

Package ‘classyfireR’

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Type Package

Title R Interface to the ClassyFire REST API

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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,
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dplyr,
stringr,
methods,
rjson,
RSQLite,
tidyjson,
tidyr

Suggests testthat,
covr,
knitr,
rmarkdown,
stringi

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
```

R topics documented:

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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>
-------------	--------------------

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/'. The optional local cache function enables classification requests with less waiting time. Furthermore, there will be fewer traffic on the classyFire servers. For best high efficiency there is an option for creating a SQLite database to cache results.

Usage

```
get_classification(inchi_key, conn = NULL)
```

Arguments

inchi_key	a character string of a valid InChIKey
conn	a DBIConnection object, as produced by dbConnect

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
--------	-------------------

open_cache

Open Cache

Description

Creates a SQLite database for the local caching. This database includes already queried InChIkeys and the serialized classification object.

Usage

```
open_cache(dbname = ":memory:")
```

Arguments

dbname	The path to the database file. SQLite keeps each database instance in one single file. The name of the database is the file name, thus database names should be legal file names in the running platform. There are two exceptions: "" will create a temporary on-disk database. The file will be deleted when the connection is closed. ":memory:" or "file::memory:" will create a temporary in-memory database.
--------	--

Value

conn a DBIConnection object, as produced by dbConnect

Query-class

ClassyFire Query Class

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

<code>object</code>	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

<code>label</code>	a string the label of the query.
<code>input</code>	a named list or vector of SMILES strings.
<code>type</code>	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)
```

unclassified

unclassified

Description

Get the identifiers of any inputs that were not classified

Usage

```
unclassified(object)

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

Arguments

object a Query S4 object

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