

# Package ‘gatom’

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**Title** Finding an Active Metabolic Module in Atom Transition Network

**Version** 1.5.0

**Description** This package implements a metabolic network analysis pipeline to identify an active metabolic module based on high throughput data. The pipeline takes as input transcriptional and/or metabolic data and finds a metabolic subnetwork (module) most regulated between the two conditions of interest. The package further provides functions for module post-processing, annotation and visualization.

**biocViews** GeneExpression, DifferentialExpression, Pathways, Network

**Depends** R (>= 4.3.0)

**Imports** data.table, igraph, BioNet, plyr, methods, XML, sna, intergraph, network, GGally, grid, ggplot2, mwcsr, pryr, htmlwidgets, htmltools, shinyCyJS (>= 1.0.0)

**Suggests** testthat, knitr, rmarkdown, KEGGREST, AnnotationDbi, org.Mm.eg.db, reactome.db, fgsea, readr, BiocStyle, R.utils

**License** MIT + file LICENCE

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abbreviateLabels	<i>Abbreviate lipid labels for lipid module</i>
------------------	---

---

### Description

Abbreviate lipid labels for lipid module

### Usage

```
abbreviateLabels(module, orig.names, abbrev.names)
```

**Arguments**

module	Module to prepare
orig.names	whether to use original names from the dataset
abbrev.names	whether to use abbreviated names for all lipids

**Value**

module object with abbreviated labels

---

addHighlyExpressedEdges

*Add reactions without highly changing genes but with high average expression*

---

**Description**

Add reactions without highly changing genes but with high average expression

**Usage**

```
addHighlyExpressedEdges(m, g, top = 3000)
```

**Arguments**

m	Metabolic module
g	Scored graph
top	Maximum rank value for the gene to be considered highly expressed

**Value**

module with added edges that correspond to high average expression

**Examples**

```
data(mEx)
data(gEx)
m <- addHighlyExpressedEdges(m = mEx, g = gEx)
```

---

```
collapseAtomsIntoMetabolites
```

*Collapse atoms belonging to the same metabolite into one vertex*

---

**Description**

Collapse atoms belonging to the same metabolite into one vertex

**Usage**

```
collapseAtomsIntoMetabolites(m)
```

**Arguments**

m                    Metabolic module

**Value**

module in which atoms of the same metabolite are collapsed into one

**Examples**

```
data(mEx)
m <- collapseAtomsIntoMetabolites(m = mEx)
```

---

```
connectAtomsInsideMetabolite
```

*Connect atoms belonging to the same metabolite with edges*

---

**Description**

Connect atoms belonging to the same metabolite with edges

**Usage**

```
connectAtomsInsideMetabolite(m)
```

**Arguments**

m                    Metabolic module

**Value**

module in which atoms of the same metabolite are connected

## Examples

```
data(mEx)
m <- connectAtomsInsideMetabolite(m = mEx)
```

---

createShinyCyJSWidget *Creates shinyCyJS widget from module*

---

## Description

Creates shinyCyJS widget from module

## Usage

```
createShinyCyJSWidget(  
  module,  
  layout = list(name = "cose-bilkent", animate = FALSE, randomize = FALSE,  
    nodeDimensionsIncludeLabels = TRUE),  
  ...  
)
```

## Arguments

module	Module
layout	Layout for the module
...	Other parameters

## Value

html widget of input module

## Examples

```
data(mEx)
hw <- createShinyCyJSWidget(module = mEx)
```

---

gatom	<i>gatom: a package for finding an active metabolic module in atom transition network</i>
-------	---

---

### Description

This package implements a metabolic network analysis pipeline to identify an active metabolic module based on high throughput data. The pipeline takes as input transcriptional and/or metabolic data and finds a metabolic subnetwork (module) most regulated between the two conditions of interest. The package further provides functions for module post-processing, annotation and visualization.

### Functions

Data preprocessing: [prepareDE](#), [getMetDEMeta](#), [getGeneDEMeta](#)

Graph creation: [makeMetabolicGraph](#)

Graph scoring: [scoreGraph](#)

Module postprocessing: [collapseAtomsIntoMetabolites](#), [connectAtomsInsideMetabolite](#), [addHighlyExpressedEdges](#), [abbreviateLabels](#)

Plotting module: [createShinyCyJSWidget](#)

Exporting module: [saveModuleToHtml](#), [saveModuleToDot](#), [saveModuleToPdf](#), [saveModuleToXgml](#)

For detailed pipeline analysis, see `gatom` vignette: `vignette("gatom-tutorial", package = "gatom")`

### Example Data

Example data provided by `gatom` consists of: metabolite differential abundance data ([met.de.rawEx](#)), gene differential expression data ([gene.de.rawEx](#)), KEGG-based network object ([networkEx](#)), KEGG-based metabolite database object ([met.kegg.dbEx](#)), Example organism annotation object ([org.Mm.eg.gatom.annoEx](#)), metabolic graph with atom topology ([gEx](#)), scored metabolic graph with atom topology ([gsEx](#)), and metabolic module ([mEx](#)).

---

gene.de.rawEx	<i>Example gene differential expression data.</i>
---------------	---

---

### Description

See file <https://github.com/ctlab/gatom/blob/master/inst/scripts/example.R> for details.

### Format

tibble/data.frame object

---

getGeneDEMeta	<i>Finds columns in gene differential expression table required for gatom analysis</i>
---------------	--

---

### Description

Default values for all columns are NULL which mean they are determined automatically.

### Usage

```
getGeneDEMeta(
  gene.de.raw,
  org.gatom.anno,
  idColumn = NULL,
  idType = NULL,
  pvalColumn = NULL,
  logPvalColumn = NULL,
  log2FCColumn = NULL,
  baseMeanColumn = NULL,
  signalColumn = NULL,
  signalRankColumn = NULL
)
```

### Arguments

gene.de.raw	A table with differential expression results, an object convertible to data.frame.
org.gatom.anno	Organsim-specific annotation obtained from makeOrgGatomAnnotation function.
idColumn	Specifies column name with gene identifiers.
idType	Specifies type of gene IDs (one of the supported by annotation).
pvalColumn	Specifies column with p-values.
logPvalColumn	Specifies column with log p-values, if there is no such column one will be generated automatically.
log2FCColumn	Specifies column with log2-fold changes.
baseMeanColumn	Specifies column with average expression across samples.
signalColumn	Specifies column with identifier of the measured entity (such as gene ID for RNA-seq and probe ID for microarrays). Could be NULL (automatic, set from based on pval and log2FC columns), character (column name), or function (evaluated in a scope of original data frame)
signalRankColumn	Specifies how the genes are ranked from highly to lowly expressed, used in 'addHighlyExpressedEdgues' function. Could be NULL (automatic), character (column name) function (evaluated in a scope of original data frame).

**Value**

object with prepared columns for the analysis for gene data

**Examples**

```
data("org.Mm.eg.gatom.annoEx")
data("gene.de.rawEx")
de.meta <- getGeneDEMeta(gene.de.rawEx, org.gatom.anno = org.Mm.eg.gatom.annoEx)
```

---

getMetabolicPathways *Generate list of metabolic pathways from Reactome and KEGG databases*

---

**Description**

Generate list of metabolic pathways from Reactome and KEGG databases

**Usage**

```
getMetabolicPathways(  
  universe,  
  metGenes,  
  keggOrgCode,  
  threshold = 0.01,  
  includeReactome = TRUE,  
  includeKEGG = TRUE  
)
```

**Arguments**

universe	list of genes
metGenes	list of metabolic genes
keggOrgCode	KEGG organism code, like mmu or hsa
threshold	threshold for Fisher test to filter out non-metabolic pathways
includeReactome	whether to include Reactome pathways (only works for Entrez ID universe)
includeKEGG	whether to include KEGG pathways and modules

**Value**

list of metabolic pathways for given organism and list of genes



---

getMetDEMeta	<i>Finds columns in differential expression table for metabolites required for gatom analysis</i>
--------------	---

---

### Description

Finds columns in differential expression table for metabolites required for gatom analysis

### Usage

```
getMetDEMeta(  
  met.de.raw,  
  met.db,  
  idColumn = NULL,  
  idType = NULL,  
  pvalColumn = NULL,  
  logPvalColumn = NULL,  
  log2FCColumn = NULL,  
  signalColumn = NULL  
)
```

### Arguments

met.de.raw	A table with differential expression results, an object convertible to data.frame.
met.db	Metabolite database
idColumn	Specifies column name with metabolite identifiers.
idType	Specifies type of metabolite IDs (one of the supported by annotation).
pvalColumn	Specifies column with p-values.
logPvalColumn	Specifies column with log p-values, if there is no such column one will be generated automatically.
log2FCColumn	Specifies column with log2-fold changes.
signalColumn	Specifies column with identifier of the measured entity Could be NULL (automatic, set from based on pval and log2FC columns), character (column name), or function (evaluated in a scope of original data frame)

### Value

object with prepared columns for the analysis for metabolite data

### Examples

```
data("met.kegg.dbEx")  
data("met.de.rawEx")  
de.meta <- getMetDEMeta(met.de.rawEx, met.db = met.kegg.dbEx)
```

---

gEx *Example metabolic graph with atom topology.*

---

**Description**

See file <https://github.com/ctlab/gatom/blob/master/inst/scripts/example.R> for details.

**Format**

igraph object

---

gsEx *Example scored metabolic graph with atom topology.*

---

**Description**

See file <https://github.com/ctlab/gatom/blob/master/inst/scripts/example.R> for details.

**Format**

igraph object

---

makeMetabolicGraph *Creates metabolic graph based on specified data*

---

**Description**

Creates metabolic graph based on specified data

**Usage**

```
makeMetabolicGraph(
  network,
  topology = c("atoms", "metabolites"),
  org.gatom.anno,
  gene.de,
  gene.de.meta = getGeneDEMeta(gene.de, org.gatom.anno),
  gene.keep.top = 12000,
  met.db,
  met.de,
  met.de.meta = getMetDEMeta(met.de, met.db),
  met.to.filter = fread(system.file("extdata", "mets2mask.lst", package = "gatom"))$ID,
  gene2reaction.extra = NULL,
  keepReactionsWithoutEnzymes = FALSE,
  largest.component = TRUE
)
```

**Arguments**

network	Network object
topology	Way to determine network vertices
org.gatom.anno	Organism annotation object
gene.de	Table with the differential gene expression, set to NULL if absent
gene.de.meta	Annotation of 'gene.de' table
gene.keep.top	Only the 'gene.keep.top' of the most expressed genes will be kept for the network
met.db	Metabolite database
met.de	Table with the differential expression for metabolites, set to NULL if absent
met.de.meta	Annotation of 'met.de' table
met.to.filter	List of metabolites to filter from the network
gene2reaction.extra	Additional gene to reaction mappings. Should be a data.table with 'gene' and 'reaction' columns
keepReactionsWithoutEnzymes	If TRUE, keep reactions that have no annotated enzymes, thus expanding the network but including some reactions which are not possible in the considered species.
largest.component	If TRUE, only the largest connected component is returned

**Value**

igraph object created from input data

**Examples**

```
data("gene.de.rawEx")
data("met.de.rawEx")
data("met.kegg.dbEx")
data("networkEx")
data("org.Mm.eg.gatom.annoEx")
g <- makeMetabolicGraph(network = networkEx, topology = "atoms",
  org.gatom.anno = org.Mm.eg.gatom.annoEx,
  gene.de = gene.de.rawEx, met.db = met.kegg.dbEx,
  met.de = met.de.rawEx)
```

---

`makeOrgGatomAnnotation`*Create an organism annotation object for network analysis*

---

**Description**

Create an organism annotation object for network analysis

**Usage**

```
makeOrgGatomAnnotation(  
  org.db,  
  idColumns = c(Entrez = "ENTREZID", RefSeq = "REFSEQ", Ensembl = "ENSEMBL", Symbol =  
    "SYMBOL"),  
  nameColumn = "SYMBOL",  
  enzymeColumn = "ENZYME",  
  appendEnzymesFromKegg = TRUE,  
  appendOrthologiesFromKegg = TRUE,  
  filterNonSpecificEnzymes = TRUE,  
  keggOrgCode = NULL  
)
```

**Arguments**

<code>org.db</code>	Bioconductor <code>org.db</code> object, e.g. <code>org.Mm.eg.db</code>
<code>idColumns</code>	vector of column names from 'org.db' object to create ID mappings. First ID will be used as a base identifier, should be compatible with KEGG and Reactome databases.
<code>nameColumn</code>	column with a human readable gene symbol. Default to "SYMBOL".
<code>enzymeColumn</code>	column with an Enzyme Commission ID. Default to "ENZYME".
<code>appendEnzymesFromKegg</code>	if TRUE, KEGG databases will be used to extend gene to enzyme mappings obtained from org.db package.
<code>appendOrthologiesFromKegg</code>	if TRUE, KEGG database will be used to extend gene to orthology mappings obtained from org.db package
<code>filterNonSpecificEnzymes</code>	if TRUE, will filter out non-specific enzymes from gene to enzyme mappings obtained from org.db package
<code>keggOrgCode</code>	KEGG organism code, e.g. "mmu". If set to NULL, the code is determined automatically.

**Value**

organism annotation object that will be used for network analysis

**Examples**

```
library(org.Mm.eg.db)
org.Mm.eg.gatom.anno <- makeOrgGatomAnnotation(org.db = org.Mm.eg.db)
```

---

met.de.rawEx	<i>Example metabolite differential abundance data.</i>
--------------	--

---

**Description**

See file <https://github.com/ctlab/gatom/blob/master/inst/scripts/example.R> for details.

**Format**

tibble/data.frame object

---

met.kegg.dbEx	<i>Example KEGG-based metabolite database object</i>
---------------	--

---

**Description**

See file <https://github.com/ctlab/gatom/blob/master/inst/scripts/example.R> for details.

**Format**

list object

---

mEx	<i>Example metabolic module.</i>
-----	----------------------------------

---

**Description**

See file <https://github.com/ctlab/gatom/blob/master/inst/scripts/example.R> for details.

**Format**

igraph object

---

networkEx	<i>Example KEGG-based network object</i>
-----------	--

---

**Description**

See file <https://github.com/ctlab/gatom/blob/master/inst/scripts/example.R> for details.

**Format**

list object

---

org.Mm.eg.gatom.annoEx	<i>Example organism annotation object</i>
------------------------	---

---

**Description**

See file <https://github.com/ctlab/gatom/blob/master/inst/scripts/example.R> for details.

**Format**

list object

---

prepareDE	<i>Makes data.table with differential expression results containing all columns required for gatom and in the expected format based on metadata object</i>
-----------	--

---

**Description**

Makes data.table with differential expression results containing all columns required for gatom and in the expected format based on metadata object

**Usage**

```
prepareDE(de.raw, de.meta)
```

**Arguments**

de.raw	Table with differential expression results, an object convertible to data.frame
de.meta	Object with differential expression table metadata acquired with getGeneDEMeta or getMetDEMeta functions

**Value**

data.table object with converted differential expression table

**Examples**

```
data("org.Mm.eg.gatom.annoEx")
data("gene.de.rawEx")
de.meta <- getGeneDEMeta(gene.de.rawEx, org.gatom.anno = org.Mm.eg.gatom.annoEx)
de <- prepareDE(gene.de.rawEx, de.meta)
```

---

saveModuleToDot	<i>Save module to a graphviz dot file</i>
-----------------	---

---

**Description**

Save module to a graphviz dot file

**Usage**

```
saveModuleToDot(
  module,
  file,
  name = NULL,
  extra.node.attrs = NULL,
  extra.edge.attrs = NULL
)
```

**Arguments**

module	Module to save
file	File to save to
name	Name of the module
extra.node.attrs	Table with additional node attributes to be written to the dot file as is
extra.edge.attrs	Table with additional edge attributes to be written to the dot file as is

**Value**

Returns NULL

**Examples**

```
data(mEx)
saveModuleToDot(module = mEx, file = "module.dot")
```

---

saveModuleToHtml      *Save module to a html widget*

---

### Description

Save module to a html widget

### Usage

```
saveModuleToHtml(
    module,
    file,
    name = "",
    sizingPolicy = htmlwidgets::sizingPolicy(defaultWidth = "100%", defaultHeight =
        "90vh", padding = 10),
    ...
)
```

### Arguments

module	Module to save
file	File to save to
name	Name of the module
sizingPolicy	A widget sizing policy
...	Other parameters

### Value

Returns NULL

### Examples

```
data(mEx)
saveModuleToHtml(module = mEx, file = "module.html")
```

---

saveModuleToPdf      *Save module to a nice pdf file*

---

### Description

Save module to a nice pdf file



**Usage**

```
saveModuleToPdf(module, file, name = NULL, n_iter = 100, force = 1e-05)
```

**Arguments**

module	Module to save
file	File to save to
name	Name of the module
n_iter	Number of repel algorithm iterations
force	Value of repel force

**Value**

Returns NULL

**Examples**

```
data(mEx)
saveModuleToPdf(module = mEx, file = "module.pdf")
```

---

saveModuleToXgmml      *Save module to an XGMML file*

---

**Description**

Save module to an XGMML file

**Usage**

```
saveModuleToXgmml(module, file, name = NULL)
```

**Arguments**

module	Module to save
file	File to save to
name	Name of the module

**Value**

Returns NULL

**Examples**

```
data(mEx)
saveModuleToXgmml(module = mEx, file = "module.xgmml")
```

---

scoreGraph	<i>Score metabolic graph</i>
------------	------------------------------

---

**Description**

Score metabolic graph

**Usage**

```
scoreGraph(
  g,
  k.gene,
  k.met,
  vertex.threshold.min = 0.1,
  edge.threshold.min = 0.1,
  met.score.coef = 1,
  show.warnings = TRUE,
  raw = FALSE
)
```

**Arguments**

<code>g</code>	Metabolic graph obtained with <code>makeMetabolic graph</code> function
<code>k.gene</code>	Number of gene signals to be scored positively, the higher is the number, the larger will be the resulting module. If set to <code>NULL</code> , genes will not be used for scoring.
<code>k.met</code>	Number of metabolite signals to be scored positively, the higher is the number, the larger will be the resulting module. If set to <code>NULL</code> , metabolites will not be used for scoring.
<code>vertex.threshold.min</code>	The worst acceptable estimated FDR for vertices. If necessary number of positive metabolite signals will be decreased from 'k.met' to reach this threshold. Default value is 0.1.
<code>edge.threshold.min</code>	The worst acceptable estimated FDR for vertices. If necessary number of positive metabolite signals will be decreased from 'k.gene' to reach this threshold. Default value is 0.1.
<code>met.score.coef</code>	Coefficient on which all vertex weights are multiplied. Can be used to balance vertex and edge weights. Default values is 1.
<code>show.warnings</code>	whether to show warnings
<code>raw</code>	whether to return raw scored graph, not a SGMWCS instance. Default to <code>FALSE</code> .

**Value**

SGMWCS instance or scored igraph object

**Examples**

```
data("gEx")
gs <- scoreGraph(g = gEx, k.gene = 25, k.met = 25)
```

---

`styleWidget`*code adopted from <https://github.com/ramnathv/htmlwidgets/issues/231>*

---

**Description**

code adopted from <https://github.com/ramnathv/htmlwidgets/issues/231>

**Usage**

```
styleWidget(hw, style = "", addl_selector = "", elementId = NULL)
```

**Value**

styled html widget

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