

Package ‘classyfireR’

May 7, 2020

Type Package

Title R Interface to the ClassyFire RESTful API

Version 0.3.4

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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, cli, purrr, dplyr, stringr, methods, rjson

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 7.1.0

Roxygen list(markdown = TRUE)

Collate 'allGenerics.R' 'allClasses.R' 'accessor-methods.R'
'get_classification.R' 'internals.R' 'query.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 ClassyFire S4 object.

See Also

ClassyFire-class

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')

## End(Not run)
```

get_query	<i>Retrieves the classification results for a given query.</i>
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Description

Retrieves the classification results for a given query.

Usage

```
get_query(query_id, format = c("json", "sdf", "csv"))
```

Arguments

query_id	query_id a numeric value for the ID of the query.
format	a string of the format of the query (either JSON, CSV, or SDF)

Value

the parsed text output displaying the classification results for

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

show-ClassyFire

Description

show-ClassyFire

Usage

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

Arguments

object a ClassyFire S4 object

submit_query

Submits a ClassyFire query in a JSON format.

Description

Submits a ClassyFire query in a JSON format.

Usage

```
submit_query(label, input, type = "STRUCTURE")
```

Arguments

label a string the label of the query.
input a named list or vector of SMILES strings.
type a string the type of the query.

Value

A list of tibbles named by input name.

Examples

```
## Not run:
input <- c(MOL1 = 'CCCOCC', MOL2 = 'COCC=CCC')
submit_query(label = 'query_test', input = input, type = 'STRUCTURE')

## End(Not run)
```

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