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**nifti-mrs**

***Release 1.3.3***

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This is the API documentation for the `nifti-mrs` Python package.

Source code is available at [https://github.com/wtclarke/nifti\\_mrs\\_tools](https://github.com/wtclarke/nifti_mrs_tools).



## NIFTI\_MRS

## 1.1 nifti\_mrs.nifti\_mrs

Core Nifti-MRS class. For more information on NIFTI-MRS see [https://github.com/wtclarke/mrs\\_nifti\\_standard](https://github.com/wtclarke/mrs_nifti_standard)

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**exception** nifti\_mrs.nifti\_mrs.NIFTIMRS\_DimDoesntExist

**exception** nifti\_mrs.nifti\_mrs.NotNIFTI\_MRS

**class** nifti\_mrs.nifti\_mrs.NIFTI\_MRS(\*args, validate\_on\_creation=True, \*\*kwargs)

A class to load and represent Nifti-MRS formatted data. Utilises the fslpy Image class and nibabel nifti headers.

Access the underlying fslpy Image object for useful attributes using obj.image.

**property header**

Returns NIFTI-MRS header object

**property ndim**

Returns number of dimensions in the NIFTI-MRS object

**property shape**

Returns the data shape. Singleton dimensions implied by header extension keys are included. Use obj.image.shape to get the shape of the stored data

**property dtype**

Returns data type

**property nifti\_mrs\_version**

Get NIFTI-MRS version string.

**set\_version\_info(major, minor)**

Puts mrs\_v{major}\_{minor} into intent\_name

**property dwelltime**

Return dwelltime in seconds

**property spectralwidth**

Return spectral width in Hz

**property bandwidth**

Alias for spectralwidth (Hz)

**property nucleus**

Returns resonant nucleus string(s) - returns list

**property spectrometer\_frequency**

Central or spectrometer frequency in MHz - returns list

**property field\_strength**

Field strength in tesla. NaN returned if unrecognised nucleus.

**getAffine(\*args)**

Return an affine transformation which can be used to transform coordinates from `from_` to `to`.

Valid values for the `from_` and `to` arguments are:

- `'voxel'`: The voxel coordinate system
- `'world'`: The world coordinate system, as defined by the image `sform/qform`
- `'fsl'`: The FSL coordinate system (scaled voxels, with a left-right flip if the `sform/qform` has a positive determinant)

**Parameters**

- **from** – Source coordinate system
- **to** – Destination coordinate system

**Returns**

A numpy array of shape (4, 4)

**property worldToVoxMat**

Returns a numpy array of shape (4, 4) containing an affine transformation from world coordinates to voxel coordinates.

**property voxToWorldMat**

Returns a numpy array of shape (4, 4) containing an affine transformation from voxel coordinates to world coordinates.

**property hdr\_ext**

Return MRS JSON header extension object.

**add\_hdr\_field(key, value, doc=None)**

Add a field to the header extension

**Parameters**

- **key** (*str*) – Field key
- **value** – Value of field to add
- **doc** (*optional*, *str*) – Use to convey meaning of user-defined header value.

**remove\_hdr\_field(key)**

Remove a field from the header extension

**Parameters**

- **key** (*str*) – Key to remove

**property file****property filename**

Name of file object was generated from. Returns empty string if N/A.



**property dim\_tags**

Return the three higher dimension tags

**dim\_position(dim\_tag)**

Return position of dim if it exists.

**set\_dim\_tag(dim, tag, info=None, header=None)**

Set or update the dim\_N, dim\_N\_info, and dim\_N\_header fields

Tag must be one of the standard-defined tags (e.g. DIM\_DYN)

**Parameters**

- **dim** (*str* or *int*) – The existing dim tag or python dimension index (i.e. N-1)
- **tag** (*str*) – New tag
- **info** (*str*) – New info string
- **header** (*dict*) – dict containing the dimension headers

**copy(remove\_dim=None)**

Return a copy of this image, optionally with a dimension removed.

**Parameters**

**remove\_dim** (*str* or *int*, *optional*) – dimension index (4, 5, 6) or tag to remove. Takes first index. Defaults to None/no removal

**Returns**

Copy of object

**Return type**

*NIFTI\_MRS*

**save(filepath)**

Save NIFTI-MRS to file

**Parameters**

**filepath** (*str* or *pathlib.Path*) – Name and path of save location

**iterate\_over\_dims(dim=None, iterate\_over\_space=False, reduce\_dim\_index=False, voxel\_index=None)**

Return generator to iterate over all indices or one dimension (and FID).

**Parameters**

- **dim** (*str* or *int*, *optional*) – None, dimension index (4, 5, 6) or tag. None iterates over all indices. Defaults to None
- **iterate\_over\_space** (*bool*, *optional*) – If True also iterate over spatial dimension, defaults to False
- **reduce\_dim\_index** (*bool*, *optional*) – If True the returned slice index will have the selected dimension removed. Defaults to False.
- **voxel\_index** (*slice* or *tuple*, *optional*) – slice or tuple of first three spatial dimensions., defaults to None

**Returns**

yeilds array of sliced data

**Return type**

np.array

**Returns**

data location slice object.

**Return type**

slice

**iterate\_over\_spatial()**

Iterate over spatial voxels yeilding a data array the shape of the FID and any higher dimensions + index.

**Yield**

Complex FID data with any higher dimensions. Index to data.

**Return type**

tuple

**dynamic\_hdr\_vals()**

Return representations of the dynamic header values

**Returns**

List of dicts containing labelled header parameters

**Returns**

List of tuples containing header values

**Returns**

Flattened numpy array for each generated spectrum containing header values

**plot**(*display\_dim=None, ppmlim=None, plot\_avg=False, mask=None, legend=True*)

## 1.2 nifti\_mrs.create\_nmrs

Generate new NIfTI-MRS objects and files from data blocks.

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**nifti\_mrs.create\_nmrs.gen\_nifti\_mrs**(*data, dwelltime, spec\_freq, nucleus='1H', affine=None, dim\_tags=[None, None, None], nifti\_version=2, no\_conj=False*)

Generate NIFTI-MRS from data and required metadata

**Parameters**

- **data** (*numpy.array*) – Complex-typed numpy array of at least 4 dimensions (max 7)
- **dwelltime** (*float*) – Spectral (4th dimension) dwelltime in seconds
- **spec\_freq** (*float*) – Spectrometer Frequency in MHz
- **nucleus** (*str, optional*) – Resonant Nucleus string (e.g. 1H, 31P, 2H), defaults to '1H'
- **affine** (*numpy.array, optional*) – 4x4 orientation/position affine, defaults to None which will use default (scaled identity).
- **dim\_tags** (*list, optional*) – List of dimension tags (e.g. DIM\_DYN), defaults to [None, None, None]
- **nifti\_version** (*int, optional*) – Version of NIFTI header format, defaults to 2
- **no\_conj** (*bool, optional*) – If true stops conjugation of data on creation, defaults to False

**Returns**

NIFTI-MRS object

**Return type***nifti\_mrs.nifti\_mrs.NIFTI\_MRS*

`nifti_mrs.create_nmrs.gen_nifti_mrs_hdr_ext(data, dwelltime, hdr_ext, affine=None, nifti_version=2, no_conj=False)`

Generate NIFTI-MRS from data and header extension object

**Parameters**

- **data** (*numpy.array*) – Complex-typed numpy array of at least 4 dimensions (max 7)
- **dwelltime** (*float*) – Spectral (4th dimension) dwelltime in seconds
- **hdr\_ext** (*nifti\_mrs.hdr\_ext.Hdr\_Ext*) – Populated NIFTI-MRS header extension
- **affine** (*numpy.array, optional*) – 4x4 orientation/position affine, defaults to None which will use default (scaled identity).
- **dim\_tags** (*list, optional*) – List of dimension tags (e.g. DIM\_DYN), defaults to [None, None, None]
- **nifti\_version** (*int, optional*) – Version of NIFTI header format, defaults to 2
- **no\_conj** (*bool, optional*) – If true stops conjugation of data on creation, defaults to False

**Returns**

NIFTI-MRS object

**Return type***nifti\_mrs.nifti\_mrs.NIFTI\_MRS*

## 1.3 nifti\_mrs.definitions

Translate the JSON definitions of NIFTI-MRS standard meta data and dimension tags to python usable formats.

Type fields should either be generic python types: float, int, str or a tuple indicating an array type and element type : (list, float) or (list, str)

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`nifti_mrs.definitions.field_def`

alias of HeaderExtensionField

`nifti_mrs.definitions.translate_definitions(obj)`

Translate the JSON defined object to python dicts with python types

## 1.4 nifti\_mrs.validator

**exception** `nifti_mrs.validator.Error`

Base class for other exceptions

**exception** `nifti_mrs.validator.headerExtensionError`

Raised if problems with header extension are found.

**exception** `nifti_mrs.validator.niftiHeaderError`

Raised if problems with nifti header are found.

**exception** `nifti_mrs.validator.niftiDataError`

Raised if problems with nifti data are found.

`nifti_mrs.validator.validate_nifti_mrs(nifti_mrs)`

Validate a full NIFTI MRS image.

`nifti_mrs.validator.validate_nifti_data(nifti_img_data)`

Validate the data inside a nibabel nifti image 1. Check data is complex 2. Check number of dimensions is at least 4 but less than 8.

`nifti_mrs.validator.validate_nifti_header(nifti_header)`

Validate the header of a nibabel nifti image Check data type is complex Check orientation data. - How? TO DO Check dwell time Check intent name

`nifti_mrs.validator.validate_hdr_ext(header_ex, dimension_sizes, data_dimensions=None)`

Validate the header extension 1. Check that it is json formatted string. 2. Check that it contains the required meta-data 3. Check that it contains any required dimension information. 4. Check that standard-defined data is of correct type.

**Parameters**

- **header\_ex** (*str*) – NIFTI-MRS header extensions as a json deserialisable string
- **dimension\_sizes** (*tuple of ints*) – Size of the NIFTI-MRS dimensions
- **data\_dimensions** (*int, optional*) – Total number of data dimensions in corresponding nifti-mrs data, defaults to None When None the dimensions are inferred from the tags and size

`nifti_mrs.validator.check_type(value, json_type)`

Checks that values is of type json\_type json\_type may be a tuple to handle array types e.g. (list, str) indicates a list of strings.

`nifti_mrs.validator.validate_spectralwidth(header_ex, dwelltime)`

If a SpectralWidth field is present, check that it matches the dwell time

Dwell time is stored in pixdim[4].

**Parameters**

- **header\_ex** (*str*) – NIFTI-MRS header extensions as a json deserialisable string
- **dwelltime** (*float*) – Dwell time as stored in pixdim[4] to check against any SpectralWidth definition. In seconds.

## 1.5 nifti\_mrs.hdr\_ext

**class** `nifti_mrs.hdr_ext.Hdr_Ext(spec_frequency, resonant_nucleus, dimensions=None)`

Class to hold meta data stored in a NIFTI MRS header extension. Required fields must be passed to initialise, Default dimension information automatically generated, but may be modified by set\_dim\_info method. Standard defined meta-data and user-defined data can be added using set\_standard\_def and set\_user\_def respectively.

**classmethod** `from_header_ext(hdr_ext_dict)`

Create a Hdr\_Ext object from a json string deserialised into a python dict

**Parameters**

**hdr\_ext\_dict** (*dict*) – header extension as a dict.

**Returns**

Class object

**Return type***Hdr\_Ext***property ndim**

Returns the number of dimensions implied by the 'dim\_{5,6,7}' tags

**set\_dim\_info(dim, tag, info=None, hdr=None)**

Set information associated with the optional, higher data dimensions.

**Parameters**

- **dim** (*str* or *int*) – May be (0,1,2) or (“5th”, “6th”, “7th”)
- **tag** (*str*) – Must be one of the defined dimension tag strings. E.g. DIM\_DYN or None
- **info** (*str*, *optional*) – Optional, free-form for documentation, defaults to None
- **hdr** (*dict*, *optional*) – Dict containing relevant header value names and values. Defaults to None

**remove\_dim\_info(dim)**

Set a dimension’s information to None

**Parameters**

**dim** (*str* or *int*) – 0,1,2 or “5th”, “6th”, “7th”

**set\_standard\_def(key, value)**

Add a single standard-defined bit of meta-data to the object.

**set\_user\_def(key, value, doc)**

Add user-defined metadata keys to the header extension. add keys and values one at a time using key, value and doc.

**remove\_standard\_def(key)**

Remove key from list of standard defined key-value pairs

**Parameters**

**key** (*str*) – Key name

**remove\_user\_def(key)**

Remove key from list of user defined key-value pairs

**Parameters**

**key** (*str*) – Key name

**to\_dict()**

Generate dictionary representation from properties.

**property current\_keys****to\_json()****copy()**

## 1.6 nifti\_mrs.tools.misc

Miscellaneous tools for NIFTI-MRS

Author: Will Clarke <[william.clarke@ndcn.ox.ac.uk](mailto:william.clarke@ndcn.ox.ac.uk)> Copyright (C) 2021 University of Oxford

`nifti_mrs.tools.misc.conjugate(nmrs)`

Conjugate a nifti-mrs object.

**Parameters**

**nmrs** (`NIFTI_MRS`) – NIFTI\_MRS object to conjugate

**Returns**

Conjugated NIFTI\_MRS

**Return type**

`NIFTI_MRS`

## 1.7 nifti\_mrs.tools.reshape

Tools for reshaping the higher dimensions of NIFTI-MRS

Author: Will Clarke <[william.clarke@ndcn.ox.ac.uk](mailto:william.clarke@ndcn.ox.ac.uk)> Copyright (C) 2021 University of Oxford

`nifti_mrs.tools.reshape.reshape(nmrs, reshape, d5=None, d6=None, d7=None)`

Reshape the higher dimensions (5-7) of an nifti-mrs file. Uses numpy reshape syntax to reshape. Use -1 for automatic sizing.

If the dimension exists after reshaping a tag is required. If None is passed but one already exists no change will be made. If no value exists then an exception will be raised.

**Parameters**

- **nmrs** (`NIFTI_MRS`) – Input NIFTI-MRS file
- **reshape** (`tuple`) – Tuple of target sizes in style of `numpy.reshape`, higher dimensions only.
- **d5** (`str`, *optional*) – Dimension tag to set dim\_5, defaults to None
- **d6** (`str`, *optional*) – Dimension tag to set dim\_6, defaults to None
- **d7** (`str`, *optional*) – Dimension tag to set dim\_7, defaults to None

## 1.8 nifti\_mrs.tools.split\_merge

Tools for merging and splitting the dimensions of NIFTI-MRS

Author: Will Clarke <[william.clarke@ndcn.ox.ac.uk](mailto:william.clarke@ndcn.ox.ac.uk)> Copyright (C) 2021 University of Oxford

`nifti_mrs.tools.split_merge.split(nmrs, dimension, index_or_indices)`

Splits, or extracts indices from, a specified dimension of a NIFTI\_MRS object. Output is two NIFTI\_MRS objects. Header information preserved.

**Parameters**

- **nmrs** (`fsl_mrs.core.nifti_mrs.NIFTI_MRS`) – Input nifti\_mrs object to split
- **dimension** (`str` or `int`) – Dimension along which to split. Dimension tag or one of 4, 5, 6 (for 0-indexed 5th, 6th, and 7th)
- **index\_or\_indices** (`int` or `[int]`) – Single integer index to split after, or list of integer indices to insert into second array. E.g. '0' will place the first index into the first output and 1 -> N in the second. '[1, 5, 10]' will place 1, 5 and 10 into the second output and all other will remain in the first.

**Returns**

Two NIFTI\_MRS object containing the split files

**Return type**

fsl\_mrs.core.nifti\_mrs.NIFTI\_MRS

nifti\_mrs.tools.split\_merge.**merge**(*array\_of\_nmrs, dimension*)

Concatenate NIFTI-MRS objects along specified higher dimension

**Parameters**

- **array\_of\_nmrs** (*tuple or list of fsl\_mrs.core.nifti\_mrs.NIFTI\_MRS*) – Array of NIFTI-MRS objects to concatenate
- **dimension** (*int or str*) – Dimension along which to concatenate. Dimension tag or one of 4, 5, 6 (for 0-indexed 5th, 6th, and 7th).

**Returns**

Concatenated NIFTI-MRS object

**Return type**

fsl\_mrs.core.nifti\_mrs.NIFTI\_MRS

## 1.9 nifti\_mrs.utils

Utility functions for NIFTI-MRS utilities

Author: Will Clarke &lt;william.clarke@ndcn.ox.ac.uk&gt; Copyright (C) 2021 University of Oxford

**exception** nifti\_mrs.utils.NIFTI\_MRSIncompatiblenifti\_mrs.utils.**modify\_hdr\_ext**(*new\_hdr\_ext, nifti\_header*)

Generate a new NIFTI header with a modified header extension. New header is a copy of the one passed

**Parameters**

- **new\_hdr\_ext** (*Hdr\_Ext object*) – Modified header extension
- **nifti\_header** (*nibabel.nifti2.Nifti2Header*) – NIFTI header

**Returns**

Copied header with modified hdr extension

**Return type**

nibabel.nifti2.Nifti2Header

nifti\_mrs.utils.**check\_type**(*in\_format*)

Return type of header: long (list) or short (dict)

**Parameters****in\_format** (*list or dict*) – Value of header key**Returns**

‘long’ or ‘short’

**Return type**

str

nifti\_mrs.utils.**dim\_n\_header\_short\_to\_long**(*in\_format, elements*)nifti\_mrs.utils.**dim\_n\_header\_long\_to\_short**(*in\_format*)





## MRS\_TOOLS

**The command-line tool for manipulation of NIFTI-MRS files.**

usage: mrs\_tools [-h] [-v] {info,vis,merge,split,reorder,conjugate} ...

NIFTI-MRS (Magnetic Resonance Spectroscopy) tools

**optional arguments:**

<b>-h, --help</b>	show this help message and exit
<b>-v, --version</b>	show program's version number and exit

**subcommands:**

Available tools

{info, vis, merge, split, reorder, conjugate}

## 2.1 info

Information about the NIFTI-MRS file.

usage: mrs\_tools info [-h] FILE or list of FILEs [FILE or list of FILEs ...]

**positional arguments:**

**FILE or list of FILEs**  
NIFTI MRS file(s)

**optional arguments:**

<b>-h, --help</b>	show this help message and exit
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## 2.2 vis

Quick visualisation of a NIFTI-MRS file or FSL-MRS basis set.

usage: mrs\_tools vis [-h] [--ppmlim LOW HIGH] [--mask MASK] [--save SAVE] [--display\_dim DISPLAY\_DIM] [--no\_mean] FILE or DIR

**positional arguments:**

**FILE or DIR**  
NIFTI file or directory of basis sets

**optional arguments:**

<b>-h, --help</b>	show this help message and exit
<b>--ppmlim LOW-HIGH</b>	limit the fit to a freq range (default=(.2,4.2))

<b>--mask MASK</b>	Mask for MRSI
<b>--save SAVE</b>	Save fig to path
<b>--display_dim</b>	DISPLAY_DIM. A NIFTI-MRS tag. Do not average across this dimension.
<b>--no_mean</b>	Do not plot the mean signal line in the case of multiple spectra.

## 2.3 merge

Merge NIFTI-MRS along higher dimensions.

```
usage: mrs_tools merge [-h] --files FILES [FILES ...] --dim DIM [--newaxis] [--output OUTPUT] [--filename FILENAME]
```

**optional arguments:**

<b>-h, --help</b>	show this help message and exit
<b>--newaxis</b>	Join files along a new axis (tag specified by <code>--dim</code> ).
<b>--output OUTPUT</b>	output folder (defaults to current directory)
<b>--filename FILENAME</b>	Override output file name.

**required arguments:**

<b>--files FILES [FILES ...]</b>	List of files to merge
<b>--dim DIM</b>	NIFTI-MRS dimension tag to merge across.

## 2.4 split

Split NIFTI-MRS along higher dimensions.

```
usage: mrs_tools split [-h] --file FILE --dim DIM (--indices INDICES [INDICES ...] | --index INDEX) [--output OUTPUT] [--filename FILENAME]
```

**optional arguments:**

<b>-h, --help</b>	show this help message and exit
<b>--indices INDICES [INDICES ...]</b>	List of indices to extract into second file. All indices are zero-indexed.
<b>--index INDEX</b>	Index to split at (split after index, zero-indexed).
<b>--output OUTPUT</b>	output folder (defaults to current directory)
<b>--filename FILENAME</b>	Override output file names.

**required arguments:**

<b>--file FILE</b>	File to split
<b>--dim DIM</b>	NIFTI-MRS dimension tag to split across.

## 2.5 reorder

Reorder higher dimensions of NIFTI-MRS.

```
usage: mrs_tools reorder [-h] --file FILE --dim_order DIM_ORDER [DIM_ORDER ...] [--output OUTPUT] [--filename FILENAME]
```

**optional arguments:**

- h, --help** show this help message and exit
- output OUTPUT** output folder (defaults to current directory)
- filename FILENAME** Override output file names.

**required arguments:**

- file FILE** File to reorder
- dim\_order DIM\_ORDER [DIM\_ORDER ...]**  
NIFTI-MRS dimension tags in desired order. Enter as strings (min:1, max:3). Can create singleton dimension at end.

## 2.6 reshape

Reshapes the higher dimensions of a NIFTI-MRS file.

usage: `mrs_tools reshape [-h] --file FILE --shape SHAPE [SHAPE ...] [--d5 D5] [--d6 D6] [--d7 D7] [--output OUTPUT] [--filename FILENAME]`

**optional arguments:**

- h, --help** show this help message and exit
- d5 D5** 5th dimension tag (e.g. DIM\_DYN).
- d6 D6** 6th dimension tag (e.g. DIM\_DYN).
- d7 D7** 7th dimension tag (e.g. DIM\_DYN).
- output OUTPUT** output folder (defaults to current directory)
- filename FILENAME** Override output file names.

**required arguments:**

- file FILE** File to reshape
- shape SHAPE [SHAPE ...]**  
Numpy-like target shape. Enter as integers, -1 is used for any. Only enter shape for higher (5th-7th) dimensions.

## 2.7 conjugate

Conjugate data to correct phase/frequency convention in a NIFTI-MRS file.

usage: `mrs_tools conjugate [-h] --file FILE [--output OUTPUT] [--filename FILENAME]`

**optional arguments:**

- h, --help** show this help message and exit
- output OUTPUT** output folder (defaults to current directory)
- filename FILENAME** Override output file names.

**required arguments:**

- file FILE** File to conjugate



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