

# MeTime R Package

July 18, 2022

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add\_col\_normality      *Function to check normality and add data to col data*

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## Description

A method applied on the s4 object of class "metime\_analyser" to check normality of the metabolites and add it to corresponding columns

## Usage

```
add_col_normality(object, which_data, type, metab_names)
```

## Arguments

object	An object of class metime_analyser
which_data	dataset on which the method is to be applied
type	type of test, currently only shapiro-wilk test is available under the choice "shapiro"
metab_names	column that has the metabolite names in col_data.

## Value

S4 object with shapiro wilk test related data in the col\_data

## Examples

```
object <- add_col_normality(object=data, which_data=c("lipid_data", "nmr_data"), type="shapiro", metab_names=c("m
```

`add_screening_vars`      *Function to add measurements taken at screening time for samples to be added to all timepoints*

### Description

A method applied on the s4 object of class "metime\_analyser" to add all those datapoints that were measured only during screening to all the respective samples at all timepoints

### Usage

```
add_screening_vars(object, vars)
```

### Arguments

<code>object</code>	An object of class metime_analyser
<code>vars</code>	A character naming the vars of interest

### Value

phenotype data which can be replaced into the original object or use it separately with a different object

### Examples

```
# adding APOEGrp, PTGENDER to all data points
new_with_apoegrp_sex <- add_screening_vars(object=metime_analyser_object, vars=c("APOEGrp", "PTGENDER"))
```

`calc_conservation_metabolite`      *Function to calculate metabolite conservation index*

### Description

Method applied on the object metime\_analyser to calculate the metabotype conservation index

### Usage

```
calc_conservation_metabolite(object, which_data, verbose)
```

### Arguments

<code>object</code>	An object of class metime_analyser
<code>which_data</code>	Name of the dataset to be used
<code>verbose</code>	Information provided on steps being processed

**Value**

List of conservation index results

**Examples**

```
#calculating metabolite_conservation_index  
out <- calc_metabolite_conservation(object=metime_analyser_object, which_data="Name of the dataset")
```

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**calc\_conservation\_metabotype**

*Function to calculate metabotype conservation index*

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**Description**

Method applied on the object metime\_analyser to calculate the metabotype conservation index

**Usage**

```
calc_conservation_metabotype(object, which_data, verbose)
```

**Arguments**

object	An object of class metime_analyser
which_data	Name of the dataset to be used
verbose	Information provided on steps being processed

**Value**

List of conservation index results

**Examples**

```
#calculating metabotype_conservation_index  
out <- calc_metabotype_conservation(object=metime_analyser_object, which_data="Name of the dataset")
```

**calc\_correlation\_pairwise***Function to calculate correlation***Description**

calculate pairwise correlations This function creates a dataframe for plotting from a dataset.

**Usage**

```
calc_correlation_pairwise(object, which_data, method)
```

**Arguments**

- |            |   |
|------------|---|
| object     | S4 Object of class metime_analyser                                      |
| which_data | specify datasets to calculate on. One or more possible                  |
| method     | default setting: method="pearson", Alternative "spearman" also possible |

**Value**

data.frame with pairwise results

**Examples**

```
# Example to calculate correlations
dist <- calc_correlation(object=metime_analyser_object, which_data="name of the dataset",
                           method="pearson")
```

**calc\_dimensionality\_reduction***Function to calculate dimensionality reduction methods such as tsne, umap and pca.***Description**

A method to apply on s4 object of class metime\_analyse in order to obtain information after dimensionality reduction on a dataset/s

**Usage**

```
calc_dimensionality_reduction(object, which_data, type)
```

**Arguments**

object	An object of class metime_analyser
which_data	a character vector - Names of the dataset from which the samples will be extracted
type	type of the dimensionality reduction method to be applied. Accepted inputs are "UMAP", "tSNE", "PCA"

**Value**

a list with two dataframes containing the dimensionality reduction information 1) samples - data of the individuals(".samples") 2) metabs - data of the metabolites(".metabs")

**Examples**

```
#calculate PCA
pca <- calc_dimensionality_reduction(object=metime_analyser_object, which_data="name/s of the dataset/s", type="PCA")
#calculate UMAP
pca <- calc_dimensionality_reduction(object=metime_analyser_object, which_data="name/s of the dataset/s", type="UMAP")
#calculate tSNE
pca <- calc_dimensionality_reduction(object=metime_analyser_object, which_data="name/s of the dataset/s", type="tSNE")
```

**calc\_distance\_pairwise**

*Function to calculate dissimilarity using distance measures*

**Description**

calculate pairwise distances This function creates a dataframe for plotting from a dataset.

**Usage**

```
calc_distance_pairwise(object, which_data, method)
```

**Arguments**

object	S4 Object of class metime_analyser
which_data	specify datasets to calculate on. One or more possible
method	default setting: method="euclidean", Alternative "maximum", "minimum", "manhattan", "canberra", "minkowski" are also possible

**Value**

data.frame with pairwise results

**Examples**

```
# Example to calculate pairwise distances
dist <- calc_pairwise_distance(object=metime_analyser_object, which_data="name of the dataset",
                                 method="euclidean")
```

**calc\_featureselection\_boruta**  
*Function to calculate dependent variables*

### Description

An S4 method to be applied on the metime\_analyser object so as to calculate dependent variables

### Usage

```
calc_featureselection_boruta(
  object,
  which_x,
  which_y,
  verbose,
  output_loc,
  file_name
)
```

### Arguments

object	An object of class metime_analyser
which_x	Name of the dataset to be used for training
which_y	Name of the dataset to be used for testing
verbose	Information provided on steps being processed
output_loc	path to the parent directory where in the out file will be stored
file_name	name of the out file

### Value

List of conservation index results

**get\_append\_analyser\_object**  
*This function appends an object of class metime\_analyser with a new dataset.*

### Description

function to apply on metime\_analyse object to append a new dataset into the existing object

### Usage

```
get_append_analyser_object(object, data, col_data, row_data, name)
```

**Arguments**

object	S4 object of class metime_analyser
data	data.frame containing data
col_data	data.frame containing col_data: id column of col data has to match colnames of data
row_data	data.frame containing row_data: id column of row data has to match rownames of data
name	Name of the new dataset

**Value**

An object of class metime\_analyser

**Examples**

```
# append data frames into the metime_analyser object
appended_object <- get_append_metab_object(object=metime_analyser_object, data=data, row_data=row_data, col_data=col
```

get\_files\_and\_names     *Function to pack all the data into a single object of class "metime\_analyser"*

**Description**

This function loads all the files from the parent directory. It assumes a certain naming pattern as follows: "datatype\_Nonelcollrow\_data.rds" Any other naming pattern is not allowed. The function first writes all files into a list and each type of data is packed into its respective class i.e. col\_data, row\_data or data

**Usage**

```
get_files_and_names(path, annotations_index)
```

**Arguments**

path	Path to the parent directory
annotations_index	a list to be filled as follows = list(phenotype="Name or index of the files", medication="Name or index of the files")

**Value**

An object of class metime\_analyser

**Examples**

```
# Input in the parent directory from which the data files are to be extracted along with annotations_index to specify
get_files_and_names(path=/path/to/parent/directory, annotations_index=list(phenotype="Name of phenotype file", m
```

**get\_make\_analyser\_object**

*Function to pack all the data into a single object of class "metime\_analyser"*

**Description**

This function creates an object of class metime\_analyser from a dataset.

**Usage**

```
get_make_analyser_object(
  data,
  col_data,
  row_data,
  annotations_index,
  name = NULL
)
```

**Arguments**

data	data.frame containing data
col_data	data.frame containing col_data: id column of col data has to match colnames of data
row_data	data.frame containing row_data: id column of row data has to match rownames of data
annotations_index	a list to be filled as follows = list(phenotype="Name or index of the file/list", medication="Name or index of the files/list")
name	character. Name you want to assign to the new dataset that is being added on

**Value**

An object of class metime\_analyser

**Examples**

```
# new_metime_analyser_object <- get_make_metab_object(data=data_frame, col_data=col_data_frame, row_data=row_data)
# annotations_index=list(phenotype="name of phenotype", medication="name of medication"))
```

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**get\_make\_plotter\_object**

*Function to make a plottable object for viz functions*

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**Description**

function to generate metime\_plotter object from plot data and metadata

**Usage**

```
get_make_plotter_object(data, metadata, calc_type, calc_info, plot_type, style)
```

**Arguments**

data	dataframe of plottable data obtained from calc object
metadata	dataframe with the metadata for the plot table mentioned above. To obtain these see get_metadata_for_rows() and get_metadata_for_columns()
calc_type	A character to specify type of calculation - will be used for comp_ functions
calc_info	A string to define the information about calculation
plot_type	type of the plot you want to build. eg: "box", "dot" etc. Its a character vector
style	Style of plot, accepted inputs are "ggplot", "circos" and "visNetwork". Is a singular option.

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**get\_metadata\_for\_columns**

*Get metadata for columns(in most cases for metabolites)*

---

**Description**

function to generate a metadata list for building the MeTime plotter object

**Usage**

```
get_metadata_for_columns(object, which_data, columns, names, index_of_names)
```

**Arguments**

object	S4 object of class MeTime Analyser
which_data	Names of dataset/s to be used
columns	A list of character vectors for the columns of interest. Length of the list should be same as length of which_data
names	A Character vector with the new names for the columns mentioned above
index_of_names	character vector to define the name of the column in which names of the variables are stored

**Value**

`data.frame` with metadata information

`get_metadata_for_rows` *Get metadata for rows(in most cases for samples)*

**Description**

function to generate a metadata list for building the MeTime plotter object

**Usage**

```
get_metadata_for_rows(object, which_data, columns, names)
```

**Arguments**

<code>object</code>	S4 object of class MeTime Analyser
<code>which_data</code>	Names of dataset/s to be used
<code>columns</code>	A list of character vectors for the columns of interest. Length of the list should be same as length of <code>which_data</code>
<code>names</code>	A Character vector with the new names for the columns mentioned above

**Value**

`data.frame` with metadata information for rows

`get_palette` *Get a palette of "n" distinct colorblind friendly colors*

**Description**

Function to get a palette of distinct colorblind friendly colors, the distinctiveness is determined by the difference in their hue values.

**Usage**

```
get_palette(n)
```

**Arguments**

<code>n</code>	number of colors wanted in the palette
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**Value**

a color palette vector with colors in the form of hex codes

**Examples**


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```
# colors=get_palette(n=10)
```

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**get\_samples\_and\_timepoints**

*Function to know the number of timepoints and the total number of samples available at that point*

---

**Description**

A method applied onto s4 object of class "metime\_analyser" so as to obtain the number of unique samples available at each timepoint.

**Usage**

```
get_samples_and_timepoints(object, which_data)
```

**Arguments**

object	An object of class metime_analyser
which_data	Name of the dataset in context

**Value**

A data table with timepoints and number of samples at each timepoint

**Examples**

```
# newdata <- get_samples_and_timepoints(object=metime_analyser_object, which_data="Name of dataset of interest")
```

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**get\_text\_for\_plot**

*Function to Obtain textual information for visualization in interactive plots*

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**Description**

a standard function to be applied on data matrices or dataframes with the colnames of interest such that the information from columns is visualized in the interactive plot

**Usage**

```
get_text_for_plot(data, colnames)
```

## Arguments

data	a dataframe with plotting data along with other variables for visualization
colnames	a character vector with the names of the variables that you want to see on the plot

## Value

a vector with strings that can be parsed into plot\_ly text.

## Examples

```
# text = get_text(data=data.frame, colnames=c("names", "of", "columns", "of", "interest"))
```

**metime\_analyser-class** *Constructor to generate an object of class metime\_analyser. contains slots - list\_of\_data: For the list of all data matrices. - list\_of\_col\_data: list of all the col data files in the same order. - list\_of\_row\_data: list of all the row data files in the same order. - annotations: list with phenotype and medication. Each of which is character that represents the name of the aforementioned dataset types.*

## Description

Constructor to generate an object of class metime\_analyser. contains slots - list\_of\_data: For the list of all data matrices. - list\_of\_col\_data: list of all the col data files in the same order. - list\_of\_row\_data: list of all the row data files in the same order. - annotations: list with phenotype and medication. Each of which is character that represents the name of the aforementioned dataset types.

Constructor to generate an object of class metime\_analyser. contains slots - list\_of\_data: For the list of all data matrices. - list\_of\_col\_data: list of all the col data files in the same order. - list\_of\_row\_data: list of all the row data files in the same order. - annotations: list with phenotype and medication. Each of which is character that represents the name of the aforementioned dataset types.

Constructor to generate an object of class metime\_analyser. contains slots - list\_of\_data: For the list of all data matrices. - list\_of\_col\_data: list of all the col data files in the same order. - list\_of\_row\_data: list of all the row data files in the same order. - annotations: list with phenotype and medication. Each of which is character that represents the name of the aforementioned dataset types.

Constructor to generate an object of class metime\_analyser. contains slots - list\_of\_data: For the list of all data matrices. - list\_of\_col\_data: list of all the col data files in the same order. - list\_of\_row\_data: list of all the row data files in the same order. - annotations: list with phenotype and medication. Each of which is character that represents the name of the aforementioned dataset types.

Constructor to generate an object of class metime\_analyser. contains slots - list\_of\_data: For the list of all data matrices. - list\_of\_col\_data: list of all the col data files in the same order. -

list\_of\_row\_data: list of all the row data files in the same order. - annotations: list with phenotype and medication. Each of which is character that represents the name of the aforementioned dataset types.

metime_plotter-class	<i>creating metime_plotter class that converts calculations and metadata as a plotable object to parse into viz_plotter Contains slots - plot_data: list of Dataframe(s) with plotting data and metadata for visualization. Dataframes is an option only for visNetwork() plots. Need a list of two dataframes: Nodes dataframe and edge dataframe named as \$.node and \$.edge - plot: ggplot(), circos() or visNetwork() object - calc_type: A vector to specify type of calculation - will be used for comp_functions - calc_info: string to define the information about calculation - plot_type: A character vector to define the type of plots that are needed. - style: Character that defines the style of plot i.e. a ggplot(), circos() or visNetwork() plot. Is always a singular input. Cannot have two styles in one object.</i>
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## Description

creating metime\_plotter class that converts calculations and metadata as a plotable object to parse into viz\_plotter Contains slots - plot\_data: list of Dataframe(s) with plotting data and metadata for visualization. Dataframes is an option only for visNetwork() plots. Need a list of two dataframes: Nodes dataframe and edge dataframe named as \$.node and \$.edge - plot: ggplot(), circos() or visNetwork() object - calc\_type: A vector to specify type of calculation - will be used for comp\_functions - calc\_info: string to define the information about calculation - plot\_type: A character vector to define the type of plots that are needed. - style: Character that defines the style of plot i.e. a ggplot(), circos() or visNetwork() plot. Is always a singular input. Cannot have two styles in one object.

creating metime\_plotter class that converts calculations and metadata as a plotable object to parse into viz\_plotter Contains slots - plot\_data: Dataframe with plotting data and metadata for visualization - plot: ggplot(), circos() or visNetwork() object with predefined aesthetics - calc\_type: A vector to specify type of calculation - will be used for comp\_functions - calc\_info: string to define the information about calculation - plot\_type: A character vector to define the type of plots that are needed.

mod_convert_s4_to_s3	<i>Function to Convert S4 object of class metime_analyser to an S3 object with same architecture</i>
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## Description

converter function to be applied onto metime\_analyse object to convert into a standard list of S3 type.

**Usage**

```
mod_convert_s4_to_s3(object)
```

**Arguments**

**object** An object of class metime\_analyser

**Value**

An S3 object of the same data as metime\_analyser in other words all slots are now converted into nested lists

**Examples**

```
# convert S4 object to a list
s3_list <- mod_convert_s4_to_s3(object=metime_analyser_object)
```

**mod\_extract\_common\_samples**

*Function to get only common samples from the dataframes in list\_of\_data*

**Description**

A method applied on object of class metime\_analyse to extract common samples across datasets.  
Also has an option to split the data according timepoints(mod\_split\_acc\_time()).

**Usage**

```
mod_extract_common_samples(object, time_splitter = FALSE)
```

**Arguments**

**object** An object of class metime\_anaylser

**time\_splitter** A boolean input: True leads to splitting of the data wrt time, False returns all the dataframes as they are with common rows

**Value**

list\_of\_data with common samples across all time points

**Examples**

```
# extracting common samples across all datasets
new_list_of_data <- mod_common_sample_extractor(object=metime_analyser_object)
```

---

mod\_filter\_tp*Functions for selecting time points*

---

**Description**

a method applied onto class metime\_analyser in order to extract timepoints of interest from a dataset

**Usage**

```
mod_filter_tp(object, timepoints, full, which_data)
```

**Arguments**

object	An object of class metime_analyser
timepoints	time points to be selected
full	if TRUE subjects are only selected if measured in all selected time points
which_data	Name of the dataset to be used

**Value**

An object of class metime\_analyser with processed data

**Examples**

```
#example to use this function
object <- mod_filter_tp(object, timepoints=c(0,12,24), full=TRUE, which_data="Name of the dataset")
```

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mod\_prep\_data\_for\_ggms

*Function to prepare and preprocess S4 objects to use it for gaussian graphical models. Also converts S4 to S3*

---

**Description**

function to be applied onto metime\_analyse object to convert into a standard list of S3 type based on the type of GGM analysis to be performed.

**Usage**

```
mod_prep_data_for_ggms(object, which_type, mlp_or_temp)
```

**Arguments**

<code>object</code>	An object of class metime_analyser
<code>which_type</code>	two choices either: 1) single - converts S4 to S3 and returns the nested list 2) multi - extracts common samples across the dataframes and returns an S3 nested list
<code>mlp_or_temp</code>	boolean. If true preps data for multibipartite lasso or temporal networks

**Value**

An S3 object(nested list) with the same architecture as that of class metime\_analyser

**Examples**

```
# prepping data for genenet ggm for single dataset
object <- mod_prep_data_for_ggms(object, which_type="single", mlp_or_temp=FALSE)
```

`mod_split_acc_to_time` *Function to split data according to time*

**Description**

Function to split the list of dataframes into a nested list with each dataframe being split into into dataframes of different timepoints

**Usage**

```
mod_split_acc_to_time(object)
```

**Arguments**

<code>object</code>	An object of class metime_analyser
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**Value**

`list_of_data` with each dataframe being broken into a list of dataframes with respect to the timepoint they belong to

**Examples**

```
#splitting data according to time
new_data <- mod_split_acc_to_time(object=metime_analyser_object)
```

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mod_trans_log	<i>Function to apply log transformation</i>
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**Description**

Function to log transform data

**Usage**

```
mod_trans_log(object, which_data, base)
```

**Arguments**

object	An object of class metime_analyser
which_data	Name of the dataset to be used
base	base of log to be used

**Value**

An object of class metime\_analyser with processed data

**Examples**

```
# example to apply log transformation
object <- mod_logtrans(object, which_data="name of the dataset", base=2)
```

---

---

mod_trans_zscore	<i>Function to scale the data</i>
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---

**Description**

Functions for scaling

**Usage**

```
mod_trans_zscore(object, which_data)
```

**Arguments**

object	An object of class metime_analyser
which_data	Name of the dataset to be used

**Value**

An object of class metime\_analyser with processed data

**Examples**

```
# example to apply scaling
object <- mod_zscore(object, which_data="name of the dataset")
```

---

**set\_parallel\_cores** *register parallel backend*

---

**Description**

function to run in order to perform the analysis parallely thereby saving time

**Usage**

```
set_parallel_cores(n_cores = NULL)
```

**Arguments**

n\_cores A number of specified cores.

**Value**

set a parallel backend

---

**show,metime\_analyser-method**

*Setting new print definition for the metime\_analyser object*

---

**Description**

function to see the structure of metime\_analyser object

**Usage**

```
## S4 method for signature 'metime_analyser'
show(object)
```

**Arguments**

object S4 object of class metime\_analyser

**Value**

structure of the S4 object

**Examples**

```
structure(object)
```

---

```
show,metime_plotter-method
```

*Setting new print definition for the metime\_plotter object*

---

## Description

function to see the structure of metime\_plotter object

## Usage

```
## S4 method for signature 'metime_plotter'  
show(object)
```

## Arguments

object            S4 object of class metime\_plotter

## Value

structure of the S4 object

## Examples

```
structure(object)
```

---

```
structure,metime_plotter-method
```

*Setting new structure definition for the metime\_plotter object*

---

## Description

function to see the structure of metime\_plotter object

## Usage

```
## S4 method for signature 'metime_plotter'  
structure(object)
```

## Arguments

object            S4 object of class metime\_plotter

## Value

structure of the S4 object

**Examples**


---

```
structure(object)
```

---

**structure**

*Setting new structure definition for the metime\_analyser object*

---

**Description**

function to see the structure of metime\_analyser object

**Usage**

```
structure(object)
```

**Arguments**

<b>object</b>	S4 object of class metime_analyser
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**Value**

structure of the S4 object

**Examples**


---

```
structure(object)
```

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**viz\_dimensionality\_reduction**

*Function to dot plot any kind of dot\_plotter including for dimensionality reduction*

---

**Description**

General function to be implemented on data\_list that is obtained after applying a dimensionality reduction method

**Usage**

```
viz_dimensionality_reduction(
  data_list,
  metadata_list,
  axes_labels,
  title_metabs,
  title_samples
)
```

**Arguments**

<code>data_list</code>	list obtained after applying <code>calc_dimensionality_reduction()</code> on <code>metime_analyse</code> object
<code>metadata_list</code>	list obtained after applying <code>get_metadata_for_plotting()</code> on <code>metime_analyse</code> object
<code>axes_labels</code>	character vector to specify the labels of the axes in the order x and y.
<code>title_metabs</code>	character to specify the title of the plot of metabolites

**Value**

a list with both the plots of samples and metabolites. Can be accessed by using `".$samples"` and `".$metabs"`

**viz\_distribution\_plotter**

*Function for Plotting distributions of phenotypic variables*

**Description**

A method to be applied onto s4 object so as to obtain distributions of various phenotypic variables

**Usage**

```
viz_distribution_plotter(object, colname, which_data, strats)
```

**Arguments**

<code>object</code>	An object of class <code>metime_analyser</code>
<code>colname</code>	Name of the variable whose distribution is of interest
<code>which_data</code>	Name of the dataset from which the samples will be extracted

**Value**

a list with either 1) density plot, mean table acc to timepoint and variable type or 2) bar plot, line plot, and variable type

**Examples**

```
# extracting distribution of Age from dataset1
plot <- viz_distribution_plotter(object, colname="Age", which_data="dataset1", strats="additional columns for fac
```

`viz_plotter_circos`      *Setting up standard wrapper for all circos plots for a metime\_plotter object.*

## Description

plot function for metime\_plotter object with different inputs to specialize plots. Used for all calc outputs.

## Usage

```
viz_plotter_circos(object, aesthetics, outfile)
```

## Arguments

<code>object</code>	S4 object of class metime_plotter
<code>aesthetics</code>	list for aesthetics. eg: list(list(x="colname",y="colname",color="colname", shape="colname"), list(...)) for "dot" plot and "heatmap" plot, for heatmap: list(x="colname", y="colname", fill="colname"). Additionally two other character vectors are allowed namely .\$vis and .\$strats for text and for facet wrapping.

`viz_plotter_ggplot`      *Setting up standard wrapper for all ggplot plots for a metime\_plotter object.*

## Description

plot function for metime\_plotter object with different inputs to specialize plots. Used for all calc outputs.

## Usage

```
viz_plotter_ggplot(object, aesthetics)
```

## Arguments

<code>object</code>	S4 object of class metime_plotter
<code>aesthetics</code>	list for aesthetics. eg: list(list(x="colname",y="colname",color="colname", shape="colname"), list(...)) for "dot" plot and "heatmap" plot, for heatmap: list(x="colname", y="colname", fill="colname"). Additionally two other character vectors are allowed namely .\$vis and .\$strats for text and for facet wrapping.

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**viz\_plotter\_visNetwork**

*Setting up standard wrapper for network plots from visNetwork for a metime\_plotter object.*

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**Description**

plot function for metime\_plotter object with different inputs to specialize plots. Used for all calc outputs.

**Usage**

```
viz_plotter_visNetwork(object, title)
```

**Arguments**

object	S4 object of class metime_plotter
title	character/string that is the title of the graph output

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