NAME

readROI – NMRWish command to Read a Region of Interest (ROI)

DESCRIPTION

The **readROI** command extracts a region of interest (ROI) from a given spectrum. In this context, a region of interest is an extract or projection of all or part of a given spectrum. Some examples of ROIs include:

An individual 1D slice extracted from any dimension of a multidimensional spectrum.

A 1D summation projection of a 2D region.

A 2D region extracted from a larger 2D spectrum.

A 2D plane extracted from any pair of dimensions in a 3D or 4D spectrum.

A 2D strip created by summation projection of a 3D region.

A 3D region extracted from a larger 3D or 4D spectrum.

Extracted regions can centered or aligned automatically through interpolation, so that the extracted data corresponds to the requested chemical shift coordinates regardless of the digitization of the data. Furthermore, extracted regions which exceed the measured chemical shift window are unfolded and sign-adjusted automatically, so that regions from related spectra can be manipulated or displayed consistently even if they have differing spectral windows.

When creating an ROI, we specify the coordinates of a region to extract from an original data set. We also specify how this extracted region will be re-arranged to create the ROI output.

Axis Names

The input region is specified on the basis of axis names. The axis names are the ones specified during conversion of the spectrum (conversion arguments -xLAB -yLAB etc). The ROI commands assume that each axis in the spectrum has a unique name.

As an alternative, the "generic" axis names "X_AXIS", "Y_AXIS", etc can also be used.

Region Limits

The coordinates of the ND region to extract are specified in terms of separate coordinates for each of the dimensions. The coordinates for a given dimension can be specified as an upper and lower bound, or as a center position and a +/- width.

I. Arguments for Reading a Region

-in inName [None] 1D/2D Input Name or 3D/4D template name.
-ndim finalDim [2] Dimension Count for ROI.

II. ROI Limits By Upper and

These arguments describe the region to extract by specifying an axis name, and a starting point and ending point in that axis. The coordinates can be specified with no units (i.e. in points), or with the labels "hz", "ppm", or "%".

If no start and end points are given, the entire axis is extracted.

-x xName [x1 xn] ROI X-Axis Source and Limits.
-y yName [y1 yn] ROI Y-Axis Source and Limits.
-z zName [z1 zn] ROI Z-Axis Source and Limits.
-a aName [a1 an] ROI A-Axis Source and Limits.

III. ROI Limits By Center and +/- Width

These arguments describe a region to extract by specifying an axis name, a position on that axis, and a +/- width. The coordinate and width can be specified with no units (i.e. in points), or with the labels "hz", "ppm", or "%". If no width is given, only a single point is extracted from that axis (+/- 0).

-dx xName x0 [xW] ROI X-Axis Source, Center, Width.
-dy yName y0 [yW] ROI Y-Axis Source, Center, Width.
-dz zName z0 [zW] ROI Z-Axis Source, Center, Width.
-da aName a0 [aW] ROI A-Axis Source, Center, Width.

IV. Alignment Options

In some cases, the coordinates of the ROI may not correspond directly to exact point locations in the spectrum. So, alignment options are provided in an attempt to adjust the ROI output so that its coordinates correspond more precisely with the requested region. The alignment is currently done via a crude linear interpolation, so it may not be very accurate.

In these options, the "axisList" argument specifies which dimensions of the ROI output should be adjusted, if any. The values "X" "Y" "Z" etc can be given.

-center axisList [None] Align Center of ROI.
-left axisList [None] Align Left Edge of ROI.
-right axisList [None] Align Right Edge of ROI.
-edge axisList [None] Align Both Edges of ROI.

V. Arguments to Write a Region of Interest

-out outName Output Name for ROI result; if an output template is
desired, use a pipeline to "pipe2xyz".

-ov Allow overwrite of existing data.

VI. Arguments for Report Generation:
-noverb Verbose Mode Off.
-verb Verbose Mode On.

VII. Examples

The following command prepares an HN 1D summation projection from a 3D HNCO spectrum (note that the default default limits are the full axis):

readROI -in hnco/ft/test%03d.ft3 -out h.dat -ndim 1 -x HN -y N -z CO

The following command prepares an HN/N 2D summation projection from a 3D HNCO spectrum (note that the default output dimension count is 2, and the default limits are the full axis):

readROI -in hnco/ft/test%03d.ft3 -out hn.dat -x HN -y N -z CO

The following two commands extract complementary 2D orthogonal strips from a CBCANH 3D experiment, centered at the location HN=8.724ppm, N=132.016ppm:

readROI -in cbcanh/ft/test%03d.ft3 -out strip1.dat -ov -center X -dx HN 8.724ppm 0.12ppm -y CACB 0% 100% -dz N 132.016ppm 1

readROI -in cbcanh/ft/test%03d.ft3 -out strip2.dat -ov -center X -dz HN 8.724ppm 1 -y CACB 0% 100% -dx N 132.016ppm 1.6ppm

readROI

readROI: Read a Region of Interest (ROI). Arguments for Reading a Region of Interest (ROI):
−in inName [None] Input Name (Required).
−roi roiID [Current] ID Number for ROI.
−ndim finalDim [2] Dimension Count for ROI.
−key keyData [None] Key Data Label/Data Pairs.
ROI Limits By Upper and Lower Bounds;
−x xName [x1 xn] ROI X−Axis Source and Limits.
−y yName [y1 yn] ROI Y−Axis Source and Limits.
−z zName [z1 zn] ROI Z−Axis Source and Limits.
−a aName [a1 an] ROI A−Axis Source and Limits.
ROI Limits By Center and +/− Width:
−dx xName x0 [xW] ROI X−Axis Source, Center, Width.
−dy yName y0 [yW] ROI Y−Axis Source, Center, Width.
−dz zName z0 [zW] ROI Z−Axis Source, Center, Width.
−da aName a0 [aW] ROI A−Axis Source, Center, Width.
Alignment Options:
−center axisList [None] Align Center of ROI.
−left axisList [None] Align Left Edge of ROI.
−right axisList [None] Align Right Edge of ROI.
−edge axisList [None] Align Both Edges of ROI. Arguments for Report Generation:
−noverb Verbose Mode Off.
−verb Verbose Mode On.

writeROI

writeROI: Write a Region of Interest (ROI). Arguments to Write a Region of Interest.
−out outName Output Name for ROI result.
−roi roiID ID of ROI; Default is Current ROI.
−tty Suppress Check for I/O to TTY.
−ov Allow overwrite of existing data. Strip Append Options (2D ROIs Only):
−init Initialize (delete) existing file;
Use prior to appending strips.
−append Append to the existing file.
−offset [0.0] Strip Axis Offset.
−step [0.0] Strip Axis Step Size;
Use 0.0 for no axis adjustment. Arguments for Report Generation:
−noverb Verbose Mode Off.
−verb Verbose Mode On.