

# Package ‘fobitools’

July 9, 2025

**Title** Tools for Manipulating the FOBI Ontology

**Version** 1.16.0

**Description** A set of tools for interacting with the Food-Biomarker Ontology (FOBI). A collection of basic manipulation tools for biological significance analysis, graphs, and text mining strategies for annotating nutritional data.

**License** GPL-3

**Encoding** UTF-8

**LazyData** true

**biocViews** MassSpectrometry, Metabolomics, Software, Visualization, BiomedicalInformatics, GraphAndNetwork, Annotation, Cheminformatics, Pathways, GeneSetEnrichment

**Imports** clisymbols, crayon, dplyr, fgsea, ggplot2, ggraph, magrittr, ontologyIndex, purrr, RecordLinkage, stringr, textclean, tictoc, tidygraph, tidyr, vroom

**Suggests** BiocStyle, covr, ggrepel, kableExtra, knitr, metabolomicsWorkbenchR, POMA, rmarkdown, rvest, SummarizedExperiment, testthat (>= 2.3.2), tidyverse

**RoxygenNote** 7.3.2

**Depends** R (>= 4.1)

**URL** <https://github.com/pcastellanoescuder/fobitools/>

**BugReports** <https://github.com/pcastellanoescuder/fobitools/issues>

**VignetteBuilder** knitr

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|                |                                                                         |
|----------------|-------------------------------------------------------------------------|
| annotate_foods | <i>Text Mining Pipeline to Annotate Free Nutritional Text with FOBI</i> |
|----------------|-------------------------------------------------------------------------|

---

Description

This function provides a text mining pipeline to map nutritional free text to Food-Biomarker Ontology. This pipeline is composed of five sequential layers to map food items to FOBI with the maximum accuracy as possible.

Usage

```
annotate_foods(foods, similarity = 0.85, reference = fobitools::foods)
```

Arguments

|            |                                                                                                                                                                                                                            |
|------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| foods      | A two column data frame. First column must contain the ID (should be unique) and the second column must contain food items (it can be a word or a string).                                                                 |
| similarity | Numeric between 0 (low) and 1 (high). This value indicates the semantic similarity cutoff used at the last layer of the text mining pipeline. 1 = exact match; 0 = very poor match. Values below 0.85 are not recommended. |
| reference  | FOBI foods table obtained with ‘parse_fobi(terms = "FOBI:0001", get = "des")’. If this value is set to NULL, the last version of FOBI will be downloaded from GitHub.                                                      |

**Value**

A list containing two tibble objects: annotated and unannotated food items.

**Author(s)**

Pol Castellano-Escuder

**References**

Pol Castellano-Escuder, Raúl González-Domínguez, David S Wishart, Cristina Andrés-Lacueva, Alex Sánchez-Pla, FOBI: an ontology to represent food intake data and associate it with metabolomic data, Database, Volume 2020, 2020, baaa033, <https://doi.org/10.1093/databa/baaa033>.

**Examples**

```
# Free text annotation in FOBI
free_text <- data.frame(id = c(101, 102, 103, 104),
                        text = c("Yesterday I ate eggs and bacon with a butter toast and black tea",
                                "Crisp bread and rice crackers with wholegrain",
                                "Beef and veal, one apple", "pizza without meat"))
annotate_foods(free_text)
```

---

fobi

---

*FOBI Table File - Jul 23, 2021*


---

**Description**

FOBI table obtained with 'parse\_fobi()'

**Usage**

```
fobi
```

**Format**

A tibble: 4069 FOBI entities with their associated information.

**id\_code** FOBI entity ID.

**name** FOBI entity name.

**is\_a\_code** FOBI entity direct parent class ID.

**is\_a\_name** FOBI entity direct parent class name.

**id\_BiomarkerOf** FOBI entity associated food ID (in terms of biomarker).

**BiomarkerOf** FOBI entity associated food name (in terms of biomarker).

**ChemSpider** ChemSpider ID.

**KEGG** KEGG ID.

**PubChemCID** PubChemCID ID.

**InChIKey** InChIKey ID.

**InChICode** InChICode ID.

**FOBI** FOBI ID.

**alias** FOBI entity alias name.

**HMDB** HMDB ID.

**id\_Contains** FOBI entity associated food ID (in terms of a recipe).

**Contains** FOBI entity associated food ID (in terms of a recipe).

## Source

<https://github.com/pcastellanoescuder/FoodBiomarkerOntology>

---

fobi\_graph

*Generate FOBI Graphs*

---

## Description

This function allows users to create networks based on FOBI relationships.

## Usage

```
fobi_graph(
  terms = NULL,
  get = NULL,
  property = c("is_a", "BiomarkerOf", "Contains"),
  layout = "sugiyama",
  labels = FALSE,
  labelsSize = 3,
  legend = FALSE,
  legendSize = 10,
  legendPos = "bottom",
  curved = FALSE,
  pointSize = 3,
  fobi = fobitools::fobi
)
```

## Arguments

|          |                                                                                                                                                                                                                           |
|----------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| terms    | A character vector with FOBI term IDs.                                                                                                                                                                                    |
| get      | A character string indicating desired relationships between provided terms. Options are 'anc' (for ancestors) and 'des' (for descendants). Default is NULL and all information related with input terms will be provided. |
| property | A character vector indicating which properties should be plotted. Options are 'is_a', 'BiomarkerOf', and 'Contains'. By default all of them are included.                                                                 |

|            |                                                                                                                                   |
|------------|-----------------------------------------------------------------------------------------------------------------------------------|
| layout     | A character string indicating the type of layout to create. Options are 'sugiyama' (default) and 'lgl'.                           |
| labels     | Logical indicating if node names should be plotted or not.                                                                        |
| labelsize  | Numeric value indicating the size of labels.                                                                                      |
| legend     | Logical indicating if legend should be plotted or not.                                                                            |
| legendSize | Numeric value indicating the size of legend.                                                                                      |
| legendPos  | A character string indicating the legend position (if legend parameter is set to TRUE). Options are 'bottom' (default) and 'top'. |
| curved     | Logical indicating if the shape of the edges shape should be curved or not.                                                       |
| pointSize  | Numeric value indicating the size of graph points.                                                                                |
| fobi       | FOBI table obtained with 'parse_fobi()'. If this value is set to NULL, the last version of FOBI will be downloaded from GitHub.   |

**Value**

A ggraph object.

**Author(s)**

Pol Castellano-Escuder

**References**

Pol Castellano-Escuder, Raúl González-Domínguez, David S Wishart, Cristina Andrés-Lacueva, Alex Sánchez-Pla, FOBI: an ontology to represent food intake data and associate it with metabolomic data, Database, Volume 2020, 2020, baaa033, <https://doi.org/10.1093/databa/baaa033>.

**Examples**

```
terms <- c("CHEBI:16164", "CHEBI:16243", "FOODON:00001139", "FOODON:00003274", "FOODON:00003275")
fobi_graph(terms, get = "anc")

# Red meat related FOBI biomarkers
fobi_graph(terms = "FOBI:0193",
  property = c("is_a", "BiomarkerOf"),
  layout = "lgl", curved = TRUE) # set labels = TRUE to display node names
```

---

fobi\_terms

---

*FOBI's 'ontology\_index' object - Jul 23, 2021*


---

**Description**

FOBI terms obtained with 'ontologyIndex::get\_ontology()'

**Usage**

fobi\_terms

**Format**

An ontology\_index object with 1201 terms.

**format-version:** 1.2

**data-version:** fobi.owl

**ontology** fobi

**Properties** id: character, name: character, parents: list, children: list, ancestors: list, obsolete: logical

**Roots** FOBI:0001 - Foods, FOBI:01501 - Biomarkers, FOBI:00422 - BiomarkerOf, FOBI:00423 - HasBiomarker, FOBI:00424 - Contains, FOBI:00425 - IsIngredientOf

**Source**

<https://github.com/pcastellanoescuder/FoodBiomarkerOntology>

---

foods

*FOBI Foods Table File - Feb 02, 2021*

---

**Description**

FOBI foods table obtained with 'parse\_fobi(terms = "FOBI:0001", get = "des")'

**Usage**

foods

**Format**

A tibble: 568 FOBI food entities with their associated information.

**id\_code** FOBI entity ID.

**name** FOBI entity name.

**is\_a\_code** FOBI entity direct parent class ID.

**is\_a\_name** FOBI entity direct parent class name.

**id\_BiomarkerOf** FOBI entity associated food ID (in terms of biomarker).

**BiomarkerOf** FOBI entity associated food name (in terms of biomarker).

**ChemSpider** ChemSpider ID.

**KEGG** KEGG ID.

**PubChemCID** PubChemCID ID.

**InChIKey** InChIKey ID.

**InChICode** InChICode ID.

**FOBI** FOBI ID.

**alias** FOBI entity alias name.

**HMDB** HMDB ID.

**id\_Contains** FOBI entity associated food ID (in terms of a recipe).

**Contains** FOBI entity associated food ID (in terms of a recipe).

## Source

<https://github.com/pcastellanoescuder/FoodBiomarkerOntology>

---

|       |                                                |
|-------|------------------------------------------------|
| idmap | <i>FOBI Identifier Map File - Jul 18, 2021</i> |
|-------|------------------------------------------------|

---

## Description

Identifier mappings for FOBI metabolites

## Usage

idmap

## Format

A tibble: 590 FOBI metabolites with 8 different IDs.

**metaboliteNames** Raw metabolite names.

**FOBI** FOBI ID.

**HMDB** HMDB ID.

**KEGG** KEGG ID.

**PubChemCID** PubChemCID ID.

**InChIKey** InChIKey ID.

**InChICode** InChICode ID.

**ChemSpider** ChemSpider ID.

## Source

<https://github.com/pcastellanoescuder/FoodBiomarkerOntology>

---

`id_convert`*Convert Metabolite Identifiers*

---

## Description

This function can convert metabolite identifiers to other available IDs in FOBI. Input vector can be a combination of different IDs.

## Usage

```
id_convert(ids, to = "FOBI", fobi = fobitools::fobi)
```

## Arguments

|                   |                                                                                                                                                                                                       |
|-------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>ids</code>  | A vector with metabolite IDs to convert. Input ID types can be FOBI, raw metabolite names (used in FOBI), HMDB, KEGG, PubChemCID, InChIKey, InChIcode, ChemSpider, and a combination of them.         |
| <code>to</code>   | Target ID type. If possible, metabolites will be converted to this ID type. Options are "FOBI" (default), "metaboliteNames", "HMDB", "KEGG", "PubChemCID", "InChIKey", "InChIcode", and "ChemSpider". |
| <code>fobi</code> | FOBI table obtained with <code>'parse_fobi()'</code> . If this value is set to NULL, the last version of FOBI will be downloaded from GitHub.                                                         |

## Value

A tibble with input IDs and converted IDs.

## Author(s)

Pol Castellano-Escuder

## References

Pol Castellano-Escuder, Raúl González-Domínguez, David S Wishart, Cristina Andrés-Lacueva, Alex Sánchez-Pla, FOBI: an ontology to represent food intake data and associate it with metabolomic data, Database, Volume 2020, 2020, baaa033, <https://doi.org/10.1093/databa/baaa033>.

## Examples

```
ids <- c(fobitools::idmap$HMDB[1:10],
        fobitools::idmap$KEGG[11:23],
        fobitools::idmap$InChIKey[100:150])
fobitools::id_convert(ids, to = "FOBI")
```

---

msea*Performs a preranked metabolite set enrichment analysis (MSEA)*

---

## Description

This function performs a MSEA based on the adaptive multilevel splitting Monte Carlo approach.

## Usage

```
msea(  
  metaboliteRanks,  
  subOntology = "food",  
  pvalCutoff = 0.01,  
  fobi = fobitools::fobi  
)
```

## Arguments

|                 |                                                                                                                                 |
|-----------------|---------------------------------------------------------------------------------------------------------------------------------|
| metaboliteRanks | A named vector of FOBI metabolite identifiers with their metabolite-level stats.                                                |
| subOntology     | A character string specifying one of the two FOBI sub-ontologies: "food", or "biomarker".                                       |
| pvalCutoff      | A numeric value indicating a p-value cutoff for raw p-values generated by MSEA.                                                 |
| fobi            | FOBI table obtained with 'parse_fobi()'. If this value is set to NULL, the last version of FOBI will be downloaded from GitHub. |

## Value

A tibble with MSEA results.

## Author(s)

Pol Castellano-Escuder

## References

G. Korotkevich, V. Sukhov, A. Sergushichev. Fast gene set enrichment analysis. bioRxiv (2019), doi:10.1101/060012

Pol Castellano-Escuder, Raúl González-Domínguez, David S Wishart, Cristina Andrés-Lacueva, Alex Sánchez-Pla, FOBI: an ontology to represent food intake data and associate it with metabolomic data, Database, Volume 2020, 2020, baaa033, <https://doi.org/10.1093/databa/baaa033>.

## Examples

```

metabolites <- c(fobitools::idmap$FOBI[1:49], fobitools::idmap$FOBI[70:80])
random_pvals <- c(runif(n = length(metabolites)*0.3, min = 0.001, max = 0.05), runif(n = length(metabolites)*0.7, min = 0.001, max = 0.05))
names(random_pvals) <- metabolites
metaboliteRanks <- random_pvals[order(random_pvals)]

# Food enrichment analysis
fobitools::msea(metaboliteRanks = metaboliteRanks,
                pvalCutoff = 1)

# Chemical class enrichment analysis
fobitools::msea(metaboliteRanks = metaboliteRanks,
                subOntology = "biomarker",
                pvalCutoff = 1)

```

---

ora

---

*Classical Over Representation Analysis with FOBI*


---

## Description

This function performs a traditional over representation analysis based on hypergeometric test: classes are treated as sets of individual metabolites and all metabolites are treated as equally informative. This function uses Food-Biomarker Ontology knowledge as biological information.

## Usage

```

ora(
  metaboliteList,
  metaboliteUniverse,
  subOntology = "food",
  pvalCutoff = 0.01,
  fobi = fobitools::fobi
)

```

## Arguments

|                    |                                                                                                                                   |
|--------------------|-----------------------------------------------------------------------------------------------------------------------------------|
| metaboliteList     | A vector of FOBI metabolite identifiers that define the selected list of metabolites.                                             |
| metaboliteUniverse | A vector of FOBI metabolite identifiers that define the universe of possible metabolites (all metabolites analyzed in the study). |
| subOntology        | A character string specifying one of the two FOBI sub-ontologies: "food", or "biomarker".                                         |
| pvalCutoff         | A numeric value indicating a p-value cutoff for raw p-values generated by hypergeometric test.                                    |
| fobi               | FOBI table obtained with 'parse_fobi()'. If this value is set to NULL, the last version of FOBI will be downloaded from GitHub.   |

**Value**

A tibble with ORA results.

**Author(s)**

Pol Castellano-Escuder

**References**

G. Korotkevich, V. Sukhov, A. Sergushichev. Fast gene set enrichment analysis. bioRxiv (2019), doi:10.1101/060012

Pol Castellano-Escuder, Raúl González-Domínguez, David S Wishart, Cristina Andrés-Lacueva, Alex Sánchez-Pla, FOBI: an ontology to represent food intake data and associate it with metabolomic data, Database, Volume 2020, 2020, baaa033, <https://doi.org/10.1093/databa/baaa033>.

**Examples**

```
metaboliteUniverse <- c(fobitools::idmap$FOBI[1:200], fobitools::idmap$FOBI[400:450])
metaboliteList <- c(fobitools::idmap$FOBI[1:50], fobitools::idmap$FOBI[70:80])

# Food enrichment analysis
fobitools::ora(metaboliteList = metaboliteList,
               metaboliteUniverse = metaboliteUniverse,
               pvalCutoff = 1)

# Chemical class enrichment analysis
fobitools::ora(metaboliteList = metaboliteList,
               metaboliteUniverse = metaboliteUniverse,
               subOntology = "biomarker",
               pvalCutoff = 1)
```

---

parse\_fobi

*Parse FOBI in a Readable Tabular Format*

---

**Description**

This function allows users to download and parse the last version of the Food-Biomarker Ontology into a readable table format.

**Usage**

```
parse_fobi(terms = NULL, get = NULL)
```

**Arguments**

|       |                                                                                                                                                                                                                         |
|-------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| terms | A character vector with FOBI term IDs. Default is NULL.                                                                                                                                                                 |
| get   | A character string indicating desired relationships between provided terms. Options are 'anc' (for ancestors) and 'des' (for descendants). Default is NULL and only information of single input terms will be provided. |

**Value**

A tibble with FOBI terms information.

**Author(s)**

Pol Castellano-Escuder

**References**

Pol Castellano-Escuder, Raúl González-Domínguez, David S Wishart, Cristina Andrés-Lacueva, Alex Sánchez-Pla, FOBI: an ontology to represent food intake data and associate it with metabolomic data, Database, Volume 2020, 2020, baaa033, <https://doi.org/10.1093/databa/baaa033>.

**Examples**

```
# Download and parse whole FOBI
fobi <- parse_fobi()

# Download and parse 'apple' related terms
fobi_apple <- parse_fobi(terms = "FOODON:00002473")

# Download and parse 'apple' term ancestors
fobi_apple_anc <- parse_fobi(terms = "FOODON:00002473", get = "anc")

# Download and parse 'apple' and 'alpha-Chaconine' related terms
fobi_subset <- parse_fobi(terms = c("FOODON:00002473", "CHEBI:10219"))
```

---

reexports

*Objects exported from other packages*

---

**Description**

These objects are imported from other packages. Follow the links below to see their documentation.

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