

Package ‘classyfireR’

February 18, 2020

Type Package

Title R Interface to the ClassyFire RESTful API

Version 0.3.3

Date 2020-02-18

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 7.0.2

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 *Accessor Methods for the ClassyFire S4 class*

Description

Get the ClassyFire classification results

Usage

```
classification(object)

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

Arguments

object a ClassyFire S4 object

ClassyFire-class *ClassyFire Class*

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

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

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

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)
```

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>
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Description

show-ClassyFire

Usage

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

Arguments

object a ClassyFire S4 object

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