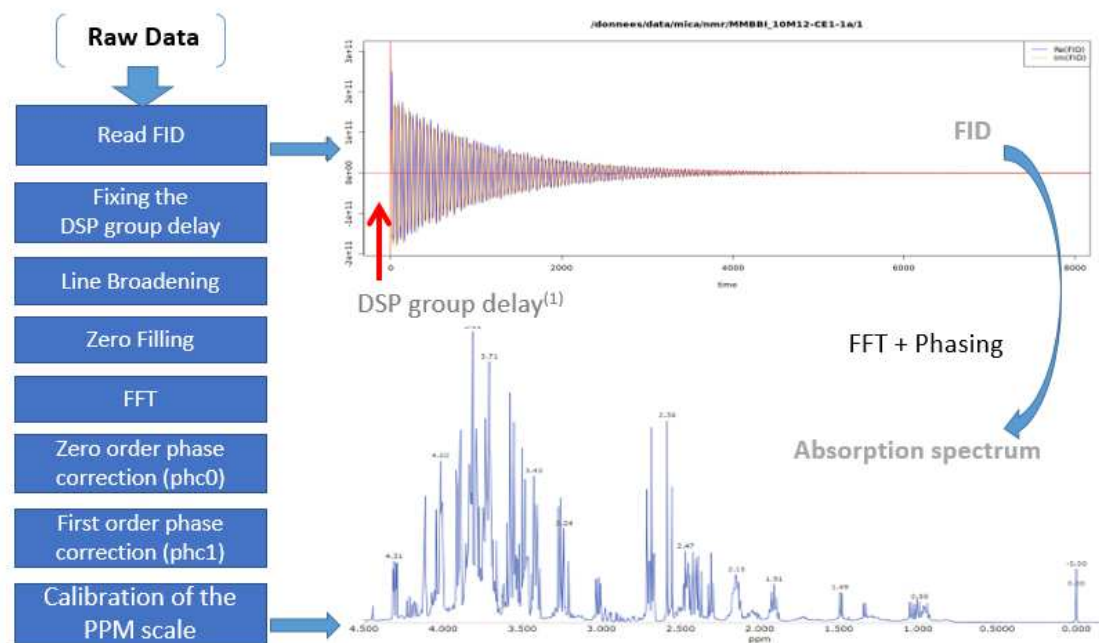


## Spectral preprocessing for 1D NMR (1H & 13C)

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](#).



<https://pmb-bordeaux.fr/nmrsec/>



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



# 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



Agilent  
Technologies



This website is optimized for:  chrome

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



## 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 (SPINet)

FID raw file

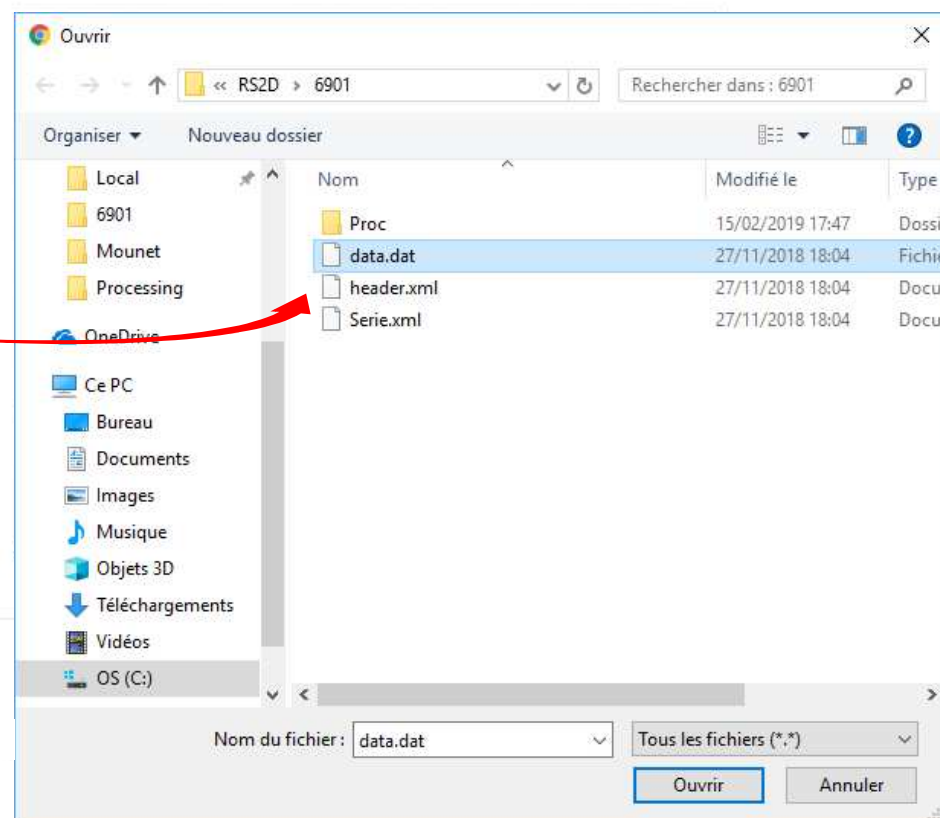
Browse...

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



## 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 (SPINet)

FID raw file

Browse...

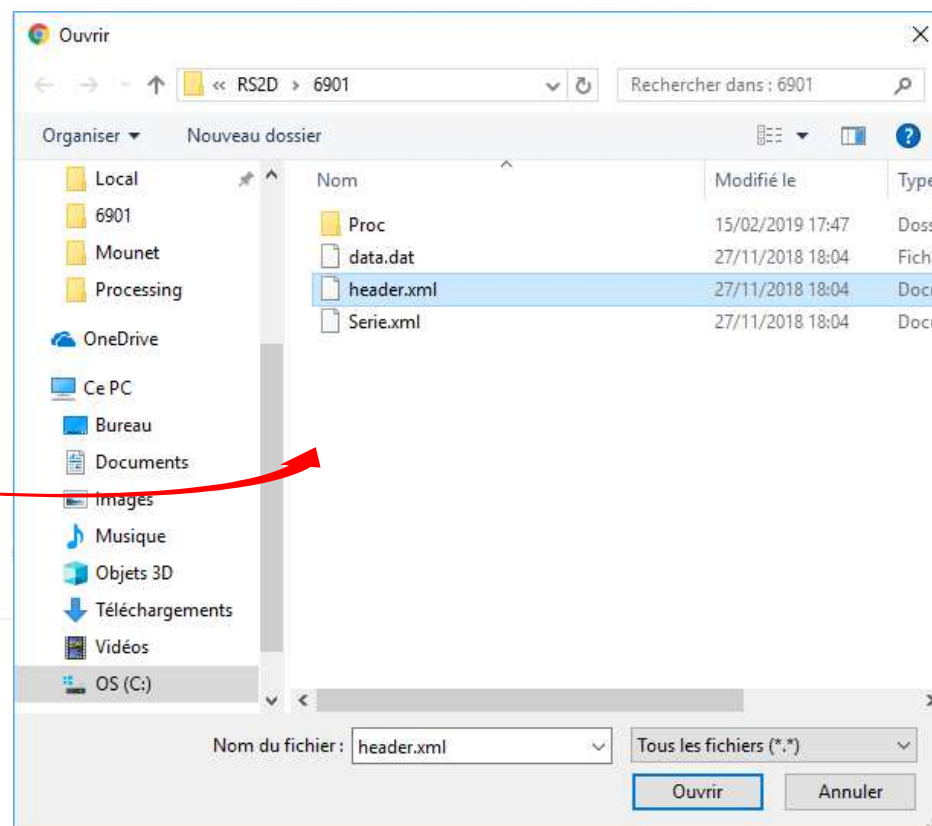
data.dat

Upload complete

Acquisition parameter file

Browse...

No file selected



This website is optimized for: chrome

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



# 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

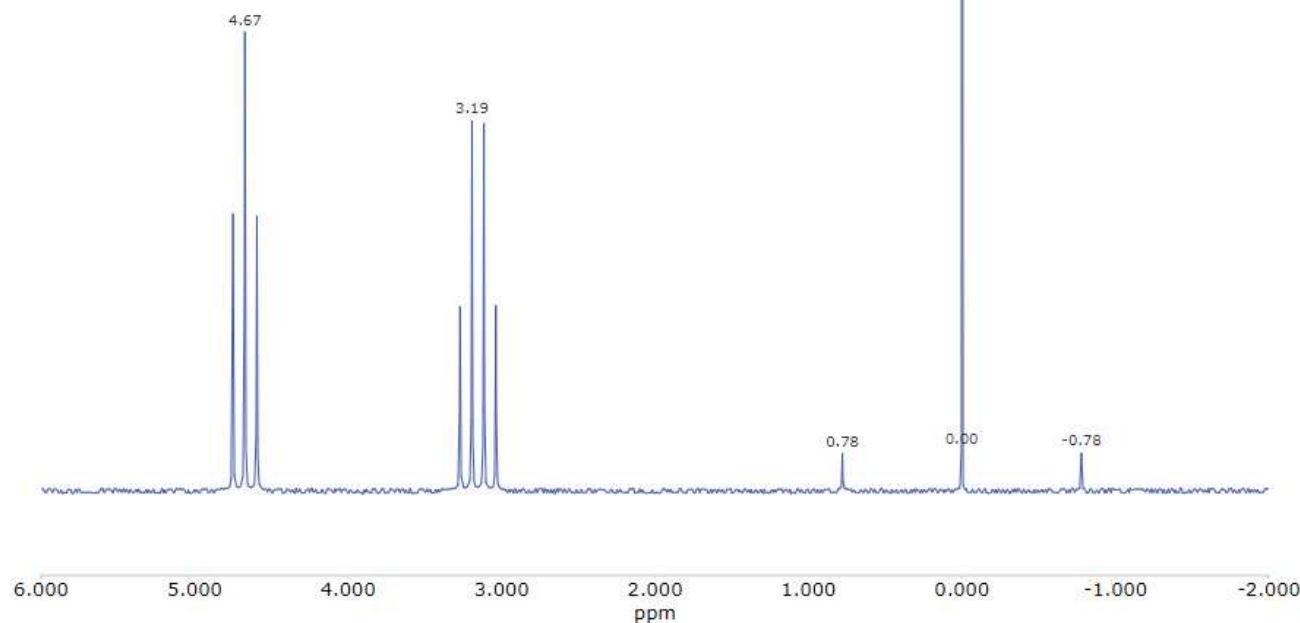
☒ TSP/TMS/DSS

☐ Zeroing

Reset

/tmp/Rtmpn0DvQ4

X 3.46



Phase 0

0

Phase 1

0



# 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

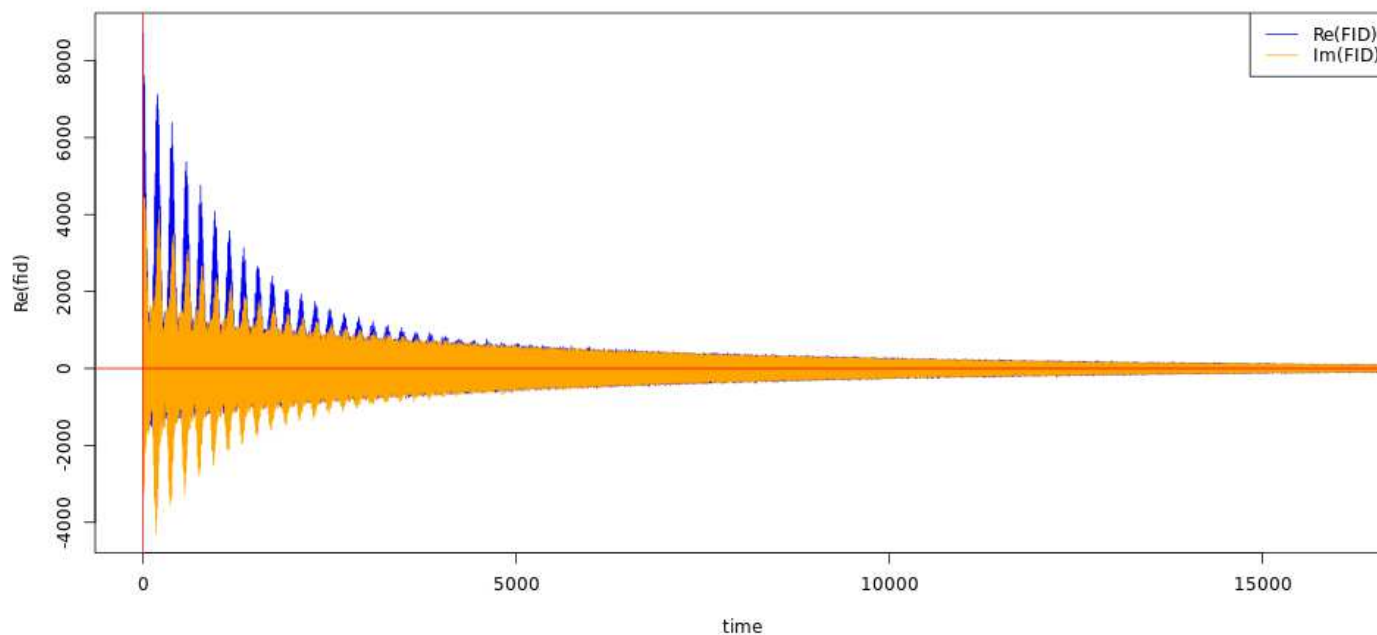
☐ Zeroing of Negative Values

☒ TSP/TMS/DSS

☐ Zeroing

Reset

/tmp/RtmpyeWo8A



Time domain (%)





	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





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

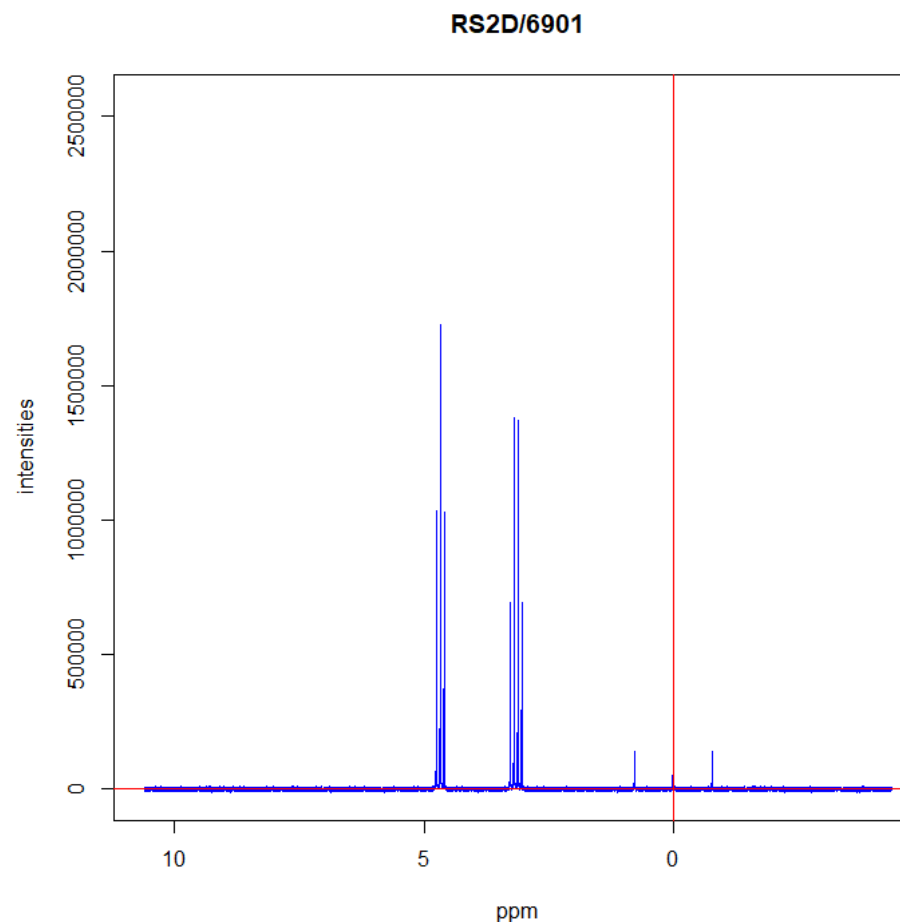


```
library(Rnmr1D)

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

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

system.time(.spec <- SpecIrDoProc(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)
```







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



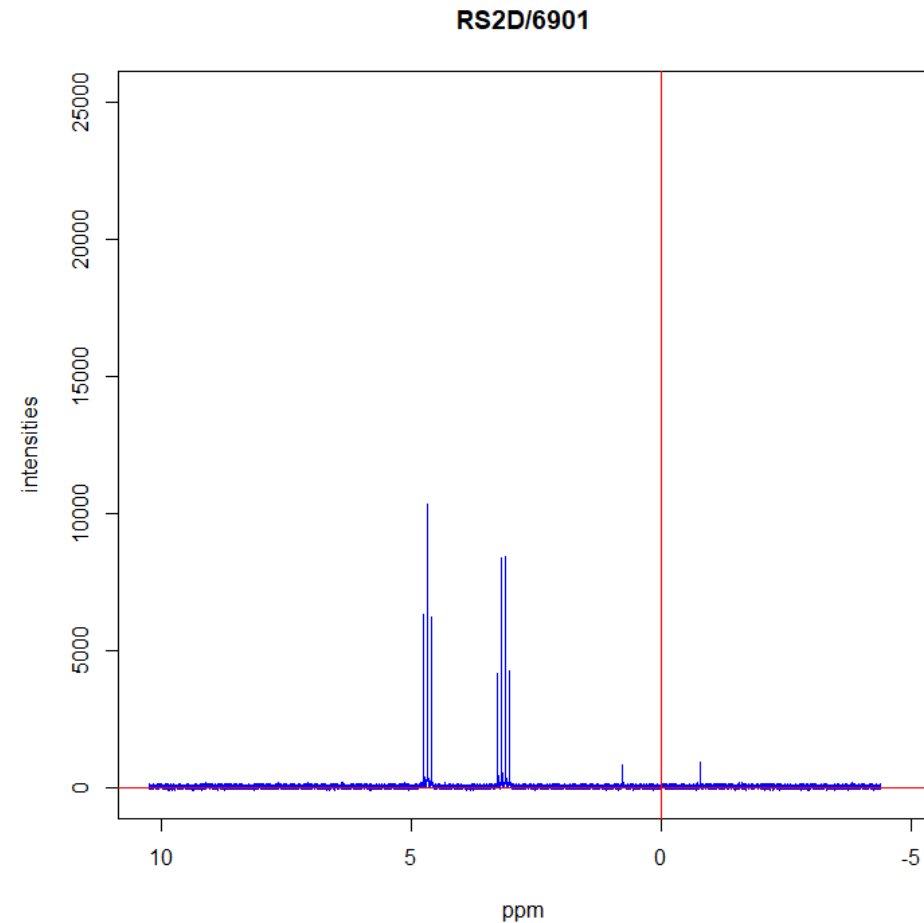
```
library(Rnmr1D)

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

procParams.<-SpecIrProcpar
procParams$VENDOR.<-.'rs2d'
procParams$INPUT_SIGNAL.<-.'1r'
procParams$PDATA_DIR.<-."Proc/0"
procParams$TSP.<-TRUE
procParams$LOGFILE.<-.""

system.time(.spec.<-SpecIrDoProc(Input=ACQDIR,param=procParams).)
# Read the 1R...OK
# utilisateur.....système.....écoulé.
# .....0.43.....0.00.....0.42.

Rnmr1D::plotSpectrum(spec)
```





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



```
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"

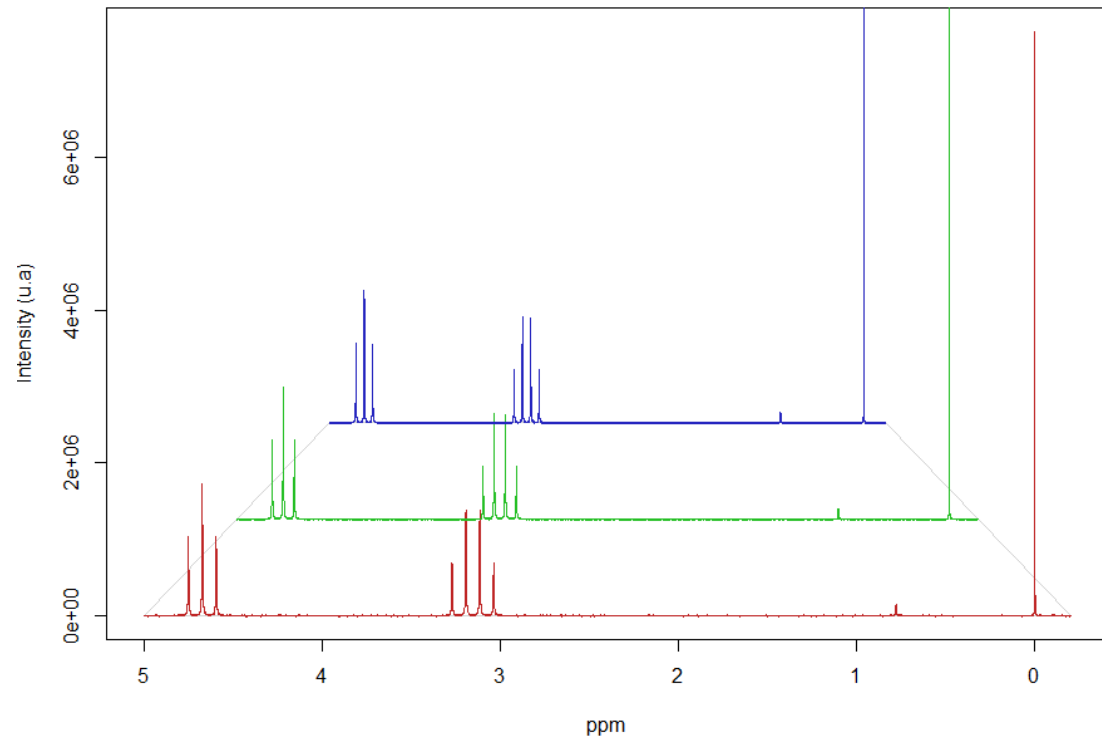
CMDFILE <- tempfile()
cat(MACROCMD"\n", .sep=' ', .file=CMDFILE, .append=FALSE)

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"
```



```
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)
```

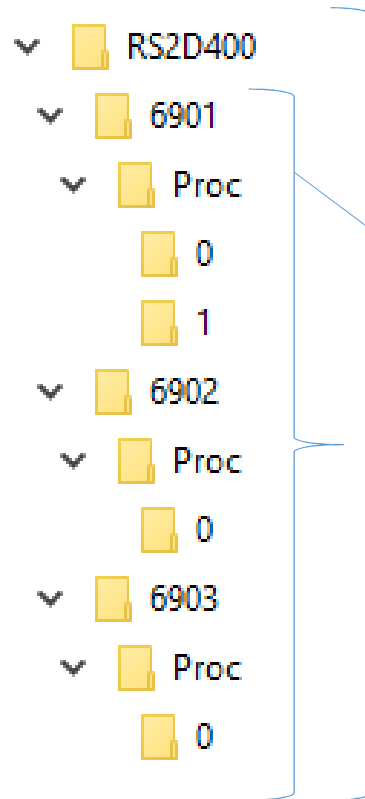




Daniel Jacob  
Feb. 2019

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

← → ↻ ⓘ Non sécurisé | openstack-192-168-100-30.genouest.org/npflow/?\_4727ff7c458eba31dc823ab4871162

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

Load Processing

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

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)

Load Processing

FID / 1r spectra  
Supported formats:  
Bruker / Jeol / Varian  
RS2D / nmrML

Parser / Converter

Internal format  
Raw Data

Macro Commands

ppm calibration

Baseline correction

Spectra Alignment

Bucketing

Bucket zones

Normalization

Data Export

Data Matrix

Input / Output information type

Supplementary importing files (optional)

Module processing

NMRProcFlow

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

```
graph TD
    subgraph Load
        A[FID / 1r spectra  
Supported formats:  
Bruker / Jeol / Varian  
RS2D / nmrML] --> B[Parser / Converter]
        B --> C[Internal format  
Raw Data]
        D[Macro Commands] --> C
    end
    subgraph Processing
        C --> E[ppm calibration]
        E --> F[Baseline correction]
        F --> G[Spectra Alignment]
        G --> H[Bucketing]
        H --> I[Normalization]
        I --> J[Data Export]
        J --> K[Data Matrix]
        L[Bucket zones] --> H
    end
    E --> F
    F --> G
    G --> H
    H --> I
    I --> J
    J --> K
```

## Preprocessing step



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

Load

Processing

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

Instrument/Vendor/Format:

RS2D (SPINIt)

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](#)

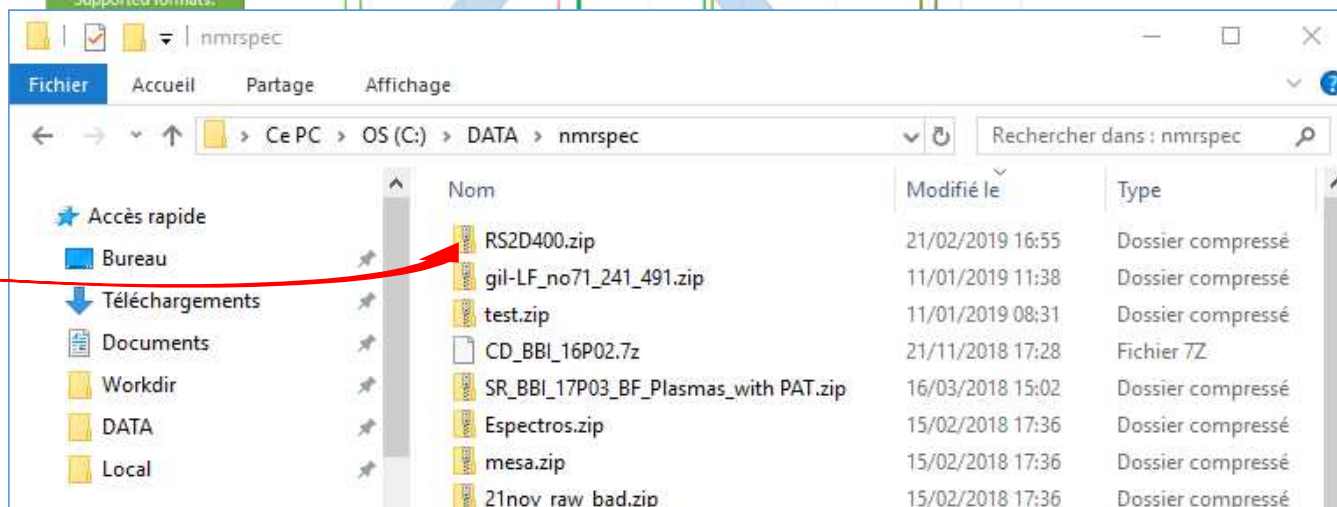
Load

Processing



NMRProcFlow


FID / 1r spectra  
Supported formats:



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



## Preprocessing step

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

Load

Processing

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

Instrument/Vendor/Format:  
RS2D (SPINIt) ▼

Spectra type:  
FID ▼


Parameters

ZIP file  
Browse... RS2D400.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

☒ Zero filling

Max factor for Zero Filling:  
x2 ▼

☐ first order phase setting


☐ Zeroing of Negative Values

☒ TSP/TMS/DSS

☐ ignore the parameter of the spectral region center (O1)

Close

## Preprocessing step

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

Load

Processing

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

Instrument/Vendor/Format:

RS2D (SPINIt) ▼

Spectra type:

FID ▼

Parameters

ZIP file

Browse... RS2D400.zip

Upload complete

Samples file (Tabular format)

Browse... No file selected


Advanced User

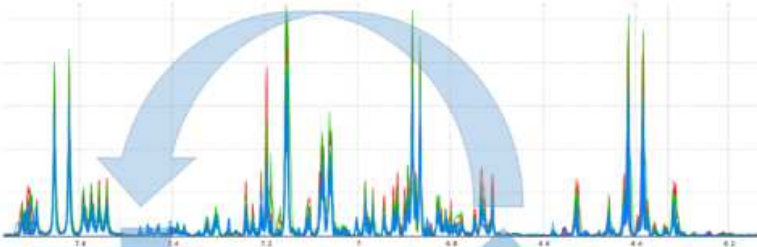
Launch

Get more information on input data format

Load

Processing

 **NMRProcFlow**



Flowchart illustrating the preprocessing steps:

- Input / Output information type** (Green box): FID / 1r spectra. Supported formats: Bruker / Jeol / Varian RS2D / nmrML.
- Module processing** (Blue box): Parser / Converter.
- Internal format Raw Data** (Light blue box).
- Supplementary Importing files (optional)** (Purple box): Macro Commands.
- Module processing** (Blue box): ppm calibration, Baseline correction, Spectra Alignment.
- Module processing** (Blue box): Bucketing.
- Supplementary Importing files (optional)** (Purple box): Bucket zones.
- Module processing** (Blue box): Normalization.
- Module processing** (Blue box): Data Export.
- Input / Output information type** (Green box): Data Matrix.

Legend:

- Input / Output information type (Green box)
- Supplementary Importing files (optional) (Purple box)
- Module processing (Blue box)

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

Job Watcher

```
[2/3]: 6902 expno=0 - procno=0 - OK
-----
Read the FID ...OK
Preprocessing ...
  Exp. Line Broadening (LB=0.300000)
  TD = 32768
  Zero Filling (x2)
  SI = 65536
  FFT ...OK
OK
Optimizing the zero order phase ...OK
PPM calibration based on TSP ... PPM min =-4.382556
OK

[3/3]: 6903 expno=0 - procno=0 - OK
-----
Read the FID ...OK
Preprocessing ...
  Exp. Line Broadening (LB=0.300000)
  TD = 32768
  Zero Filling (x2)
  SI = 65536
  FFT ...OK
OK
Optimizing the zero order phase ...OK
PPM calibration based on TSP ... PPM min =-4.382556
OK

[1/3]: 6901 expno=0 - procno=0 - OK
-----
Rnmr1D: Generate the final matrix of spectra...
Rnmr1D: Write the spec.pack file ...
Rnmr1D: Write the list_pars.csv file ...
```

Close

Shiny Server ve  
----  
Session Identif  
Instrument/Vend  
Spectra type =  
The original na  
The original na  
The macro-comm  
The number of S  
The number of F  
----  
Reset Log  
Show 10 ▼ entr  
Spectrum  
6901  
6902  
6903  
Spectrum  
Showing 1 to 3 of 3 ent  
NMRProcFlow -(C) INRA

SI  
65536  
65536  
65536  
SI  
Previous 1 Next



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

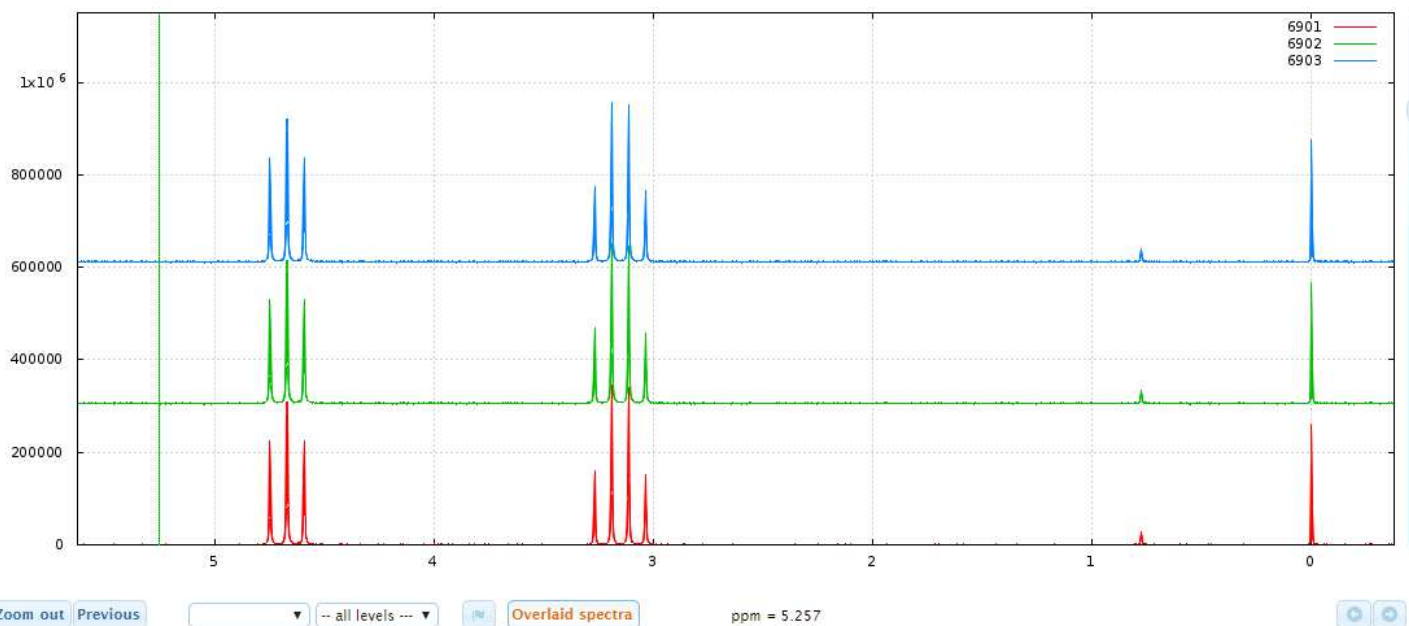
1

Next

## Data visualization / processing

Load

Processing



Processing

Bucketing

Data Export

Processing Type:

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

Type of Correction

Global Correction

Level of Correction

Soft correction

noisy PPM range:

10.5 10.2

   MD

Launch

☒ Job Watcher

Undo

Log

CMD