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# **nifti-mrs**

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**CONTENTS:**

<b>1</b>	<b>nifti_mrs</b>	<b>3</b>
1.1	nifti_mrs.nifti_mrs .....	3
1.2	nifti_mrs.create_nmrs .....	6
1.3	nifti_mrs.definitions .....	7
1.4	nifti_mrs.validator .....	8
1.5	nifti_mrs.hdr_ext .....	9
1.6	nifti_mrs.tools.misc .....	10
1.7	nifti_mrs.tools.reshape .....	10
1.8	nifti_mrs.tools.split_merge .....	11
1.9	nifti_mrs.utils .....	11
<b>2</b>	<b>mrs_tools</b>	<b>13</b>
2.1	info .....	13
2.2	vis .....	13
2.3	merge .....	14
2.4	split .....	14
2.5	reorder .....	15
2.6	reshape .....	15
2.7	conjugate .....	16
	<b>Python Module Index</b>	<b>17</b>
	<b>Index</b>	<b>19</b>



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
- **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> 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 <william.clarke@ndcn.ox.ac.uk> Copyright (C) 2021 University of Oxford

**exception** `nifti_mrs.utils.NIFTI_MRSIncompatible`

`nifti_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)`



**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
-------------------	---------------------------------

## 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:**

**-h, --help** show this help message and exit  
**--ppmlim LOW-HIGH** limit the fit to a freq range (default=(.2,4.2))  
**--mask MASK** Mask for MRSI  
**--save SAVE** Save fig to path  
**--display\_dim** DISPLAY\_DIM. A NIFTI-MRS tag. Do not average across this dimension.  
**--no\_mean** 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:**

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

**required arguments:**

**--files FILES [FILES ...]**  
List of files to merge  
**--dim DIM** 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:**

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

**required arguments:**

**--file FILE** File to split  
**--dim DIM** 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

## PYTHON MODULE INDEX

### n

- `nifti_mrs.create_nmrs`, 6
- `nifti_mrs.definitions`, 7
- `nifti_mrs.hdr_ext`, 9
- `nifti_mrs.nifti_mrs`, 3
- `nifti_mrs.tools.misc`, 10
- `nifti_mrs.tools.reshape`, 10
- `nifti_mrs.tools.split_merge`, 11
- `nifti_mrs.utils`, 11
- `nifti_mrs.validator`, 8



## A

`add_hdr_field()` (*nifti\_mrs.nifti\_mrs.NIFTI\_MRS method*), 4

## B

`bandwidth` (*nifti\_mrs.nifti\_mrs.NIFTI\_MRS property*), 3

## C

`check_type()` (*in module nifti\_mrs.utils*), 12  
`check_type()` (*in module nifti\_mrs.validator*), 8  
`conjugate()` (*in module nifti\_mrs.tools.misc*), 10  
`copy()` (*nifti\_mrs.hdr\_ext.Hdr\_Ext method*), 10  
`copy()` (*nifti\_mrs.nifti\_mrs.NIFTI\_MRS method*), 5  
`current_keys` (*nifti\_mrs.hdr\_ext.Hdr\_Ext property*), 10

## D

`dim_n_header_long_to_short()` (*in module nifti\_mrs.utils*), 12  
`dim_n_header_short_to_long()` (*in module nifti\_mrs.utils*), 12  
`dim_position()` (*nifti\_mrs.nifti\_mrs.NIFTI\_MRS method*), 5  
`dim_tags` (*nifti\_mrs.nifti\_mrs.NIFTI\_MRS property*), 5  
`dtype` (*nifti\_mrs.nifti\_mrs.NIFTI\_MRS property*), 3  
`dweltime` (*nifti\_mrs.nifti\_mrs.NIFTI\_MRS property*), 3  
`dynamic_hdr_vals()` (*nifti\_mrs.nifti\_mrs.NIFTI\_MRS method*), 6

## E

`Error`, 8

## F

`field_def` (*in module nifti\_mrs.definitions*), 7  
`field_strength` (*nifti\_mrs.nifti\_mrs.NIFTI\_MRS property*), 4  
`file` (*nifti\_mrs.nifti\_mrs.NIFTI\_MRS property*), 4  
`filename` (*nifti\_mrs.nifti\_mrs.NIFTI\_MRS property*), 4  
`from_header_ext()` (*nifti\_mrs.hdr\_ext.Hdr\_Ext class method*), 9

## G

`gen_nifti_mrs()` (*in module nifti\_mrs.create\_nmrs*), 6

`gen_nifti_mrs_hdr_ext()` (*in module nifti\_mrs.create\_nmrs*), 7  
`getAffine()` (*nifti\_mrs.nifti\_mrs.NIFTI\_MRS method*), 4

## H

`Hdr_Ext` (*class in nifti\_mrs.hdr\_ext*), 9  
`hdr_ext` (*nifti\_mrs.nifti\_mrs.NIFTI\_MRS property*), 4  
`header` (*nifti\_mrs.nifti\_mrs.NIFTI\_MRS property*), 3  
`headerExtensionError`, 8

## I

`iterate_over_dims()` (*nifti\_mrs.nifti\_mrs.NIFTI\_MRS method*), 5  
`iterate_over_spatial()` (*nifti\_mrs.nifti\_mrs.NIFTI\_MRS method*), 6

## M

`merge()` (*in module nifti\_mrs.tools.split\_merge*), 11  
`modify_hdr_ext()` (*in module nifti\_mrs.utils*), 11  
`module`  
    *nifti\_mrs.create\_nmrs*, 6  
    *nifti\_mrs.definitions*, 7  
    *nifti\_mrs.hdr\_ext*, 9  
    *nifti\_mrs.nifti\_mrs*, 3  
    *nifti\_mrs.tools.misc*, 10  
    *nifti\_mrs.tools.reshape*, 10  
    *nifti\_mrs.tools.split\_merge*, 11  
    *nifti\_mrs.utils*, 11  
    *nifti\_mrs.validator*, 8

## N

`ndim` (*nifti\_mrs.hdr\_ext.Hdr\_Ext property*), 9  
`ndim` (*nifti\_mrs.nifti\_mrs.NIFTI\_MRS property*), 3  
`NIFTI_MRS` (*class in nifti\_mrs.nifti\_mrs*), 3  
`nifti_mrs.create_nmrs`  
    *module*, 6  
`nifti_mrs.definitions`  
    *module*, 7  
`nifti_mrs.hdr_ext`

module, 9  
nifti\_mrs.nifti\_mrs  
  module, 3  
nifti\_mrs.tools.misc  
  module, 10  
nifti\_mrs.tools.reshape  
  module, 10  
nifti\_mrs.tools.split\_merge  
  module, 11  
nifti\_mrs.utils  
  module, 11  
nifti\_mrs.validator  
  module, 8  
nifti\_mrs\_version (nifti\_mrs.nifti\_mrs.NIFTI\_MRS  
  property), 3  
NIFTI\_MRSIncompatible, 11  
niftiDataError, 8  
niftiHeaderError, 8  
NIFTIMRS\_DimDoesntExist, 3  
NotNIFTI\_MRS, 3  
nucleus (nifti\_mrs.nifti\_mrs.NIFTI\_MRS property), 3

## P

plot() (nifti\_mrs.nifti\_mrs.NIFTI\_MRS method), 6

## R

remove\_dim\_info() (nifti\_mrs.hdr\_ext.Hdr\_Ext  
  method), 9  
remove\_hdr\_field() (nifti\_mrs.nifti\_mrs.NIFTI\_MRS  
  method), 4  
remove\_standard\_def() (nifti\_mrs.hdr\_ext.Hdr\_Ext  
  method), 9  
remove\_user\_def() (nifti\_mrs.hdr\_ext.Hdr\_Ext  
  method), 9  
reshape() (in module nifti\_mrs.tools.reshape), 10

## S

save() (nifti\_mrs.nifti\_mrs.NIFTI\_MRS method), 5  
set\_dim\_info() (nifti\_mrs.hdr\_ext.Hdr\_Ext method), 9  
set\_dim\_tag() (nifti\_mrs.nifti\_mrs.NIFTI\_MRS  
  method), 5  
set\_standard\_def() (nifti\_mrs.hdr\_ext.Hdr\_Ext  
  method), 9  
set\_user\_def() (nifti\_mrs.hdr\_ext.Hdr\_Ext method), 9  
set\_version\_info() (nifti\_mrs.nifti\_mrs.NIFTI\_MRS  
  method), 3  
shape (nifti\_mrs.nifti\_mrs.NIFTI\_MRS property), 3  
spectralwidth (nifti\_mrs.nifti\_mrs.NIFTI\_MRS prop-  
  erty), 3  
spectrometer\_frequency  
  (nifti\_mrs.nifti\_mrs.NIFTI\_MRS property),  
  4  
split() (in module nifti\_mrs.tools.split\_merge), 11

## T

to\_dict() (nifti\_mrs.hdr\_ext.Hdr\_Ext method), 9  
to\_json() (nifti\_mrs.hdr\_ext.Hdr\_Ext method), 10  
translate\_definitions() (in module  
  nifti\_mrs.definitions), 7

## V

validate\_hdr\_ext() (in module nifti\_mrs.validator), 8  
validate\_nifti\_data() (in module  
  nifti\_mrs.validator), 8  
validate\_nifti\_header() (in module  
  nifti\_mrs.validator), 8  
validate\_nifti\_mrs() (in module  
  nifti\_mrs.validator), 8  
validate\_spectralwidth() (in module  
  nifti\_mrs.validator), 8  
voxToWorldMat (nifti\_mrs.nifti\_mrs.NIFTI\_MRS prop-  
  erty), 4

## W

worldToVoxMat (nifti\_mrs.nifti\_mrs.NIFTI\_MRS prop-  
  erty), 4