

Package ‘classyfireR’

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Type Package

Title R Interface to the ClassyFire RESTful API

Version 0.2.0

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Description Access to the ClassyFire RESTful API <<http://classyfire.wishartlab.com>>. Retrieve existing 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/wilsontom/classyfireR>

BugReports <https://github.com/wilsontom/classyfireR/issues>

RoxygenNote 6.1.1

NeedsCompilation no

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Repository CRAN

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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',
  'TYEYBOSBBBHJIV-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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