

Vendor to nmrML Converter

- This online converter is based on the the Java tool nmrMLcreate (see [Github nmrML](#)) and allows you to convert bruker, jeol or varian vendor raw formats (1D NMR) into the standardized nmrML format. Amongst many advantages, nmrML files **1**) are readable by a variety of open source processing tools, **2**) can serve to generate an ISA metadata backbone file automatically, **3**) can be validated with the semantic validator and not the least, **4**) are annotated by a standardized terminology ([nmrCV](#)), avoiding semantic ambiguity. See Schober et al (2017), [doi:10.1021/acs.analchem.7b02795](https://doi.org/10.1021/acs.analchem.7b02795).
- Using this converter:**
 - Multiple nmr fid files should be packed into the same ZIP archive. **For Bruker and Varian**, each nmr fid file must have its own directory within the ZIP archive, along with the acquisition parameter file. **For Jeol**, each nmr fid data along with the acquisition parameter have to be embedded within a JDF format file within the ZIP archive..
 - To test, and get familiar with the expected zip folder structure, you can [download a zip file](#) that contains eleven fid spectra from Bruker

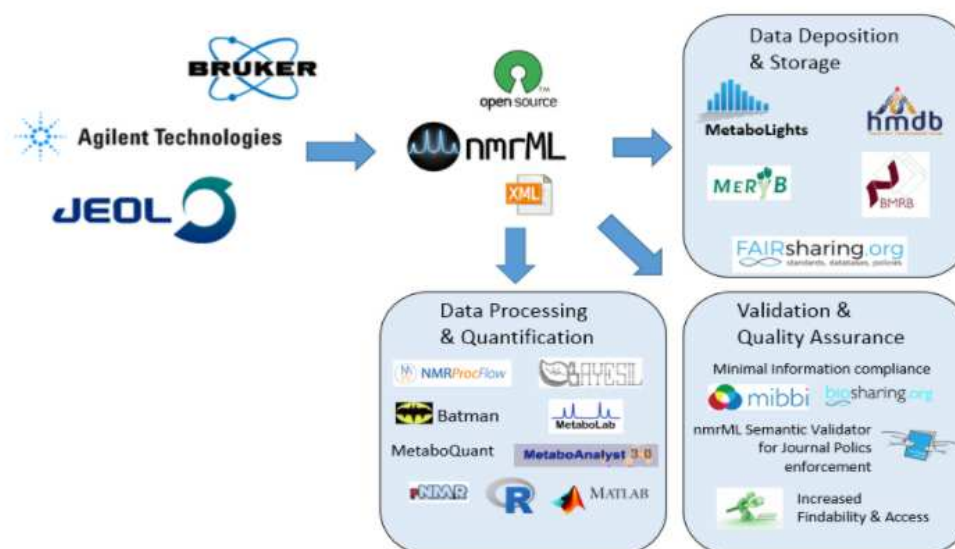
Vendor (Format):

Jeol (JDF/DELTA)

ZIP file

Browse...

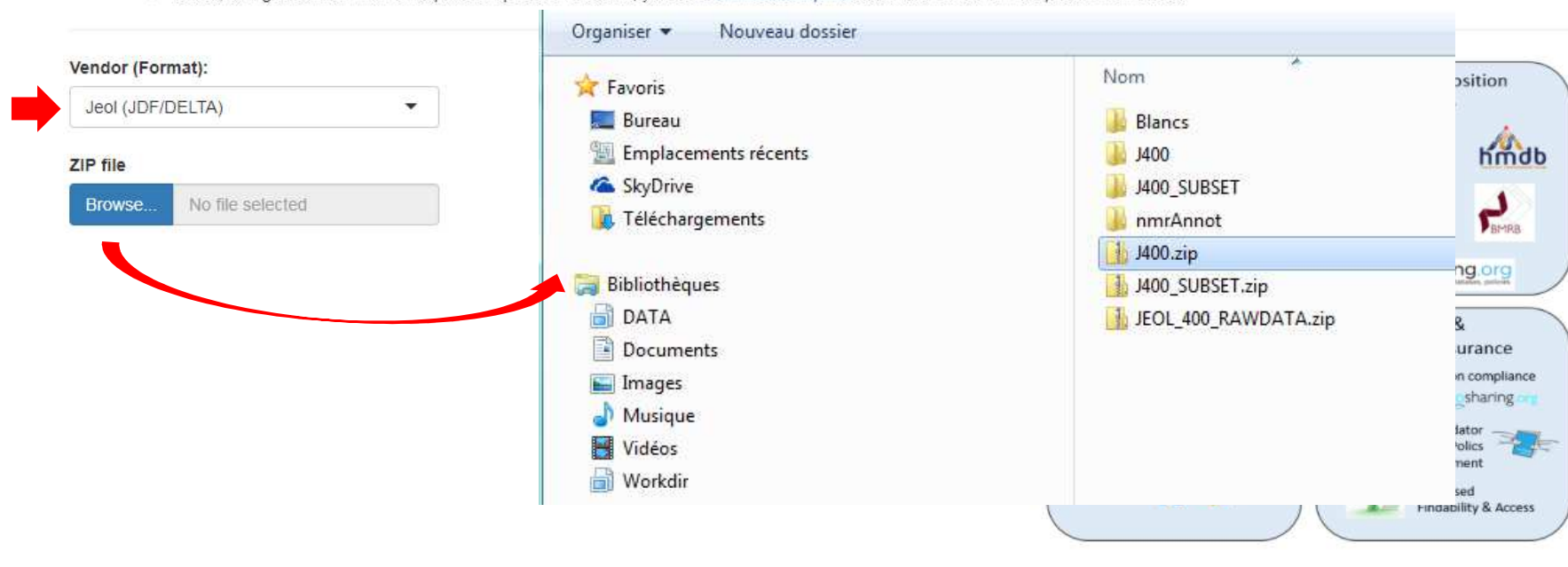
No file selected



(C) COSMOS

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The screenshot displays the nmrML Converter web interface on the left and a Windows File Explorer window on the right. In the converter interface, the 'Vendor (Format)' dropdown is set to 'Jeol (JDF/DELTA)'. Below it, the 'ZIP file' section has a 'Browse...' button and the text 'No file selected'. A red arrow points from this button to the File Explorer window. The File Explorer window shows a list of files in a folder named 'Nouveau dossier'. The files listed are: 'Blancs', 'J400', 'J400_SUBSET', 'nmrAnnot', 'J400.zip', 'J400_SUBSET.zip', and 'JEOL_400_RAWDATA.zip'. The 'J400.zip' file is selected. A red arrow points from this file back to the 'Browse...' button in the converter interface.



<http://nmrml.org/converter/>

Vendor (Format):

Jeol (JDF/DELTA) ▼

ZIP file

Browse... J400.zip
Upload complete

Launch



Converting in progress ... 3/5



Vendor (Format):

Jeol (JDF/DELTA) ▼

nmrML file name:

J400


Download nmrML file

Reset



- vn02_PROTON-1-1.nmrML
- vn03_PROTON-1-1.nmrML
- vn04_PROTON-1-1.nmrML
- vn05_PROTON-1-1.nmrML
- vn06_PROTON-1-1.nmrML

J400 (1).zip

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

Load Processing

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

Instrument/Vendor/Format:
nmrML v1.0.rc1

Spectra type:
FID

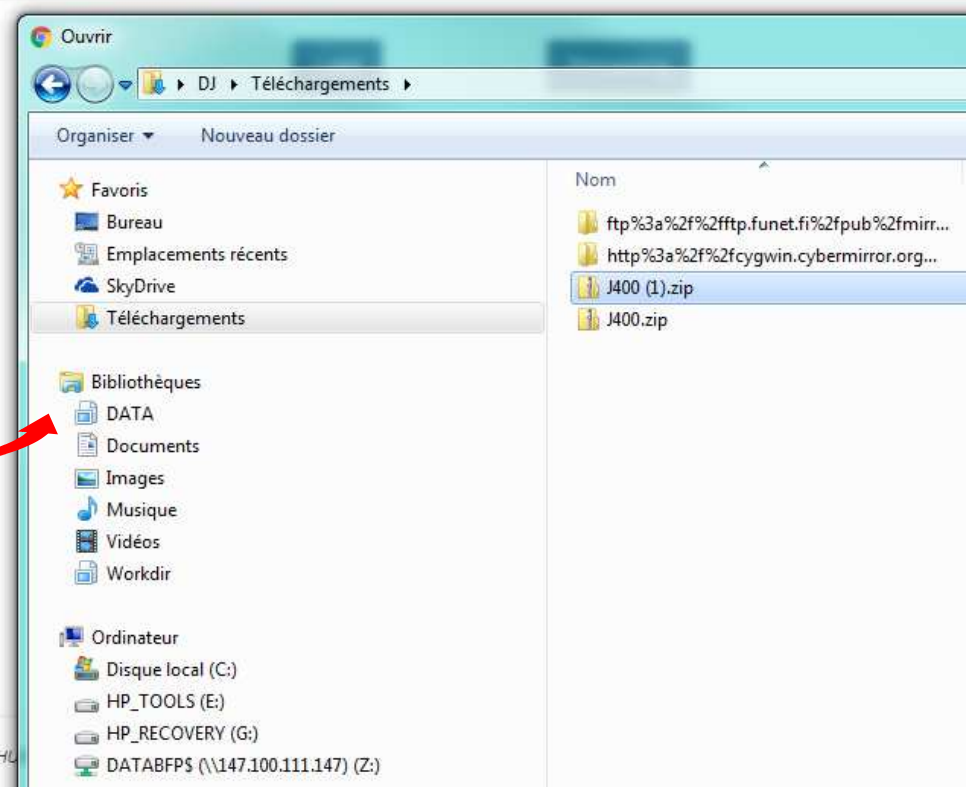
Parameters

ZIP file
Browse... No file selected

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

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

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



Load Processing

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

```

Shiny Server version 1.5.7.878
-----
Session Identifier = _795d16dc1f6398ade1dd2a39774d65
Instrument/Vendor/Format = nmrml
Spectra type = fid
The original name of the Zip file = J400 (1).zip
The original name of the Samples file = NA
The macro-command file for processing =
The number of Spectra = 5
The number of Factors = 0
-----
    
```

Reset Log Export Parameters

Show 10 entries

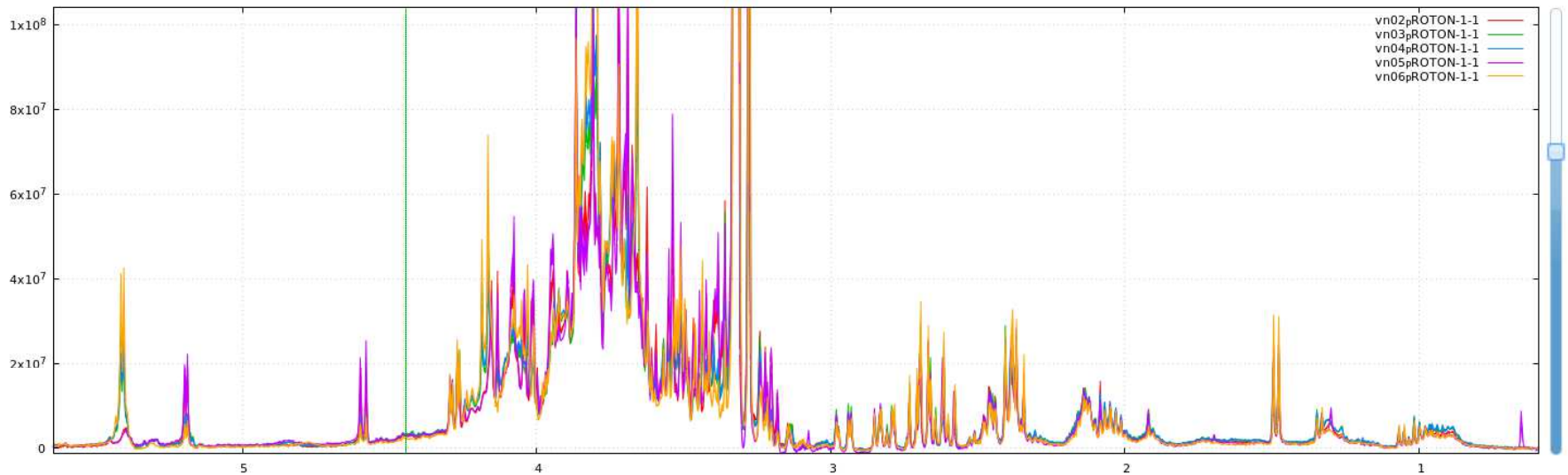
Spectrum	PULSE	NUC	SOLVENT	PHC0	PHC1	SW	SF	SI
vn02_PROTON-1-1.nmrML		1H	-	3.057477	-0.2367175	17.52636	399.7822	131072
vn03_PROTON-1-1.nmrML		1H	-	3.063629	-0.1762600	17.52636	399.7822	131072
vn04_PROTON-1-1.nmrML		1H	-	3.057467	-0.1976226	17.52636	399.7822	131072
vn05_PROTON-1-1.nmrML		1H	-	2.809759	-0.1706490	17.52636	399.7822	131072
vn06_PROTON-1-1.nmrML		1H	-	2.827423	-0.1974291	17.52636	399.7822	131072

Showing 1 to 5 of 5 entries

Previous 1 Next



Load Processing



zoom out previous
Samplecode ▼ -- all levels --- ▼
Stacked spectra
ppm = 4.445
↶ ↷

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