

Package ‘classyfireR’

November 11, 2019

Type Package

Title R Interface to the ClassyFire RESTful API

Version 0.3.0

Date 2019-011-11

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, cli, purrr, dplyr, stringr, methods

Suggests testthat, covr

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)

Collate 'allGenerics.R' 'allClasses.R' 'accessor-methods.R' 'get_classification.R' 'internals.R' 'show-method.R' 'zzz.R'

NeedsCompilation no

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alternative_parents	<i>alternative_parents</i>
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Description

Get the alternative_parents

Usage

```
alternative_parents(object)

## S4 method for signature 'ClassyFire'
alternative_parents(object)
```

Arguments

object a ClassyFire S4 object

chebi	<i>chebi</i>
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Description

Get the predicted ChEBI identifications

Usage

```
chebi(object)

## S4 method for signature 'ClassyFire'
chebi(object)
```

Arguments

object a ClassyFire S4 object

classification	<i>Accessor Methods for the ClassyFire S4 class</i>
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Description

Get the ClassyFire classification results

Usage

```
classification(object)

## S4 method for signature 'ClassyFire'
classification(object)
```

Arguments

object a ClassyFire S4 object

ClassyFire-class	<i>ClassyFire Class</i>
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Description

A S4 class to store the results from the ClassFire RESTful API

Slots

meta a list of the input SMILE, InChI Key and classification version used
classification a tibble of the ClassyFire classification results
direct_parent a list of the direct parent
alternative_parents a tibble of alternative parents
predicted_chebi a character vector of the predicted ChEBI terms
external_descriptors a tibble of any external identifications
description a character string of the compound description

description	<i>description</i>
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Description

Get the ClassyFire description

Usage

```
description(object)
```

```
## S4 method for signature 'ClassyFire'  
description(object)
```

Arguments

object	a ClassyFire S4 object
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descriptors	<i>descriptors</i>
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Description

Get the external descriptors

Usage

```
descriptors(object)
```

```
## S4 method for signature 'ClassyFire'  
descriptors(object)
```

Arguments

object	a ClassyFire S4 object
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direct_parent	<i>direct_parent</i>
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Description

Get the direct_parent

Usage

```
direct_parent(object)
```

```
## S4 method for signature 'ClassyFire'  
direct_parent(object)
```

Arguments

object	a ClassyFire S4 object
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get_classification	<i>Get Entity Classification</i>
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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
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Value

a tibble containing the following;

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

Examples

```
## Not run:

# 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',
  'TYEYBOSBBHJIV-UHFFFAOYSA-N',
  'AFENDNXGAFYKQO-UHFFFAOYSA-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)

## End(Not run)
```

meta	<i>meta</i>
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Description

Get the ClassyFire meta data

Usage

```
meta(object)

## S4 method for signature 'ClassyFire'
meta(object)
```

Arguments

object a ClassyFire S4 object

show,ClassyFire-method
<i>show-ClassyFire</i>

Description

show-ClassyFire

Usage

```
## S4 method for signature 'ClassyFire'
show(object)
```

Arguments

object a ClassyFire S4 object

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