Package 'classyfireR'

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Type Package

Title R Interface to the ClassyFire RESTful API

Version 0.2.1

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Description Access to the ClassyFire RESTful API <http://classyfire.wishartlab.com>. Retrieve exist-
ing entity classifications and submit new entities for classification.

Depends magrittr

Imports httr, jsonlite, tibble, crayon, clisymbols, purrr, dplyr,
stringr

Suggests testthat, covr, tidyr

License GPL (>= 3)

Encoding UTF-8

LazyData true

URL https://github.com/aberHRML/classyfireR

BugReports https://github.com/aberHRML/classyfireR/issues

RoxygenNote 6.1.1

Roxygen list(markdown = TRUE)

NeedsCompilation no

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R topics documented:

get_classification   *Get Entity Classification*

Description

Retrieve entity classification from 'http://classyfire.wishartlab.com/entities/'

Usage

```
get_classification(inchi_key)
```

Arguments

inchi_key   a character string of a valid InChIKey

Value

a `tibble` containing the following;

- **Level** Classification level (kingdom, superclass, class and subclass)
- **Classification** The compound classification
- **CHEMONT** Chemical Ontology Identification code

Examples

```
# Valid InChI key where all four classification levels are available
get_classification('BRMWTNUJHUMWMS-LURJTMIESA-N')

# Valid InChI key where only three classification levels are available
get_classification('MDHYEMXUFSJLGV-UHFFFAOYSA-N')

# Invalid InChI key
get_classification('MDHYEMXUFSJLGV-UHFFFAOYSA-B')


# Using `dplyr` a vector of InChI Keys can be submitted and easily parsed
  library(dplyr)
  library(purrr)
  library(tidyr)

 keys <- c(
'BRMWTNUJHUMWMS-LURJTMIESA-N',
'XFNJVJPLKCPIBV-UHFFFAOYSA-N',
'TYEYBOSBBBBHJIV-UHFFFAOYSA-N',
'AFENDNXGAFYKQO-UHFFFAOYSA-N',
'WHEUWNKSCXYKBU-QPWUGHHJSA-N',
'WHBMMWSBFZVSSR-GSVOUGTGSA-N')
```

```
classification_list <- map(keys, get_classification)

classification_list <- map(classification_list, ~{select(.,-CHEMONT)})

spread_tibble <- purrr:::map(classification_list, ~{
                spread(., Level, Classification)
                }) %>% bind_rows() %>% data.frame()

rownames(spread_tibble) <- keys

classification_tibble <-  tibble(
    InChIKey = rownames(spread_tibble),
    Kingdom = spread_tibble$kingdom,
    SuperClass = spread_tibble$superclass,
    Class = spread_tibble$class,
    SubClass = spread_tibble$subclass,
    Level5 = spread_tibble$level.5,
    Level6 = spread_tibble$level.6,
    Level7 = spread_tibble$level.7
   )

print(classification_tibble)
```

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