Package 'rgoslin'

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Type Package

Title Lipid Shorthand Name Parsing and Normalization

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Description The R implementation for the Grammar of Succint Lipid Nomenclature
parses different short hand notation dialects for lipid names. It
normalizes them to a standard name. It further provides calculated
monoisotopic masses and sum formulas for each successfully parsed lipid name and supplements it with LIPID MAPS
Category and Class information. Also, the structural level and further structural
details about the head group, fatty acyls and functional groups are returned, where applicable.

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Imports Rcpp (>= 1.0.3), dplyr

LinkingTo Rcpp

Suggests testthat (>= 2.1.0), BiocStyle, knitr, rmarkdown, kableExtra,
BiocManager, stringr, stringi, ggplot2, tibble, lipidr

RoxygenNote 7.1.2

Encoding UTF-8

VignetteBuilder knitr

biocViews Software, Lipidomics, Metabolomics, Preprocessing,
Normalization, MassSpectrometry

BugReports https://github.com/lifs-tools/rgoslin/issues

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`rgoslin-package` *rgoslin: Lipid Shorthand Name Parsing and Normalization*

Description

The R implementation for the Grammar of Succint Lipid Nomenclature parses different short hand notation dialects for lipid names. It normalizes them to a standard name. It further provides calculated monoisotopic masses and sum formulas for each successfully parsed lipid name and supplements it with LIPID MAPS Category and Class information. Also, the structural level and further structural details about the head group, fatty acyls and functional groups are returned, where applicable.

Details

rgoslin is the R implementation of the "grammar of succint lipid nomenclature". It provides implementations for parsing of shorthand lipid names from LipidMAPS, SwissLipids and other common sources of lipid names.

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References

NA

See Also

Useful links:

- https://github.com/lifs-tools/rgoslin
- Report bugs at https://github.com/lifs-tools/rgoslin/issues

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`isValidLipidName` *Check lipid name.*

Description

`isValidLipidName` checks the provided lipid name against the built-in grammars. Will return FALSE if none of the parsers was able to parse the provided name successfully. Will stop execution via `stop` if non character input is detected.

Usage

```
isValidLipidName(lipidName)
```

Arguments

`lipidName`	The lipid name to check.

Value

TRUE if the lipidName could be parsed, FALSE otherwise.

Examples

```
isValidLipidName("PC 32:1")
isValidLipidName("PC(32:1)")
isValidLipidName("PCX(32:1)")
```

`listAvailableGrammars` *Return the list of grammars supported by goslin.*

Description

`listAvailableGrammars` returns the list of grammars that the underlying cppgoslin library supports.

Usage

```
listAvailableGrammars()
```

Value

the list of grammars

Examples

```
listAvailableGrammars()
```

`parseLipidNames` *Parse multiple lipid names and return a data frame with the results.*

Description

`parseLipidNames` reads the provided lipid names vector and returns structural information as a data frame. Will return a cell with the "Grammar" column set to "NOT_PARSEABLE" if none of the parsers was able to parse the provided name successfully. Will stop execution via `stop` if invalid non character input is detected or fatal errors are encountered during parsing.

Usage

```
parseLipidNames(lipidNames, grammar = NULL)
```

Arguments

`lipidNames`	The vector of lipid names to parse.
`grammar`	The grammar to use. One of "Goslin", "GoslinFragments", "SwissLipids", "LipidMaps", "HMDB", "FattyAcids". Call `listAvailableGrammars()` for a complete list of available grammars. If `grammar` is omitted or `NULL` is passed as a parameter, all available grammars / parsers will be tested. The first successful one will win. If all parsers fail, the "Messages" column in the returned data frame will contain the last parsers message.

Value

Data frame where each row reports the parsing result of each element in lipidNames.

Examples

```
parseLipidNames(c("PC 32:1","LPC 34:1","TG(18:1_18:0_16:1)"))
parseLipidNames(c("Cer(d18:1(8Z)/24:0)", grammar = "LipidMaps"))
```

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