Package 'classyfireR'

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Type Package

Title R Interface to the ClassyFire RESTful API

Version 0.3.5

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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, tidyjson, tidyr

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

Author Tom Wilson [aut, cre] (<https://orcid.org/0000-0003-3112-4682>), Jasen Finch [aut], Gordon Getzinger [ctb]

Maintainer Tom Wilson <tpw2@aber.ac.uk>

R **topics documented:**

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alternative_parents   *alternative_parents*

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   *ClassyFire Class*

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

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description   *description*

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 *descriptors*

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 *direct_parent*

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

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get_classification   *Get Entity Classification*

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)
```

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get_query   *Retrieves the classification results for a given query.*

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`	*meta*

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`	*ClassyFire Query Class*

Description

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

Slots

`meta` a list of the input SMILE, InChI Key and classification version used

`classification` a list of `tibbles` of the ClassyFire classification results

`direct_parent` a list of `tibbles` the direct parent

`alternative_parents` a list of `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 identificatons

`description` a character string of the compound description

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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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