http://nmrml.org/converter/

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. Amongs many avantages, 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.

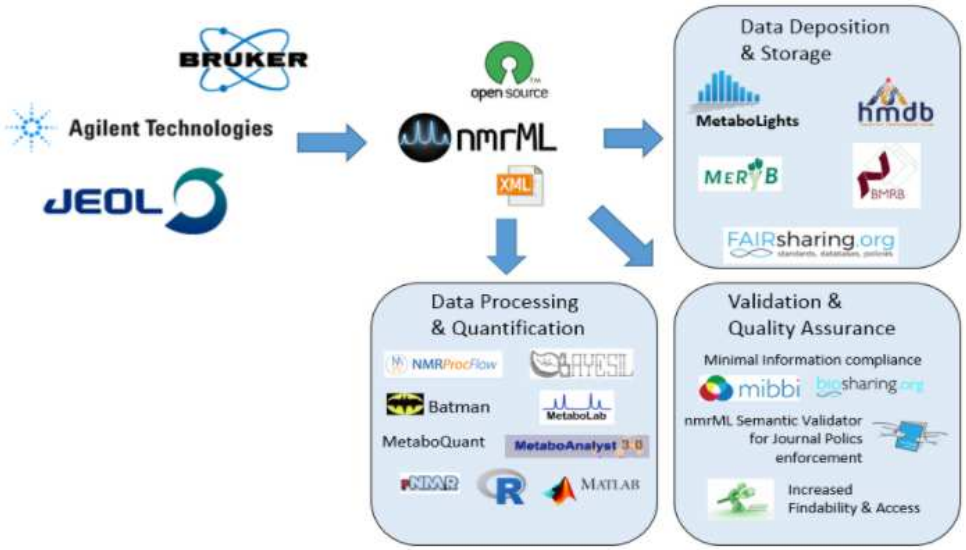
- **Using this converter**:
  - Multiple nmr fid files should be packed into the same ZIP archive. **For Bruker and Varian**, each nmr fid file must have its own directory within the ZIP archive, along with the acquitisition parameter file. **For Jeol**, each nmr fid data along with the acquitisition 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

nmrML

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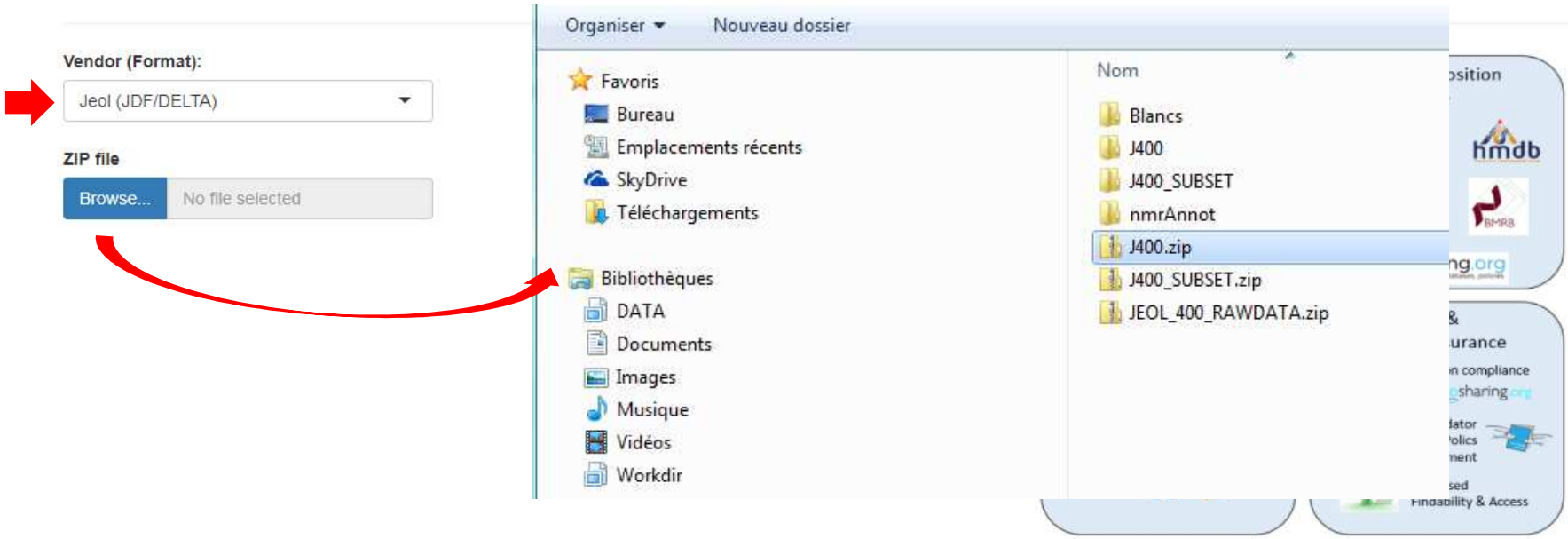


(C) COSMOS

INRA SCIENCE & IMPACT

nmrML

http://nmrml.org/converter/

JEOL

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

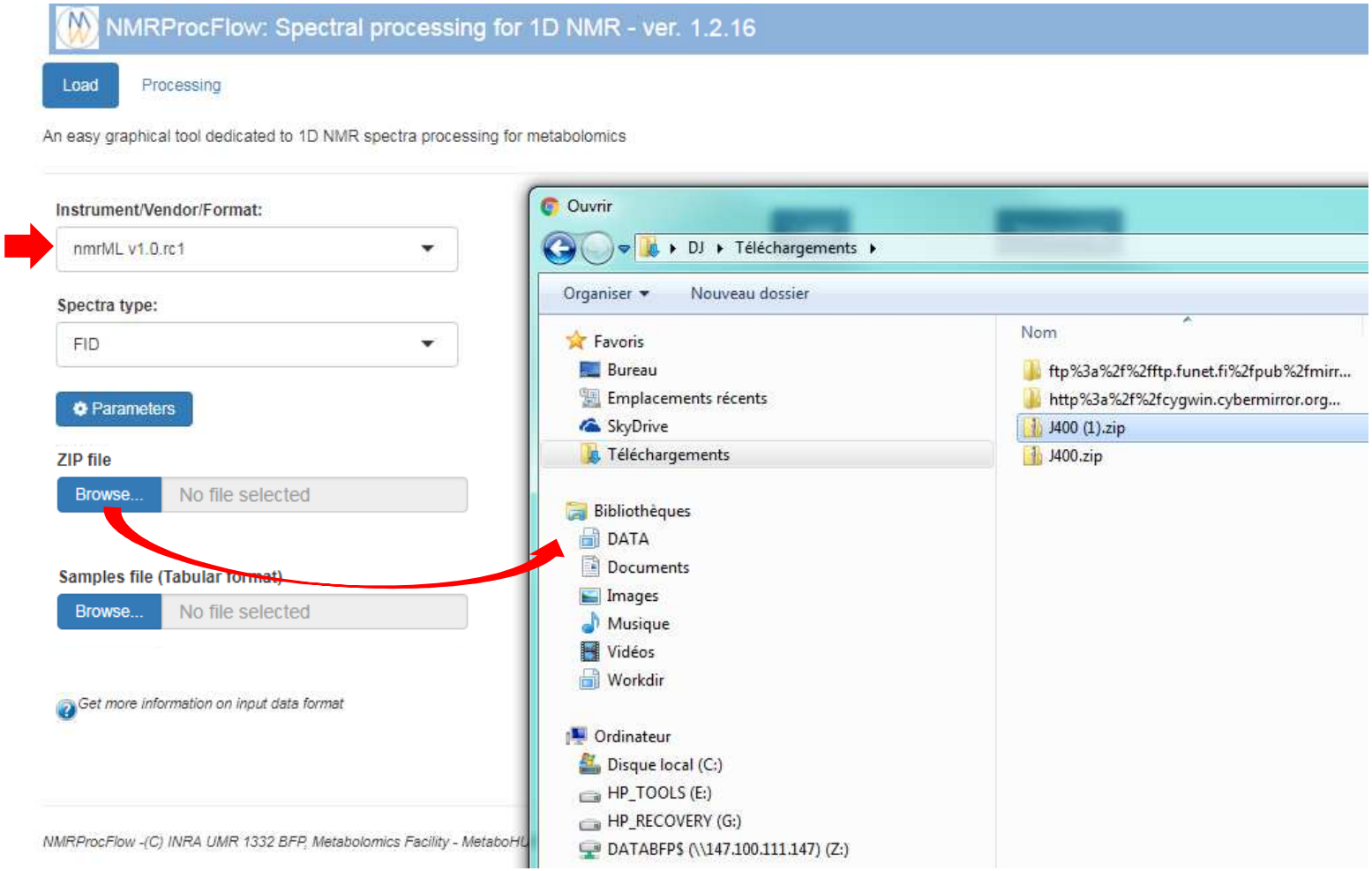
nmrML

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

INRA SCIENCE & IMPACT

nmrML → NMRProcFlow



INRA SCIENCE & IMPACT

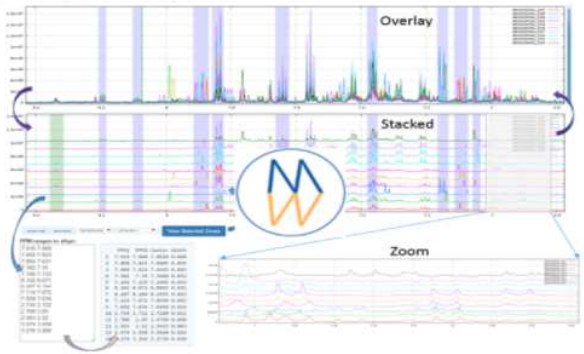
nmrML → NMRProcFlow

NMRProcFlow: Spectral processing for 1D NMR - ver. 1.2.16 J400 (1)

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

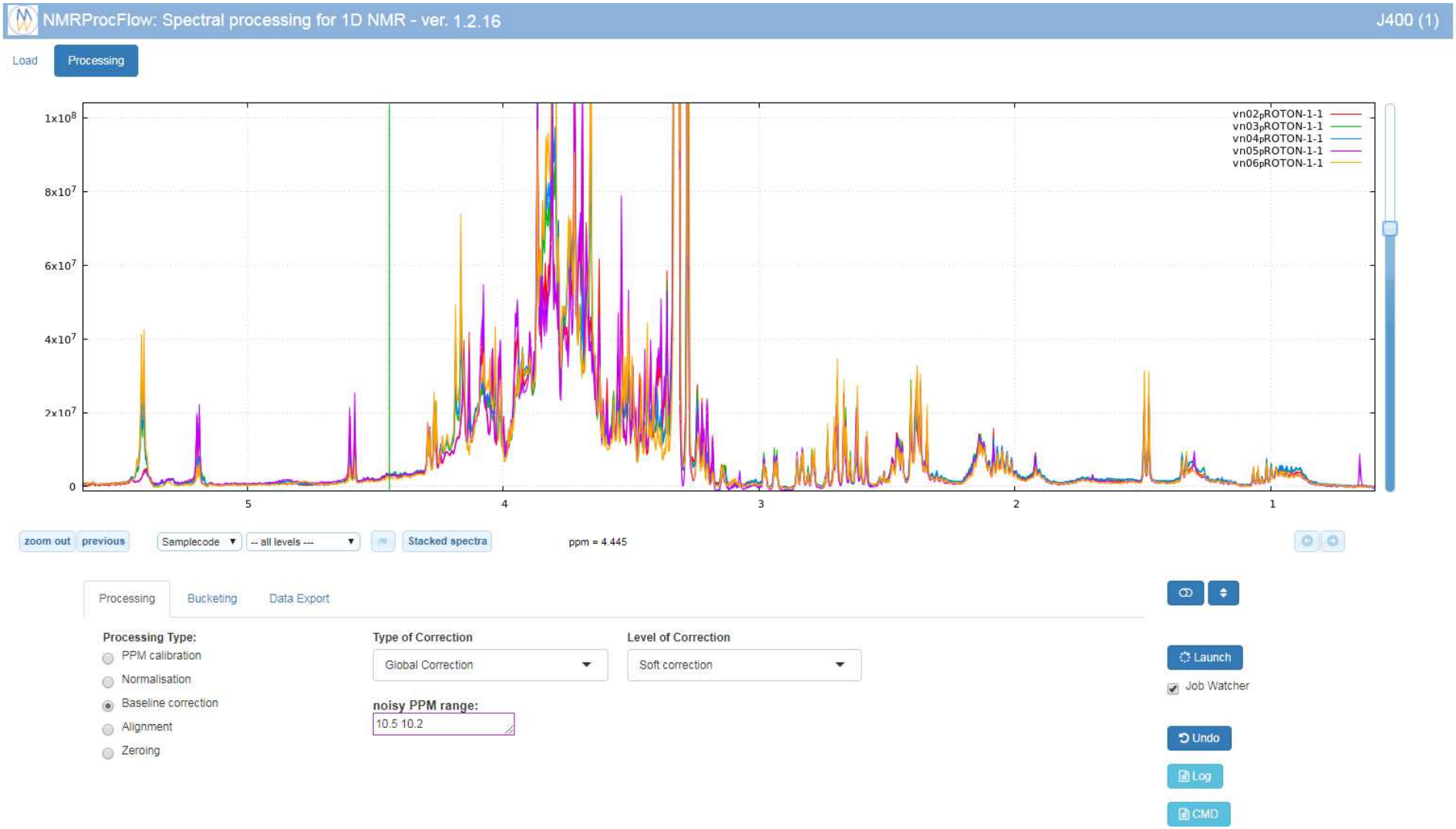
Show 10 entries Search:

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
Spectrum	PULSE	NUC	SOLVENT	PHC0	PHC1	SW	SF	SI

Showing 1 to 5 of 5 entries Previous 1 Next

INRA SCIENCE & IMPACT

nmrML → NMRProcFlow



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