Package 'lipidmaps'

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Type Package

Title R Interface to the LIPID MAPS RESTful API

Version 0.1.0

Author Tom Wilson <tpw2@aber.ac.uk>

Maintainer Tom Wilson <tpw2@aber.ac.uk>

Description Simple searching of the LIPID MAPS database using Molecular Formulae or an InChiKey as an input.

Imports RCurl, jsonlite

Suggests testthat

License GPL (>= 3)

LazyData TRUE

RoxygenNote 5.0.0

NeedsCompilation no

R topics documented:

`LMsearch` *Seach LIPID MAPS*

Description

Retrieve data from the LIPID MAPS database using either an `InChiKey` or `Molecular Formula` as an input

Usage

```
LMsearch(x)
```

Arguments

x	a character of a valid InChiKey or Molecular Formula

Value

a data.frame containing the following fields for each returned entry

name Systematic name

id LIPID MAPS database id

mz Monoisotopic accurate mass

inchi InChi Code

inchi_key InChiKey

smiles Smiles

formula Molecular formula

core_class core

main_class main

sub_clss sub

Author(s)

Tom Wilson <tpw2@aber.ac.uk>

Examples

```
## Not run:
    LMsearch("C18H32O2")
    LMsearch("ZKRPGPZHULJLKJ-JHRQRACZSA-N")

## End(Not run)
```

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