

Package ‘classyfireR’

April 14, 2021

Type Package

Title R Interface to the ClassyFire REST API

Version 0.3.7

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Description Access to the ClassyFire REST 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,
tidyjson,
tidyr

Suggests testthat,
covr,
knitr,
rmarkdown

License GPL (>= 3)

Encoding UTF-8

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

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

RoxygenNote 7.1.1

Roxygen list(markdown = TRUE)

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

VignetteBuilder knitr

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alternative_parents	<i>alternative_parents</i>
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Description

Get the alternative_parents
Get the alternative_parents

Usage

alternative_parents(object)

S4 method for signature 'ClassyFire'
alternative_parents(object)

S4 method for signature 'Query'
alternative_parents(object)

Arguments

object a Query S4 object

chebi

chebi

Description

Get the predicted ChEBI identifications

Get the predicted ChEBI identifications

Usage

```
chebi(object)
```

```
## S4 method for signature 'ClassyFire'
```

```
chebi(object)
```

```
## S4 method for signature 'Query'
```

```
chebi(object)
```

Arguments

object a Query S4 object

classification

Accessor Methods for the ClassyFire S4 class

Description

Get the ClassyFire classification results

Get the ClassyFire classification results

Usage

```
classification(object)
```

```
## S4 method for signature 'ClassyFire'
```

```
classification(object)
```

```
## S4 method for signature 'Query'
```

```
classification(object)
```

Arguments

object a Query S4 object

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

A S4 class to store the results from the ClassyFire 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 identificatons
 description a character string of the compound description

description	<i>description</i>
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Description

Get the ClassyFire description

Get the ClassyFire description

Usage

```
description(object)

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

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

Arguments

object a Query S4 object

descriptors	<i>descriptors</i>
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Description

Get the external descriptors
Get the external descriptors

Usage

```
descriptors(object)

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

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

Arguments

object a Query S4 object

direct_parent	<i>direct_parent</i>
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Description

Get the direct_parent
Get the direct_parent

Usage

```
direct_parent(object)

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

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

Arguments

object a Query S4 object

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

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
- Get the ClassyFire meta data

Usage

```
meta(object)

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

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

Arguments

- object a Query S4 object

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

A S4 class to store the results from the ClassyFire RESTful API Queries

Slots

meta a 'tibble' of the input SMILE, InChI Key and classification version used
classification a tibbles of the ClassyFire classification results
direct_parent a tibbles the direct parent
alternative_parents a tibbles of alternative parents
predicted_chebi a list of character vectors of the predicted ChEBI terms
external_descriptors a list of tibbles of any external identifications
description a list of character vectors for the compound descriptions
unclassified a character string of any input structures that failed the ClassyFire classification

show, ClassyFire-method

show-ClassyFire

Description

show-ClassyFire

show-Query

Usage

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

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

Arguments

object a Query 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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