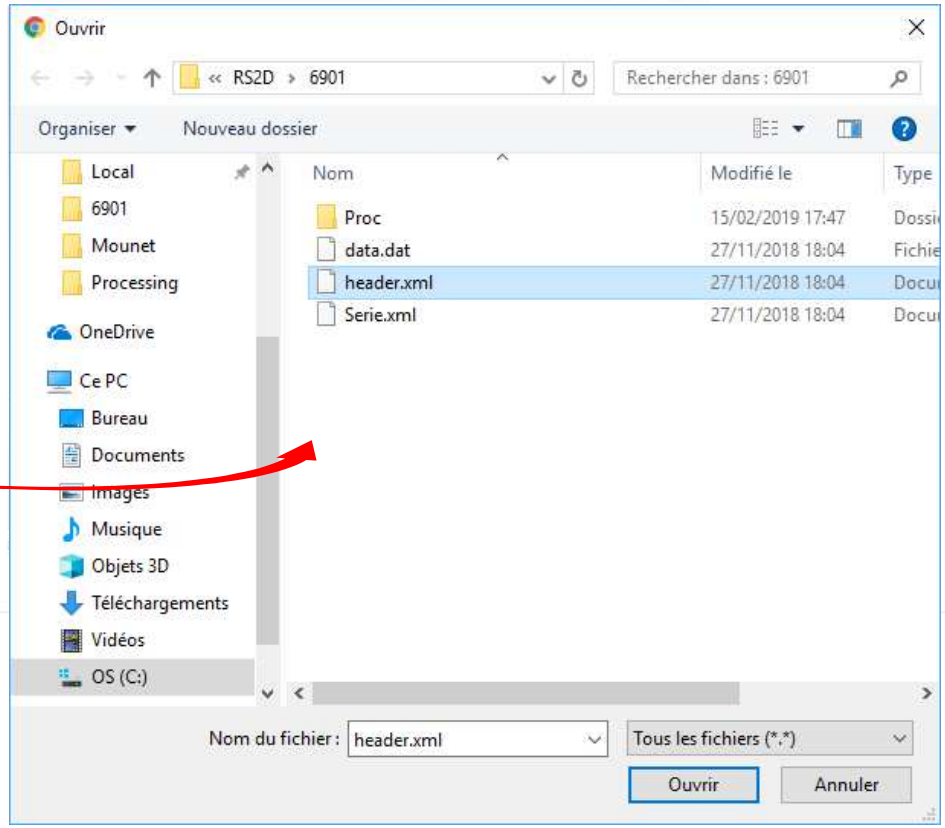
FID raw file

Browse... data.dat

Upload complete

Acquisition parameter file

Bro se... No file selected



This website is optimized for: chrome

(C) Daniel Jacob - INRA UMR 1332, PMB, MetaboHUB, 2019

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Spectral preprocessing for 1D NMR (1H & 13C)

Processing | Export | Help

Spectrum | FID | Acquisition Parameters | Processing Parameters | Log

Line Broadening:

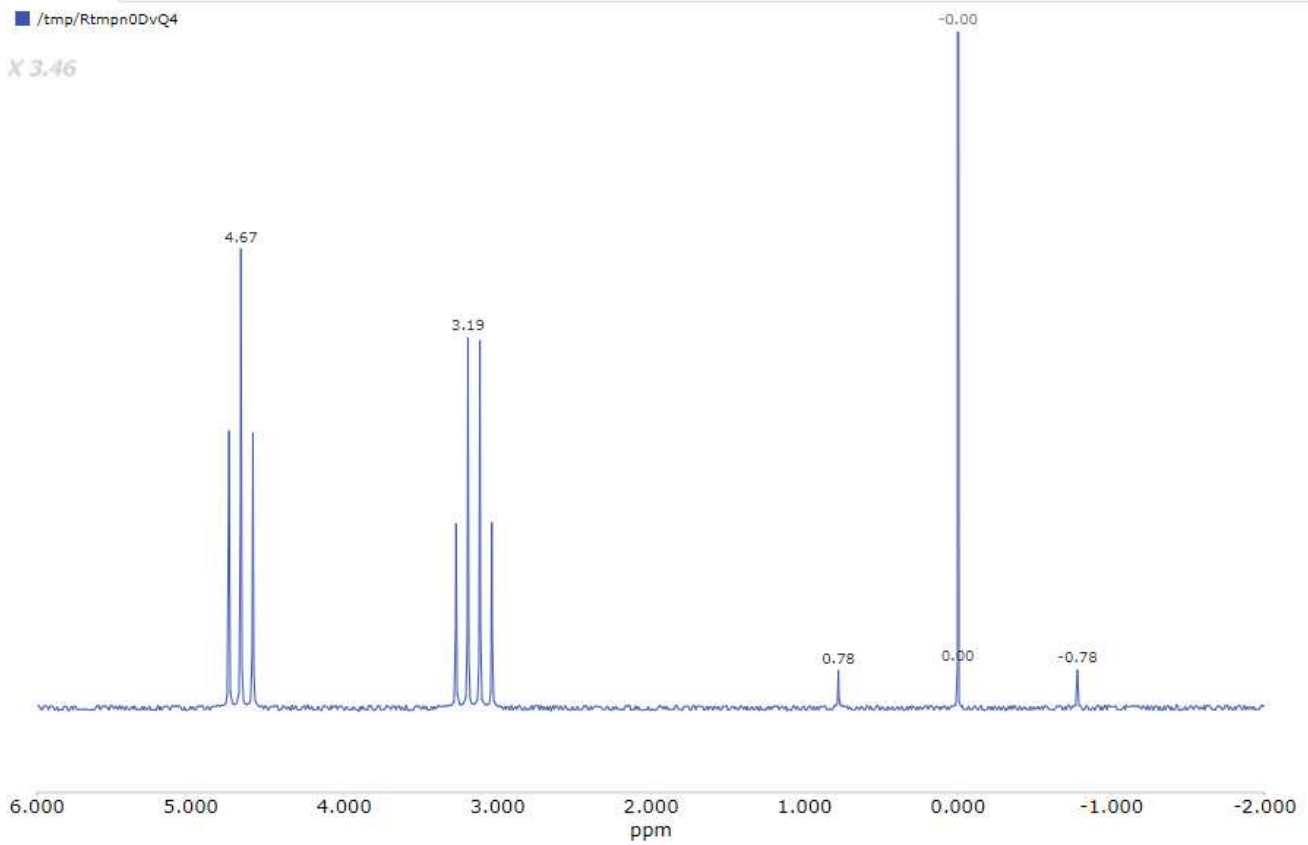
0.3

Gaussian Broadening:

0

- [ ] Zero filling
- [ ] Zero order phase setting
- [ ] First order phase setting
- [ ] Baseline correction
- [ ] Zeroing of Negative Values
- [x] TSP/TMS/DSS
- [ ] Zeroing

Reset



Phase 0

0

Phase 1

0

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Spectral preprocessing for 1D NMR (1H & 13C)

Processing | Export | Help

Spectrum | FID | Acquisition Parameters | Processing Parameters | Log

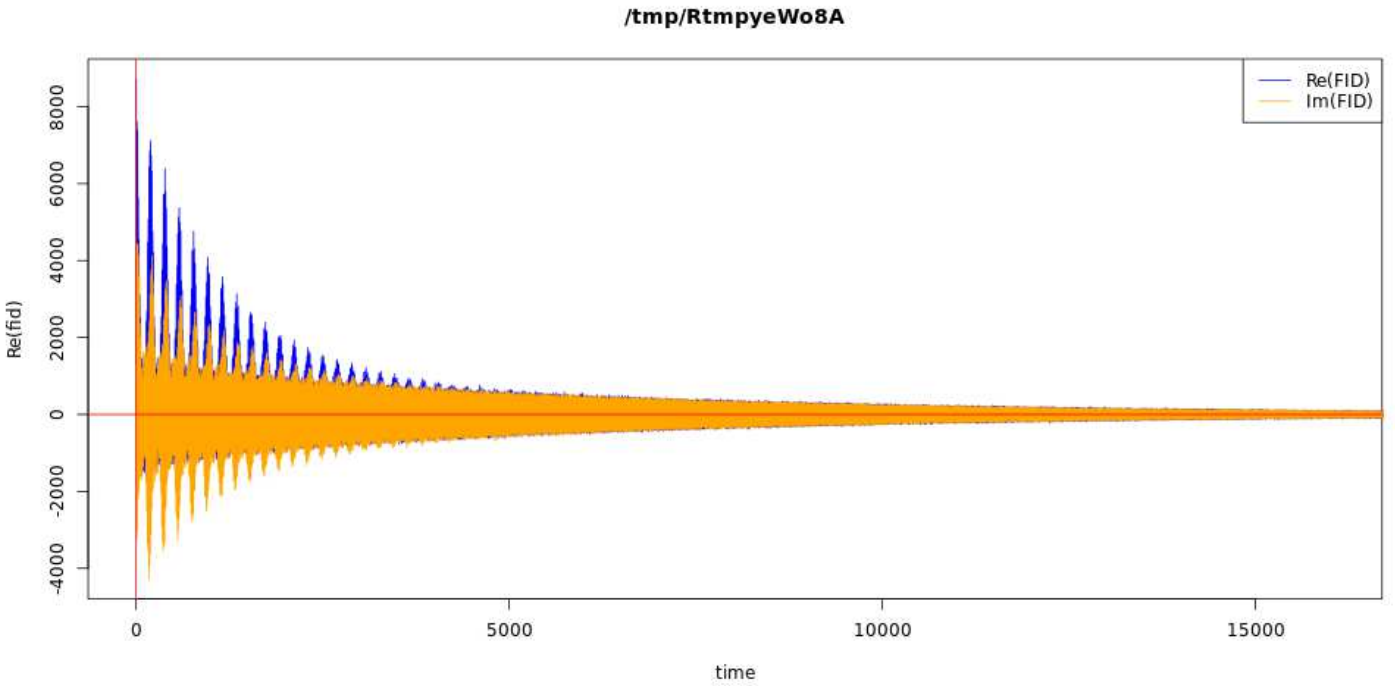
Line Broadening:

0.3

Gaussian Broadening:

0

- [ ] Zero filling
- [ ] Zero order phase setting
- [ ] First order phase setting
- [ ] Baseline correction
- [ ] Zeroing of Negative Values
- [x] TSP/TMS/DSS
- [ ] Zeroing



Time domain (%)

0 | 49 | 100

Reset

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Spectrum | FID | Acquisition Parameters | Processing Parameters

	Parameters	Values	Corresponding fields in the Header.xml file
Manufacturer	VENDOR	RS2D	MANUFACTURER
Software version	SOFTWARE	1.218-SNAPSHOT	SOFTWARE_VERSION
Origin of the sample (Name or Path)	NAME	/tmp/Rtmpn0DvQ4/c92c46e906c18ef5e75b0e77	No found
Instrument / Model	INSTRUMENT	RS2D NMRCube	MODEL_NAME
Probe name	PROBE	Dual 5mm	PROBES
Pulse sequence used for the acquisition	PULSE		SEQUENCE_NAME
nucleus for frequency channel f1	NUC	1H	OBSERVED_NUCLEUS
Number of Scans	TOTAL SCANS	0	NUMBER_OF_AVERAGES
Number of Steady State Scans	STEADY STATE SCANS	0	DUMMYSCANS
Sample solvent name	SOLVENT	D2O	SOLVENT
Temperature (K)	TEMP(K)	293.15	SAMPLE_TEMPERATURE
Relaxation delay (s)	RELAX. DELAY	1	Last delay
Spinning rate	SPINNINGRATE	0	SPIN_RATE
Pulse width (ms)	PULSEWIDTH	10	P1.width * 1e6
Number of data points	TD	32768	Nb Point
Group delay	GRPDLY	0	No found – It seems not necessary
Spectral width (ppm)	SW	14.9950516333052	*=SWH/SFO1*
Spectral width (Hz)	SWH	6000	SPECTRAL_WIDTH
Transmitter frequency (MHz)	SFO1	400.131999990819	OBSERVED_FREQUENCY / 1e6
Frequency offset in Hz	O1	1100.16198730469	OFFSET_FREQ_1

Rnmr1D

Installation of the Rnmr1D package
See : **https://github.com/INRA/Rnmr1D/**

RS2D

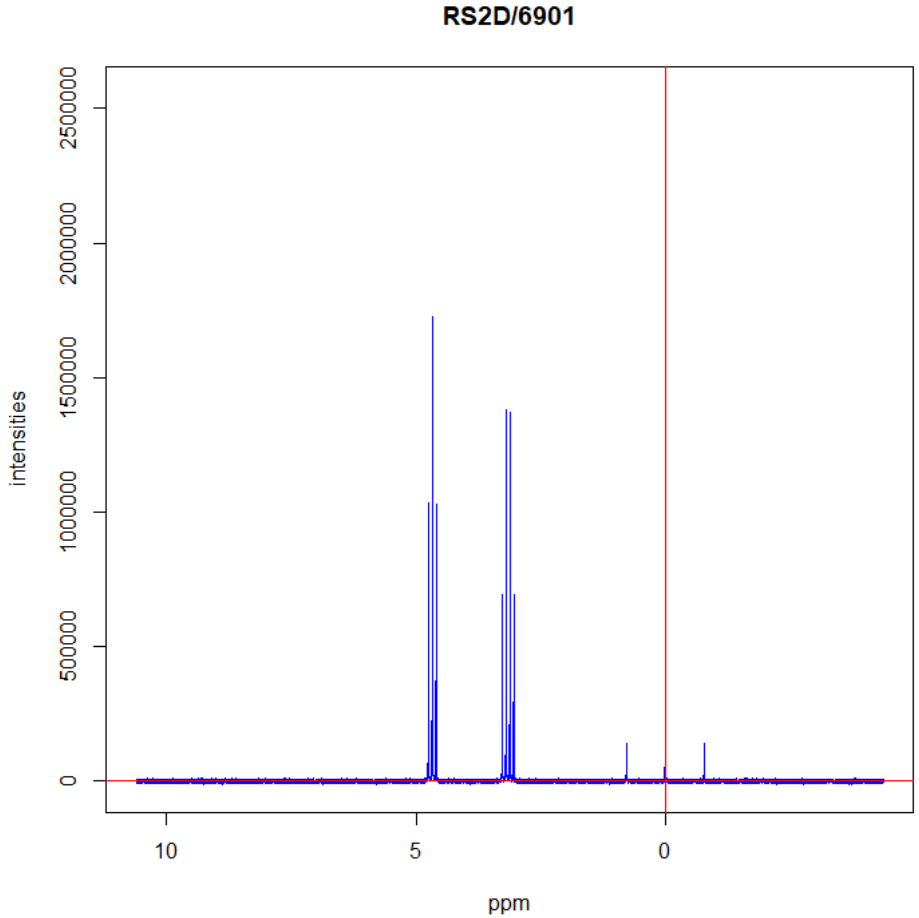
RStudio

```
library(Rnmr1D)

ACQDIR <- "C:/DATA/nmr_examples/RS2D/6901"

procParams <- SpecInrProcpar
procParams$VENDOR <- 'rs2d'
procParams$INPUT_SIGNAL <- 'fid'
procParams$LB <- 0.3
procParams$ZEROFILLING <- TRUE
procParams$ZFFAC <- 2
procParams$OPTPHC0 <- FALSE
procParams$OPTPHC1 <- FALSE
procParams$TSP <- TRUE
procParams$LOGFILE <- ""

system.time( spec <- SpecInrDoProc(Input=ACQDIR,param=procParams) )
# Read the FID ...OK
# Preprocessing ...
# →Exp. Line Broadening (LB=0.300000)
# →TD = 32768
# →Zero Filling (x2)
# →SI = 65536
# →FFT ...OK
# OK
# PPM calibration based on TSP .... PPM min =-4.382556
# OK
# utilisateur     système     écoulé
#        0.46        0.00        0.45
Rnmr1D:::plotSpectrum(spec)
```



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Rnmr1D

Installation of the Rnmr1D package
See : **https://github.com/INRA/Rnmr1D/**

RS2D

RStudio

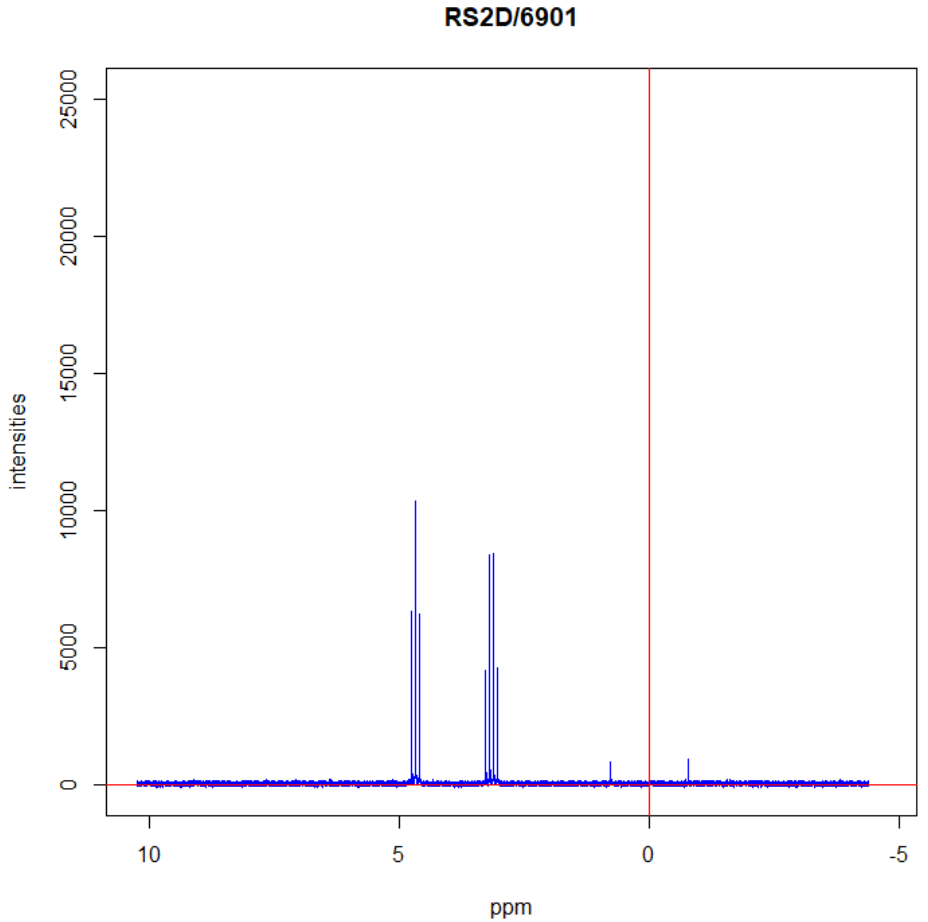
```
library(Rnmr1D)

ACQDIR <- "C:/DATA/nmr_examples/RS2D/6901"

procParams <- SpecIrProcpar
procParams$VENDOR <- 'rs2d'
procParams$INPUT_SIGNAL <- 'lr'
procParams$PDATA_DIR <- "Proc/0"
procParams$TSP <- TRUE
procParams$LOGFILE <- ""

system.time( spec <- SpecIrDoProc(Input=ACQDIR,param=procParams) )
# Read the lR ...OK
# utilisateur     système     écoulé
#        0.43        0.00        0.42

Rnmr1D:::plotSpectrum(spec)
```



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Rnmr1D

Installation of the Rnmr1D package
See : https://github.com/INRA/Rnmr1D/

RS2D

RStudio

```
library(Rnmr1D)

raw_dir <- 'C:/Workdir/Share/tmp'

DIR <- 'RS2D400'
RAWDIR <- file.path(raw_dir, DIR)

MACROCMD <-
"### Vendor=rs2d; Type=fid; LB=0.3; GB=0; ZF=2; BLPHC=FALSE; PHC0=FALSE; PHC1=FALSE; FP=0; TSP=TRUE"

CMDFILE <- tempfile()
cat(MACROCMD"\n", sep='', file=CMDFILE, append=FALSE)

metadata <- generateMetadata(RAWDIR, procParams, NULL)
metadata
#  $`samples`
#       [,1]  [,2]
#  [1,] "6901" "6901"
#  [2,] "6902" "6902"
#  [3,] "6903" "6903"
#
#  $rawids
#       [,1]                                  [,2] [,3]
#  [1,] "C:/Workdir/Share/tmp/RS2D400/6901" "0"  "0"
#  [2,] "C:/Workdir/Share/tmp/RS2D400/6902" "0"  "0"
#  [3,] "C:/Workdir/Share/tmp/RS2D400/6903" "0"  "0"
#
#  $factors
#       [,1] [,2]
#  [1,] "1"  "Samplecode"
```

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Rnmr1D

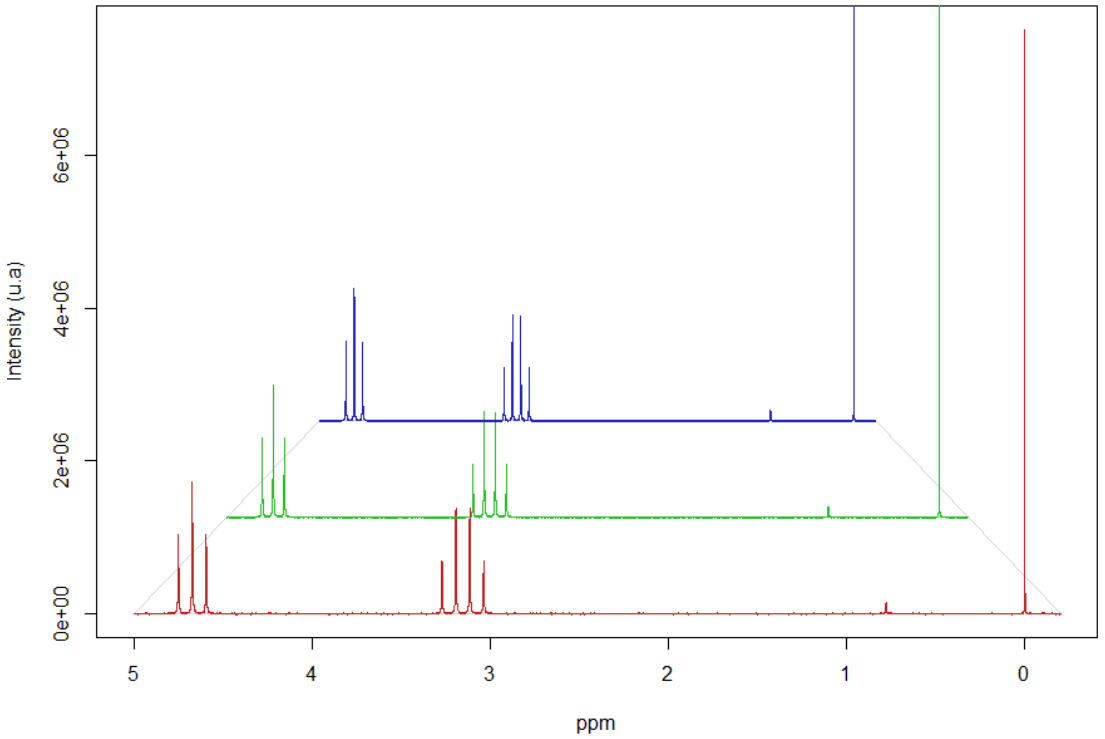
Installation of the Rnmr1D package
See : **https://github.com/INRA/Rnmr1D/**

RS2D

RStudio

```
system.time( out <- Rnmr1D::doProcessing(RAWDIR, cmdfile=CMDFILE, samplefile=NULL, ncpu=3) )
# Rnmr1D:  ----READING and CONVERTING---
# Rnmr1D:  Vendor=rs2d, Type=fid, LB=0.3, GB=0, ZF=2, BLPHC=FALSE, PHC0=FALSE, PHC1=FALSE, FP=0, TSP=TRUE
# Rnmr1D:  Generate the 'samples' & 'factors' files from the list of
# Rnmr1D:  ---Nb Spectra = 3 -- Nb Cores = 3
#
# Rnmr1D:  Generate the final matrix of spectra...
# Rnmr1D: -------------------------------------
# Rnmr1D: Process the Macro-commands file
# Rnmr1D: -------------------------------------
# Rnmr1D:
# utilisateur     système      écoulé
#        0.50        0.08        5.77

plotSpecMat(out$specMat, ppm_lim=c(-0.2,5), K=0.33)
```



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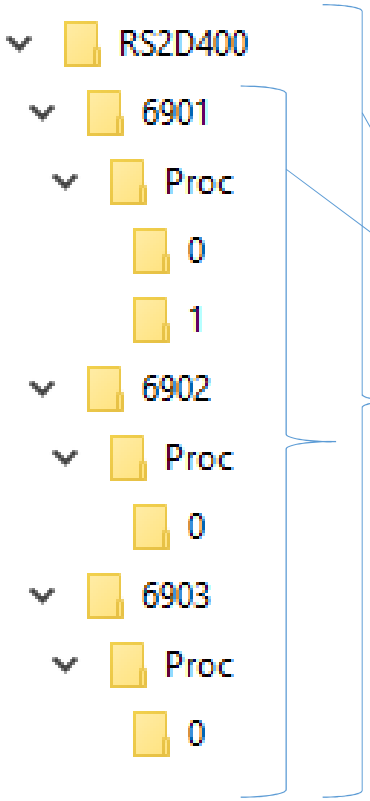
Daniel Jacob
Feb. 2019

Bordeaux Metabolome Facility

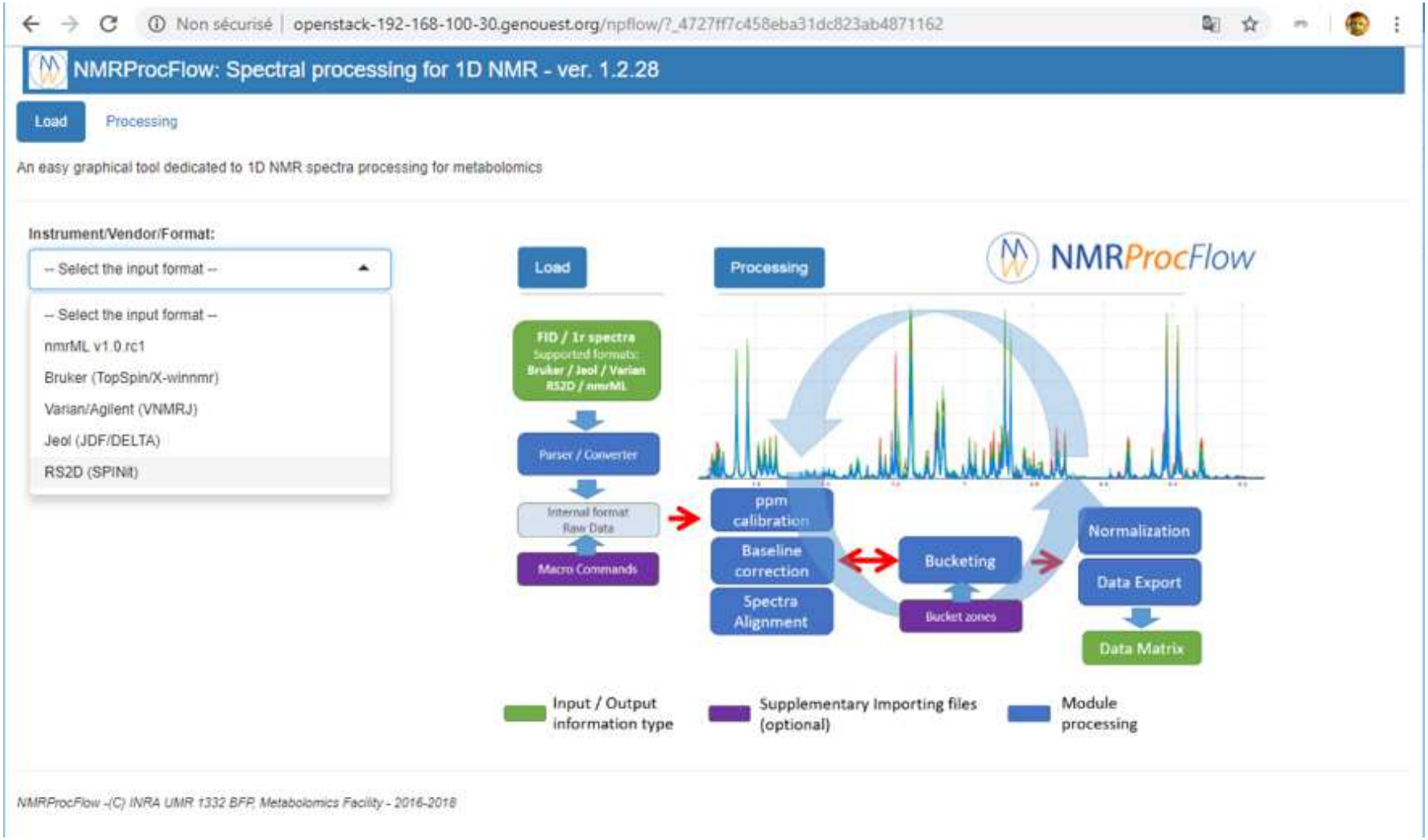
Data preparation step



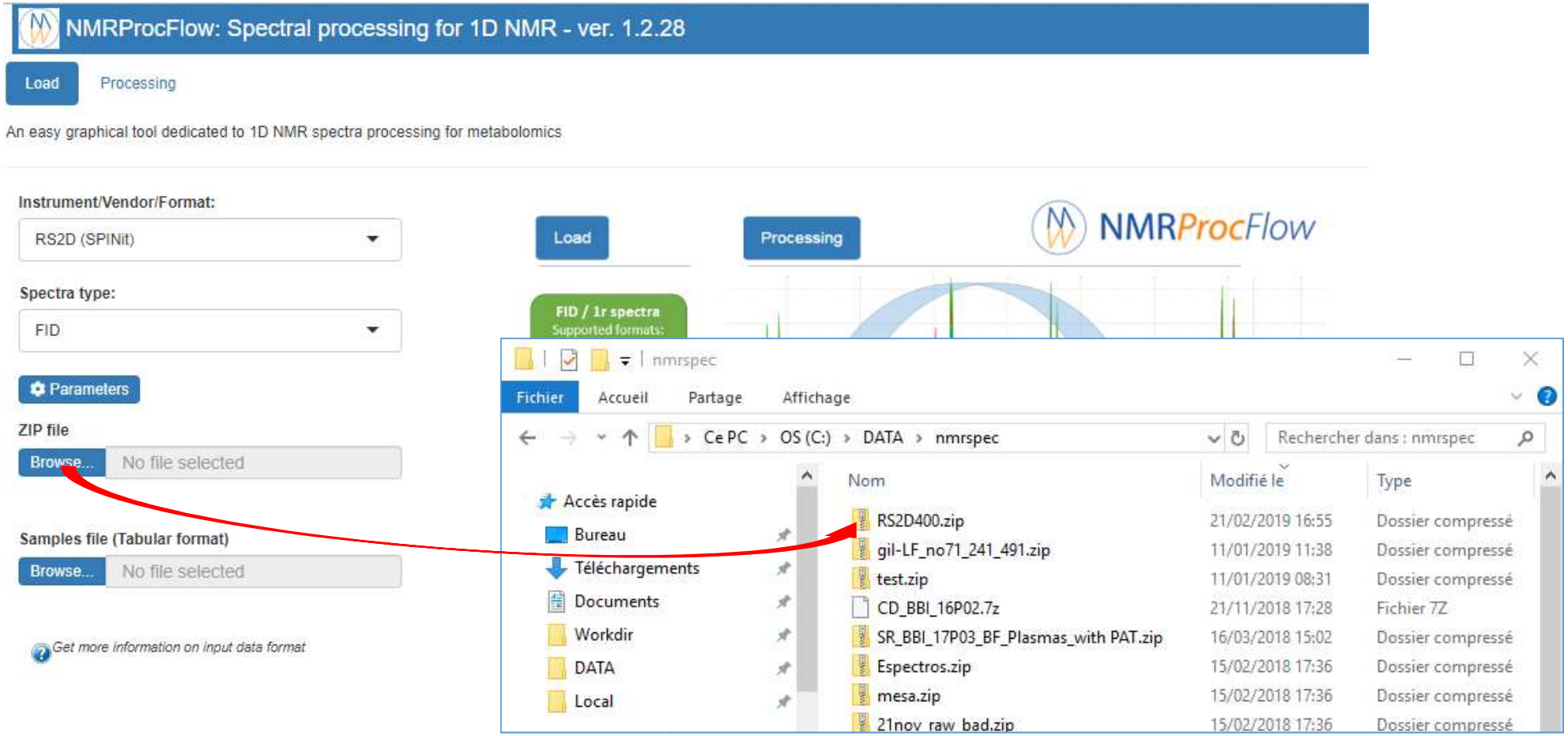
Simply zip the entire directories including all spectra of the experiment

- **possibly including (or not) a root directory**

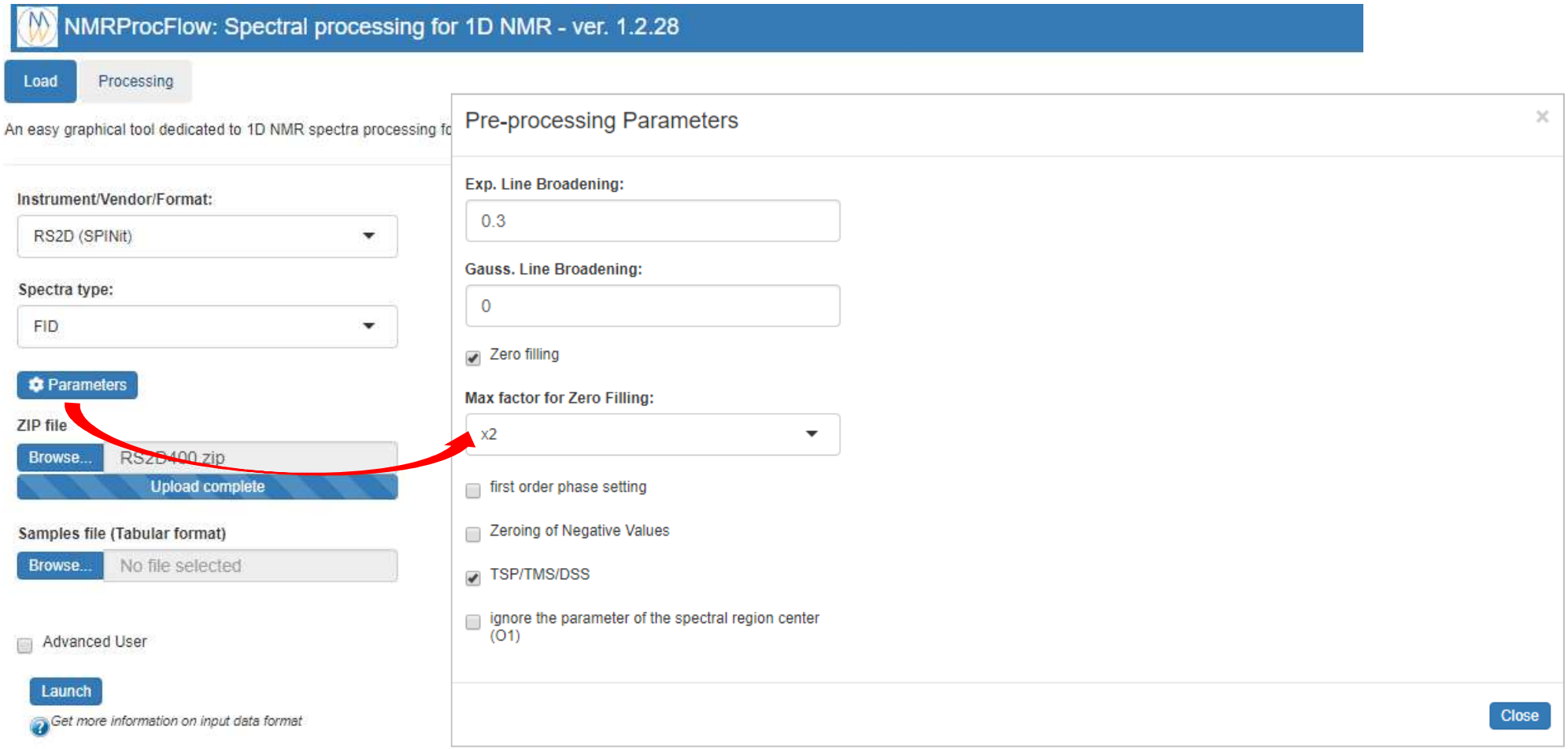
Preprocessing step



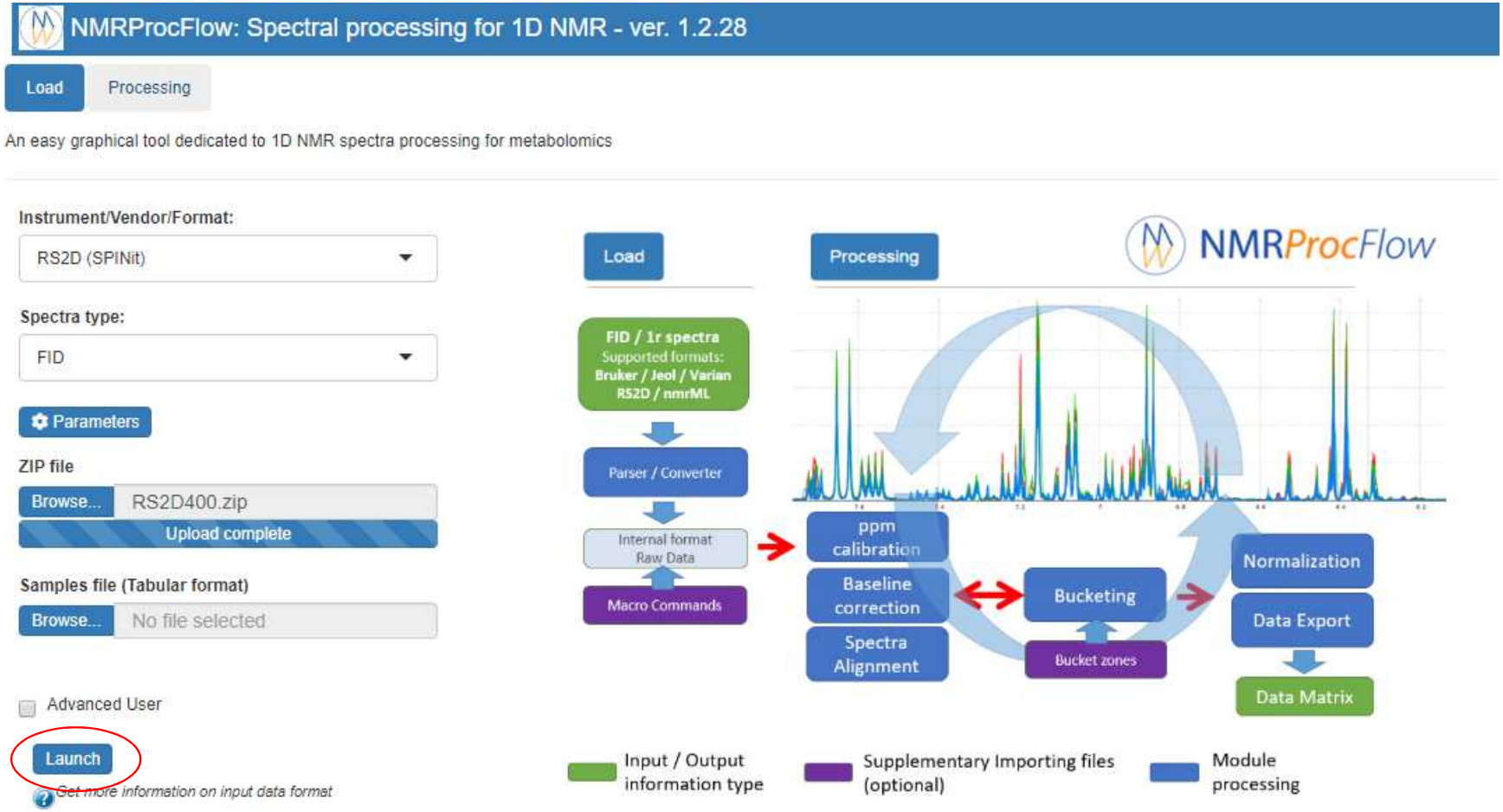
Preprocessing step



Preprocessing step

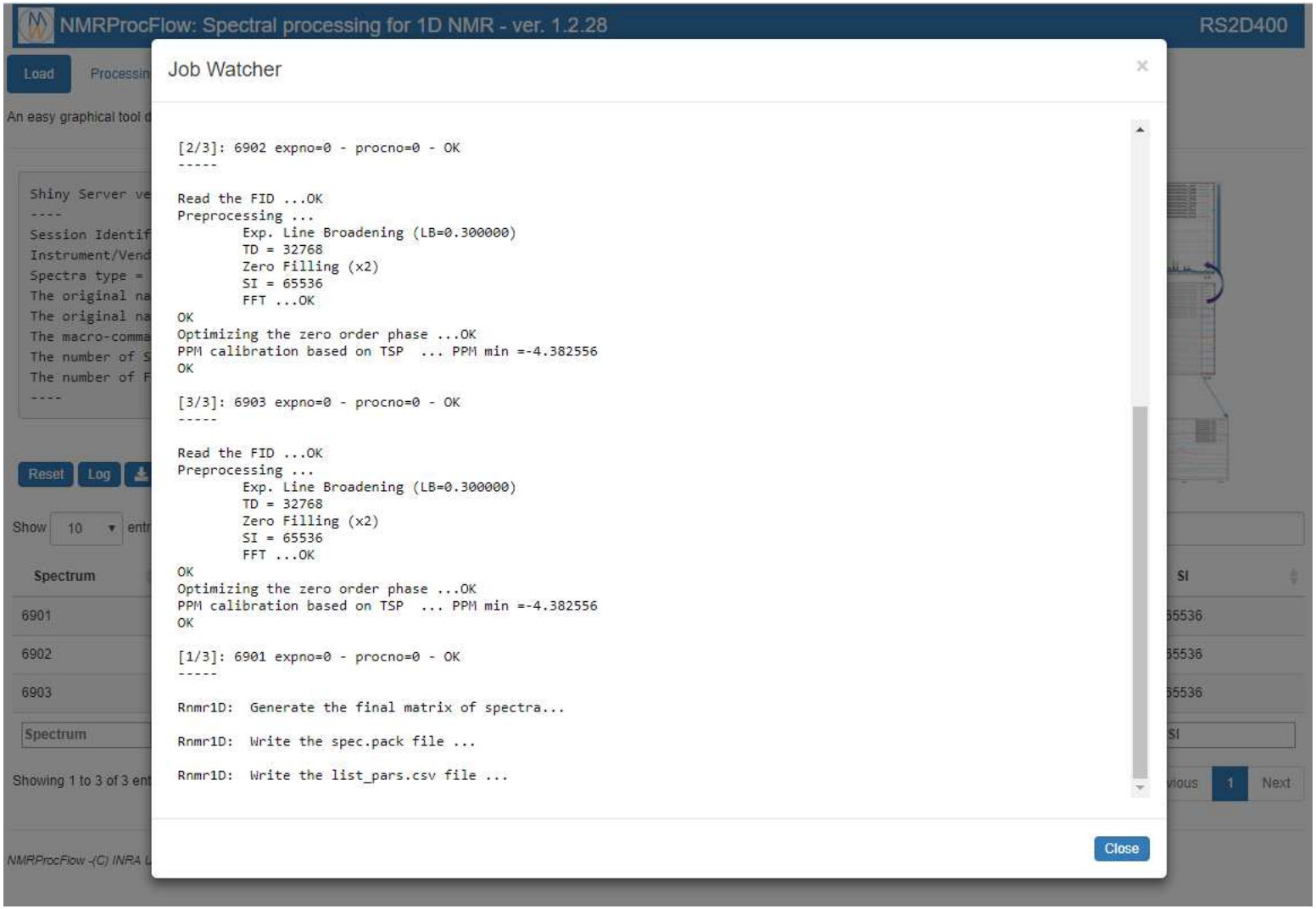


Preprocessing step



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

Preprocessing step



NMRProcFlow: Spectral processing for 1D NMR - ver. 1.2.28 RS2D400

Load | Processing

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

```
Shiny Server version 1.5.9.923
----
Session Identifier = _4727ff7c458eba31dc823ab4871162
Instrument/Vendor/Format = rs2d
Spectra type = fid
The original name of the Zip file = RS2D400.zip
The original name of the Samples file = NA
The macro-command file for processing =
The number of Spectra = 3
The number of Factors = 1
----
```

Reset | Log | Export Parameters

Show 10 entries Search:

Spectrum	PULSE	NUC	SOLVENT	PROCNO	PHC0	PHC1	SW	SF	SI
6901		1H	D2O	0	6.266027	0	14.99505	400.132	65536
6902		1H	D2O	0	6.266027	0	14.99505	400.132	65536
6903		1H	D2O	0	6.266027	0	14.99505	400.132	65536
Spectrum	PULSE	NUC	SOLVENT	PROCNO	PHC0	PHC1	SW	SF	SI

Showing 1 to 3 of 3 entries

Previous 1 Next

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Data visualization / processing

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