

# Agilent Technologies

## **vj2pipe spectral processing utility**

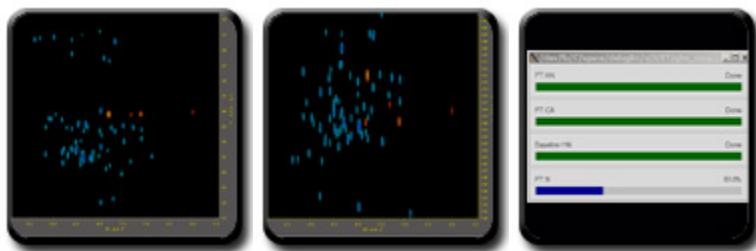
Last Updated 9/12/2014 frank\_delaglio@agilent.com

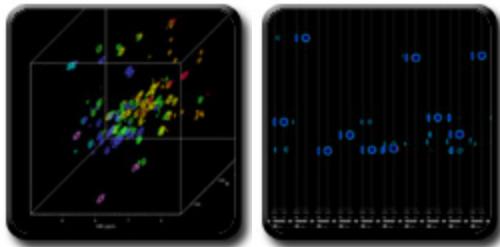
Agilent **vj2pipe** is a system of scripts and software for seamless processing and visualization of data from Agilent and Varian NMR spectrometers. The system builds scripts to process and display data via the widely-used **NMRPipe Spectral Processing System**. This version of **vj2pipe** is configured for use with **VnmrJ BioPack** for biomolecular data and **VnmrJ ChemPack** for small molecule data. The parameters and software have been enhanced specifically to support the most convenient and effective use of Agilent and Varian NMR data together with NMRPipe. The **vj2pipe** system can be used from within Agilent's **VnmrJ** software. And, like the tools of NMRPipe, **vj2pipe** can also be used directly from a C-shell command-line.

In addition to creating processing schemes for conventionally sampled data, **vj2pipe** creates schemes for reconstructing **Non-Uniformly Sampled** (NUS) data. This saves weeks of learning time by automating the creation the complex scripts needed to exploit this data. This makes NUS accessible to everyone for measuring sharper spectra with less measurement time.

**vj2pipe** uses information from the VnmrJ spectral data (the `fid` file) and parameter file (the `procpar` file) to create and execute NMRPipe scripts which are then used to process and display the data. If processing parameters such as phase correction have already been selected, the processing and display can be entirely automated. Or, the scripts and data created by **vj2pipe** can be used interactively in the usual NMRPipe-style workflow.

As an initial step, **vj2pipe** reads the VnmrJ data parameters and builds a shell-script which converts the data from VnmrJ format to NMRPipe format. This script also establishes the chemical shift calibration information. Then, depending on the type of experiment, **vj2pipe** creates one or more additional scripts to process and display the spectral data. In the case of 3D experiments, these scripts will process and display the first XY and XZ 2D planes of the 3D data, as well as processing and displaying the entire 3D spectrum as a simple cube plot and in an interactive strip viewer.





## Using **vj2pipe** from the Command-Line

The script `vj2pipe.com` can be used to run **vj2pipe** from a C-shell command-line. By default, **vj2pipe** will read files and parameters from the current directory. So, it is usually used from the directory containing the `fid` and `procpar` files. In its simplest form, it can be used without any additional command-line options. When used this way, it will automatically convert and process the data according to parameters in the `procpar` file, and display the result. For example, the following commands would automatically convert, process, and display the given 3D data:

```
cd ghn_coca_cb_3D.fid
vj2pipe.com
```

In addition, **vj2pipe** can be used to list the options and parameters it determines for the current data, without creating or executing any scripts. This makes it possible to review the settings that will be used for the given data, and adjust these as desired via command-line options. The `-info` option is used to generate the informational display, for example:

```
cd ghn_coca_cb_3D.fid
vj2pipe.com -info
```

An example of the informational output produced for a 3D spectrum is given at the bottom of this document. Besides showing the parameter settings extracted from the current data, the informational display shows the name of the NMRPipe-style command-line option which can be used to adjust that parameter.

**vj2pipe** performs the following steps in order:

- If an input data directory has been specified with the `-cd` option, change to that directory. Input for `-procpar` and `-vjfid` will be relative to this directory.
- If an output data directory has been specified with the `-pipeDir` option, create it if it does not exist, and change to that directory.

- Find the `procpar` file. If keyword `Auto` is used, **`vj2pipe`** will search for `./procpar acqfil/procpar` and `../procpar` in that order.
- Find the `fid` file. If keyword `Auto` is used, **`vj2pipe`** will search for `./fid acqfil/fid` and `../fid` in that order.
- Read the `procpar` file and extract all parameters in it.
- Replace or create `procpar` parameters with command-line values if any are given. This is done via the `-pset` option. Besides being one way to override values in `procpar`, this allows `vj2pipe` to be used with older Varian data that might be missing specific `vj2pipe` parameters. For example, to set the value used in place of the `procpar` parameter `BPPipetype`:

```
vj2pipe.com -pset BPPipetype HNCA
```

- If the spectrum is Non-Uniformly Sampled (NUS), **`vj2pipe`** will search for the sampling schedule `./sampling.sch` `../sampling.sch` or `*.hdr_3` in that order, then read and interpret the contents.
- Interpret the `procpar` parameters to extract information about experiment type, data size, acquisition modes, storage details, axis labels, chemical shift calibration, and processing parameters. These are established as arguments for NMRPipe programs and scripts. Refer to the [Big NMRPipe Reference Page](#) and other NMRPipe documentation for more details.
- Replace any of the NMRPipe parameters with command-line values if any are given. This allows control of the details of conversion and processing. For example, to reset the NMRPipe conversion parameter for the X-Axis label of the data:

```
vj2pipe.com -xLAB HMeth
```

- Besides the predefined NMRPipe parameters such as `aqORD` `xN` `xT` `xLAB` etc., additional parameter names can be defined via the `-sVar` `-lVar` and `-dVar` command-line options. This provides a way to make new parameter names available for use in scripts.
- Create a script which converts the Varian-format data to NMRPipe-format. This script uses the usual NMRPipe methods and arguments for format conversion, via the NMRPipe program `var2pipe`.
- Create one or more scripts for processing the spectral data. These are created from default **script templates** for particular tasks such as performing

3D Fourier processing. The default templates are stored in a directory of the NMRPipe installation (\$NMRBASE/vj2pipe/com).

- New scripts are created by replacing text markers in the templates with the specific NMRPipe parameter settings for the given data. The text markers have the same names as the NMRPipe options, but begin and end with the underscore character. For example, the NMRPipe -xP0 parameter specifies the P0 (Zero Order Phase) value to apply when processing the X-Axis of the given data. So, the corresponding text marker for this option would be \_xP0\_ and this text marker will be replaced where ever it appears by the actual value for P0. For example, if a line from an input script template looked like this:

```
| nmrPipe -fn PS -p0 _xP0_ -p1 180.0 -di \
```

then the text \_xP0\_ would be replaced by the value for P0, for example:

```
| nmrPipe -fn PS -p0 43.0 -p1 180.0 -di \
```

- If requested, create additional scripts for displaying the processed spectral data.
- If additional template script names have been specified via the -subs command-line option, create new versions of these replacing text markers in the same way as for the default scripts.
- Execute the conversion script.
- Execute any processing and display scripts created from the default templates. If any additional options were specified via the vj2pipe -args option, these will be passed as arguments to each script when it is executed. The same set of options will be passed to all scripts, even though all scripts might not use them.

As an example, scripts which perform IST (Iterative Soft Threshold) processing use an option -istIter ... so, in order to pass this option, use:

```
vj2pipe.com -args -istIter 1024
```

The auxiliary script vj\_clean.com can be used to delete all processed data, and optionally all scripts created by **vj2pipe** in a given data directory. For safety, the script will only clean directories where file timestamp.vj2pipe is found, a file which is created when vj2pipe.com is used. Typical use will be as follows, use the -help argument for a complete list of options:

```
vj_clean.com -com
```

## vj2pipe General Command-Line Options

Option	Default	Description
-procpar pName	procpar	Name of VNMRJ procpar Input, or Keyword Auto.
-vjfid fName	fid	Name of VNMRJ binary fid Input, or Keyword Auto.
-cd cdDir	.	Default Data Directory for Input.
-pipeDir	.	Default Data Directory for Output. It will be created if it does not exist.
-outPrefix prefix	spec	File Name Prefix for Processed Results and Related Output Files.
-msgName mName	stderr	Output File for Status Messages, or Keyword stdout stderr None.
-vjDir vName	\$NMRBASE/ vj2pipe	Directory of Auxiliary Files and Template Scripts used by vj2pipe.
-sVar sList	None	List of Additional User-Defined Single-Value Variables to Create.
-lVar lList	None	List of Additional User-Defined Multiple Value (List) Variables to Create.
-dVar dList	None	List of Additional User-Defined Dimension-Specific Variables to Create.
-subs sList	None	List of Additional User-Defined Template Scripts to Substitute.
-h2oM tSlope	-0.009552	Slope of ppm/Degree K for Water, used in some calibration schemes.
-h2oB tInter	5.011718	PPM value for water at 273 degrees K, used in some calibration schemes.
-coThresh tPPM	150.0000	PPM threshold for identifying CO dimensions of <sup>13</sup> C experiments.
-args argList	None	Optional arguments to pass to conversion and processing scripts when they are executed. Ignored when the –noexec option is used.

-fidScript fidComPrefix	vj_fid	File Name Prefix for Conversion Script.
-ft1Script ft1ComPrefix	vj_ft1	File Name Prefix for 1D Processing Script.
-ft2Script ft2ComPrefix	vj_ft2	File Name Prefix for 2D Processing Script.
-xyScript xyComPrefix	vj_xy	File Name Prefix for Processing Script for 2D XY Plane of 3D.
-xzScript xzComPrefix	vj_xz	File Name Prefix for Processing Script for 2D XZ Plane of 3D.
-xyzScript xyzComPrefix	vj_xyz	File Name Prefix for 3D Processing Script.
-scrollScript scrComPrefix	vj_scroll	File Name Prefix for Strip Viewer Display Script for 3D Spectra.
-info		List All Parameters for the Current Data, then Exit.
-clean		Delete Previous Results and Scripts Before Processing.
-cleanOnly		Delete Previous Results and Scripts, then Exit.
-exec		Execute Conversion and Processing Scripts (Default).
-noexec		Create but Do Not Execute Conversion and Processing Scripts.
-partial	celem	Accommodate Partially-Completed Acquisition.
-nopartial		No Adjustment for Partially-Completed Acquisition (Default).
-graph		Display Spectral Graphics of the Results (Default).
-nograph		Do Not Display Spectral Graphics.
-drawPlane		Use NMRDraw to Display 2D Planes.
-nodrawPlane		Do Not Use NMRDraw to Display 2D Planes.
-drawCube		Draw 3D Contour Cube for 3D Data.
-nodrawCube		Do Not Draw 3D Contour Cube.

-drawStrips		Draw Strips for 3D Data.
-nodrawStrips		Draw 3D Strips.
-progress		Display a Progress Bar During Processing (Default).
-noprogress		Do Not Use Progress Bar Display.
-noskip		List Single-Point Dimensions, as for 3D experiments acquired as 2D.
-skip		Skip Listing of Single-Point Dimensions (Default).
-vjshow		List VJNMR-Specific Parameters.
-novjshow		Do Not List VJNMR-Specific Parameters.
-vjapod		Use VJNMR Window Function Values. <i>Not yet implemented.</i>
-novjapod		Use NMRPipe Window Function Values (Default).
-verb		Verbose Mode ON (Default).
-noverb		Verbose Mode OFF.
-help		List the Command-Line Options and Defaults.
-pset pName valList --		Reset a procpar value. Can be used more than once. See below.

## vj2pipe Data-Specific Command-Line Options

The following options pertain to the parameters extracted specifically from the current data, and used to build conversion and processing schemes for the data. Options for specific parameters start with prefix `-x` `-y` `-z` etc ...

Option	Example	Related <code>procpar</code>	Description
<code>-title</code>	"hn(co)ca"	<code>seqfil BPpipetype</code>	The canonical title of the experiment.
<code>-dimension</code>	C13 N15 H1	<code>dimension</code>	Specified which nuclei are associated with a given dimension
<code>-type</code>	HN	<code>tn dn dn2 ...</code>	The general experiment type. Keywords: HN HC HOMO NMR.
<code>-ndim</code>	3	<code>np ni ni2 ...</code>	Number of dimensions in the data.
<code>-nusDim</code>	3	SAMPLING, sparse	Number of dimensions Non-Uniformly Sampled (NUS) data will have after it is expanded.
<code>-aq2D</code>	States	array	The NMRPipe 2D plane mode. Keywords: States Magnitude.
<code>-aqORD</code>	1	array	The order of loops for real,imaginary detection in the indirect dimensions.
<code>-planeHi</code>	10%	<code>BPPipedrawinfo</code>	2D Plane Contour Height, as Value, % or Fraction of Data @.
<code>-hi</code>	2.50%	<code>BPPipedrawinfo</code>	2D Spectrum Contour Height, as Value, % or Fraction of Data @.
<code>-cubeHi</code>	10.0%	<code>BPPipedrawinfo</code>	3D Cube Contour Height, as Value, % or Fraction of Data @.
<code>-stripHi</code>	3.00%	<code>BPPipedrawinfo</code>	3D Strip Contour Height, as Value, % or Fraction of Data @.
<code>-projHi</code>	10.0%	<code>BPPipedrawinfo</code>	Peak detection threshold for analyzing 2D projections for 3D strip locations.
<code>-temperature</code>	298.00	<code>temp</code>	Temperature, degrees K. Used in some PPM calibration schemes.
<code>-xN</code>	2048	<code>np ni ni2 ...</code>	Number of total points (real + imaginary) stored for the given dimension.

-xT	1024	array np ni ni2 ...	Number of valid time-domain points (complex) in the dimension.
-xMODE	Complex	array f1coef ...	Acquisition Mode for the dimension. Keywords: Complex Rance-Kay.
-xCHAN	1	dimension refsource...	Channel number the spectrometer associated with the dimension.
-xSW	12019.2000	sw sw1 sw2 ...	Spectral width, Hz.
-xAQTIME	0.085197	np ni ... sw sw1 ...	Effective acquisition time, Hz.
-xOBS	599.8896	sfrq dfrq dfrq2 ...	Observe Frequency at Zero ppm, MHz.
-xOBSMID	599.8896	sfrq dfrq dfrq2 ...	Observe Frequency at Center of Spectrum, MHz.
-xCAR	4.6300	obscenterppm h1ref... etc pipexCAR... etc	PPM position of the center point of the spectrum (point N/2 + 1 of 1 to N).
-xCARSET	0	h1ref... etc	Indicates which <code>procpar ref</code> parameter (i.e. <code>n15ref2</code> ) is set.
-xLAB	HN	BPPipetype tn dn ...	Axis label for the dimension.
-xNUC	H1	dimension tn dn dn2 ...	Nucleus associated with the dimension. 1H 13C 15N.
-xGAMMA	1.000000000	dimension tn dn dn2 ...	Gamma value (gyromagnetic ratio).
-xP0	-160.00	rp rp1 rp2 ...	Zero-Order Phase, degrees.
-xP1	-71.80	lp lp1 lp2 ...	First-Order Phase, degrees.
-xAPOD	SP		NMRPipe Window Function Name. SP EM GM GMB TM JMOD.
-xQ1	0.500		Window Function Parameter 1.
-xQ2	0.950		Window Function Parameter 2.
-xQ3	2.000		Window Function Parameter 3.
-xELB	0.000		NMRPipe Window Function Exponential Broadening, Hz.

-xGLB	0.000		NMRPipe Window Function Gaussian Broadening, Hz.
-xGOFF	0.000		NMRPipe Window Function Gaussian Center, 0.0 (first point) to 1.0 (last point).
-xC1	1.000	lp lp1 lp2 ...	First-Point Time Domain Scale. Usually 0.5 (when P1 phase is zero) or 1.0.
-xVJSB	-0.085	sb sb1 sb2 ...	Original VnmrJ sb window value.
-xVJSBS	-0.085	sbs sbs1 sbs2 ...	Original VnmrJ sbs window value.
-xVJLB	5.000	lb lb1 lb2 ...	Original VnmrJ lb window value.
-xVJGF	0.022	gf gf1 gf2 ...	Original VnmrJ gf window value.
-xVJGFS	0.009	gfs gfs1 gfs2 ...	Original VnmrJ gfs window value.
-xSOL	SOL		NMRPipe Solvent Filter Function to use. This argument is <a href="#">expandable</a> by use of commas between options.
-xZFARG	zf=1,auto	BPpipeprocinfo	NMRPipe Zero-Fill Options. This argument is <a href="#">expandable</a> by use of commas between options.
-xFTARG	None	BPpipeprocinfo	NMRPipe Fourier Transform Options. This argument is <a href="#">expandable</a> by use of commas between options.
-xEXTX1	9.952ppm	sp wp BPpiperegion	Start Coord of Processed Region to Extract. Units pts Hz ppm %.
-xEXTXN	5.423ppm	sp wp BPpiperegion	End Coord of Processed Region to Extract. Units pts Hz ppm %.
-xLSTIME	0	lsfid lsfid1 lsfid2 ...	Shift to Apply in the Frequency Domain.
-xLSFREQ	0	lsfrq lsfrq1 lsfrq2 ...	Shift to Apply in the Frequency Domain.
-xBASEARG	None	BPpipeprocinfo	NMRPipe Baseline Correction Options. This argument is <a href="#">expandable</a> by use of commas between options.

## **Viewing and Setting vj2pipe Conversion and Processing Parameters**

Using the command `vj2pipe.com -info` or `vj2pipe.com -info -vjshow` will generate a list of the default conversion and processing parameters for the data in the current directory. An example of this output is shown below. The values for any of these parameters can be reset at the command-line. For example, to change the default setting for the `-title` option:

```
vj2pipe.com -title HNCA
```

As noted previously, it is also possible to adjust values from the `procpar` file before they are interpreted to generate NMRPipe parameters. This is done via the `-pset` option, followed by the name of the `procpar` parameter the corresponding value or value list, for example:

```
vj2pipe.com -pset BPpipetype HNCA
```

The `-pset` option can be used multiple times to reset more than one parameter. It can also be used with other options for adjusting parameters. In these cases, each use of the `-pset` option should be concluded by double-dashes `--` for example:

```
vj2pipe.com -pset BPpipetype HNHA -- -pset h1ref3 4.55 -- -xLAB HN -yLAB HA
```

If no adjustments to `procpar` parameters are needed, a simple list of conversion and processing parameter settings or adjustments can be used. Commonly, these adjustments will be regions of interest and phase correction values:

```
vj2pipe.com -xEXT1 11.3ppm -xEXTN 5.2ppm -yP0 45 -xLAB HN -yLAB HA
```

As noted in the tables above, some options, including the processing arguments `-xSOL` `-xZFARG` `-xFTARG` and `-xBASEARG` are [expandable](#). This means that when the associated values are used in processing scripts, they will be expanded at commas and equal signs to space-separated flags and argument/value pairs. For example:

<code>-xZFARG zf=1,auto</code>	is expanded to	<code>-zf 1 -auto</code>
<code>-xSOL POLY,time</code>	is expanded to	<code>POLY -time</code>

## Example output for a 3D CBCANH experiment:

```
% vj2pipe.com -info -vjshow
-cd . -outPrefix spec -vjPath . -vjfid fid -procpar procpar \
-nusSched Auto -title CBCANH -type HN -ndim 3 -nusDim 0 -celem 8192 \
-arrayDim 8192 -aq2D States -aqORD 1 -temperature 298.00 \
-h2oM -0.009552 -h2oB 5.011718 -coThresh 150.0000 -fidScript vj_fid \
-ft1Script vj_ft1 -ft2Script vj_ft2 -xyScript vj_xy -xzScript vj_xz \
-xaScript vj_xa -xyzScript vj_xyz -xyzaScript vj_xyza \
-scrollScript vj_scroll -tmpScript vj_tmp -vjAuxDir /u/fd/vj2pipe \
-inName spec.fid -outName spec.dat -auxName aux.dat \
-hi 2.5% -stripHi 3.0% -cubeHi 10% -planeHi 10% -projHi Full \
-noise Auto -tdNoise Auto -ftNoise Auto -istTMult _default_ \
-istCMult _default_ -istIter _default_ -istMaxRes _default_ \
-dimension C13 N15 H1 -nusMethods clean irls ist mdd mem ml scrub \
-xN          2048 -yN           128 -zN          64 \
-xT          1024 -yT           64 -zT          32 \
-xMODE       Complex -yMODE      Complex -zMODE      Rance-Kay \
-xCHAN        1 -yCHAN         2 -zCHAN         3 \
-xSW          13020.8000 -ySW        16084.5872 -zSW        2106.6000 \
-xAQTIME     0.078643 -yAQTIME    0.003979 -zAQTIME    0.015190 \
-xOBS         799.5969 -yOBS        201.0666 -zOBS        81.0318 \
-xOBSMID     799.5969 -yOBSMID    201.0666 -zOBSMID    81.0318 \
-xCAR         4.6330 -yCAR        45.9700 -zCAR        119.9800 \
-xCARSET      0 -yCARSET       1 -zCARSET       2 \
-xLAB          HN -yLAB         CACB -zLAB         N \
-xNUC          H1 -yNUC         C13 -zNUC         N15 \
-xGAMMA       1.0000000000 -yGAMMA    0.251449530 -zGAMMA    0.101329118 \
-xP0          78.00 -yP0          0.00 -zP0          0.00 \
-xP1          0.00 -yP1          0.00 -zP1          0.00 \
-xP0EXTRA    0.00 -yP0EXTRA    0.00 -zP0EXTRA    0.00 \
-xP1EXTRA    0.00 -yP1EXTRA    0.00 -zP1EXTRA    0.00 \
-xAPOD        SP -yAPOD        SP -zAPOD        SP \
-xQ1          0.500 -yQ1          0.500 -zQ1          0.500 \
-xQ2          0.950 -yQ2          0.950 -zQ2          0.950 \
-xQ3          2.000 -yQ3          1.000 -zQ3          1.000 \
-xELB          0.000 -yELB          0.000 -zELB          0.000 \
-xGLB          0.000 -yGLB          0.000 -zGLB          0.000 \
-xGOFF         0.000 -yGOFF         0.000 -zGOFF         0.000 \
-xC1          0.500 -yC1          0.500 -zC1          0.500 \
-xVJSB        -0.079 -yVJSB        -0.008 -zVJSB        0.061 \
-xVJSBS       -0.079 -yVJSBS       -0.008 -zVJSBS       -0.061 \
-xVJLB        5.000 -yVJLB        0.318 -zVJLB        1.000 \
-xVJGF        0.040 -yVJGF        0.016 -zVJGF        0.000 \
-xVJGFS       0.000 -yVJGFS       0.000 -zVJGFS        0.000 \
-xDECAY       0.000 -yDECAY       0.000 -zDECAY       0.000 \
-xSOL          SOL -ySOL          None -zSOL          None \
-xZFARG      zf=1,auto -yZFARG    zf=1,auto -zZFARG    zf=1,auto \
-xFTARG        None -yFTARG        None -zFTARG        None \
-xEXTX1        3% -yEXTX1        0% -zEXTX1        0% \
-xEXTXN       47% -yEXTXN       100% -zEXTXN       100% \
-xLSTIME        0 -yLSTIME        0 -zLSTIME        0 \
-xLSFREQ        0 -yLSFREQ        0 -zLSFREQ        0 \
-xBASEARG      POLY,auto -yBASEARG    NULL -zBASEARG    NULL \
-xLPARG        None -yLPARG        None -zLPARG        None
```

## Example output for a 3D Non-Uniformly Sampled Experiment:

```
% vj2pipe.com -info -vjshow
-cd . -outPrefix spec -vjPath . -vjfid fid -procpar procpar \
-nusSched sampling.sch -title HNCACB -type HN -ndim 3 \
-nusDim 0 -celem 1248 -arrayDim 1248 -mcFlag 0 -aq2D States \
-aqORD 1 -temperature 298.00 -h2oM -0.009552 -h2oB 5.011718 \
-coThresh 150.0000 -fidScript vj_fid -ft1Script vj_ft1 \
-ft2Script vj_ft2 -xyScript vj_xy -xzScript vj_xz -xaScript vj_xa \
-xyzScript vj_xyz -xyzaScript vj_xyza -scrollScript vj_scroll \
-tmpScript vj_tmp -vjAuxDir /u/delaglio/vj2pipe -inName spec.fid \
-outName spec.dat -auxName aux.dat -hi 2.5% -stripHi 3.0% \
-cubeHi 10% -planeHi 10% -projHi Full -noise Auto -tdNoise Auto \
-ftNoise Auto -istTMult _default_ -istCMult _default_ \
-istIter _default_ -istMaxRes _default_ \
-dimension C13 N15 H1 -nusMethods clean irls ist mdd mem ml scrub \
-xN          2404 -yN          1248 -zN          1 \
-xT          1202 -yT          48   -zT          26 \
-xMODE       Complex -yMODE      Complex -zMODE      Real \
-xCHAN       1     -yCHAN      2     -zCHAN      3 \
-xSW          12019.2308 -ySW         12060.0022 -zSW        1320.0000 \
-xAQTIME     0.100006 -yAQTIME    0.003980 -zAQTIME    0.019697 \
-xOBS         599.4225 -yOBS        150.7307 -zOBS        60.7459 \
-xOBSMID     599.4225 -yOBSMID    150.7307 -zOBSMID    60.7459 \
-xCAR         4.6280  -yCAR        173.9700 -zCAR        127.2100 \
-xCARSET      0     -yCARSET     1     -zCARSET     2 \
-xLAB         HN   -yLAB        CACB -zLAB        N \
-xNUC         H1   -yNUC        C13 -zNUC        N15 \
-xGAMMA       1.000000000 -yGAMMA    0.251449530 -zGAMMA    0.101329118 \
-xP0          334.84 -yP0         0.00  -zP0         0.00 \
-xP1          0.00  -yP1         0.00  -zP1         0.00 \
-xP0EXTRA    0.00  -yP0EXTRA   0.00  -zP0EXTRA   0.00 \
-xP1EXTRA    0.00  -yP1EXTRA   0.00  -zP1EXTRA   0.00 \
-xAPOD        SP   -yAPOD      SP   -zAPOD      SP \
-xQ1          0.500  -yQ1         0.500 -zQ1         0.500 \
-xQ2          0.950  -yQ2         0.950 -zQ2         0.950 \
-xQ3          2.000  -yQ3         1.000 -zQ3         1.000 \
-xELB         0.000  -yELB        0.000 -zELB        _default_ \
-xGLB         0.000  -yGLB        0.000 -zGLB        _default_ \
-xGOFF        0.000  -yGOFF       0.000 -zGOFF       _default_ \
-xC1          0.500  -yC1         0.500 -zC1         0.500 \
-xVJSB        -0.100  -yVJSB      -0.004 -zVJSB      -0.020 \
-xVJSBS       -0.090  -yVJSBS     -0.061 -zVJSBS     -0.029 \
-xVJLB        5.000  -yVJLB      0.318  -zVJLB      1.000 \
-xVJGF        0.046  -yVJGF      0.016  -zVJGF      0.000 \
-xVJGFS       0.000  -yVJGFS     0.000  -zVJGFS     0.000 \
-xDECAY       0.000  -yDECAY     0.000  -zDECAY     0.000 \
-xSOL          SOL  -ySOL        None  -zSOL        None \
-xZFARG       zf=1,auto -yZFARG    zf=1,auto -zzFARG    zf=1,auto \
-xFTARG        None  -yFTARG     None  -zFTARG     None \
-xEXTX1        3%   -yEXTX1     0%   -zEXTX1     0% \
-xEXTXN       47%   -yEXTXN    100%  -zEXTXN    100% \
-xLSTIME       0    -yLSTIME     0    -zLSTIME     0 \
-xLSFREQ       0    -yLSFREQ     0    -zLSFREQ     0 \
-xBASEARG      POLY,auto -yBASEARG NULL  -zBASEARG   NULL \
-xLPARG        None  -yLPARG     None  -zLPARG     None
```