Package 'classyfireR'

August 31, 2018

Type Package

Title R Interface to the ClassyFire RESTful API

Version 0.1.0

Date 2018-06-13

Description Access to the ClassyFire RESTful API (http://classyfire.wishartlab.com).

Depends magrittr

Imports httr, jsonlite, tibble, crayon, clisymbols

Suggests testthat, covr, dplyr, purrr

License GPL (>= 3)

Encoding UTF-8

LazyData true

URL https://github.com/wilsontom/classyfireR

BugReports https://github.com/wilsontom/classyfireR/issues

RoxygenNote 6.1.0

Roxygen list(markdown = TRUE)

NeedsCompilation no

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R topics documented:

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entity_classification   *Entity Classification*

Description

Retrive entity classification from 'http://classyfire.wishartlab.com/entities/'

Usage

```
entity_classification(inchi_key)
```

Arguments

inchi_key   a character string of a valid InChIKey

Value

a `tibble` containing the following;

- **Level** Classification level (kingdom, superclass, class and subclass)
- **Classification** The compound classification
- **CHEMONT** Chemical Ontology Identification code

Examples

```
# Valid InChI key where all four classification levels are available
entity_classification('BRMWTNUJHUMWMS-LURJTMIESA-N')

# Valid InChI key where only three classification levels are available
entity_classification('MDHYEMXUFSJLGV-UHFFFAOYSA-N')

# Invalid InChI key
entity_classification('MDHYEMXUFSJLGV-UHFFFAOYSA-B')


# Using `dplyr` a vector of InChI Keys can be submitted and easily parsed
  library(dplyr)
  library(purrr)

  keys <- c(
 'BRMWTNUJHUMWMS-LURJTMIESA-N',
 'XFNJVJPLKCPIBV-UHFFFAOYSA-N',
 'TYEYBOSBBBHJIV-UHFFFAOYSA-N',
 'AFENDNXGAFYKQO-UHFFFAOYSA-N',
 'WHEUWNKSCXYKBU-QPWUGHHJSA-N',
 'WHBMMWSBFZVSSR-GSVOUGTGSA-N')

  classification_list <- map(keys, entity_classification)
```

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get_status_code   *Get Status Code*

Description

Get Status Code

Usage

```
get_status_code(query_id)
```

Arguments

query_id   a numeric value for the query id

Value

a list of `query_id` and classification status; either `In progress` or `Done`

Examples

```
get_status_code(2813259)
```

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retrieve_classification
                        Retrieve classification results

Description

Retrieve classification results from a new submission

Usage

```
retrieve_classification(query_id)
```

Arguments

query_id   a numeric value for the query id

Value

a `tibble` containing the following;

- **Level** Classification level (kingdom, superclass, class and subclass)
- **Classification** The compound classification
- **CHEMONT** Chemical Ontology Identification code

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submit_classification   *Submit InChI Code for Classification*

Description

Submit and new entity for classification using the ClassyFire webserver

Usage

```
submit_classification(query, label, type = "STRUCTURE")
```

Arguments

query	a charatcer string of InChI Code or SMILE
label	a character string of the query name
type	the label type (Default = STRUCTURE)

Value

if the classification has completed; a `tibble` containing the following;

- **Level** Classification level (kingdom, superclass, class and subclass)
- **Classification** The compound classification
- **CHEMONT** Chemical Ontology Identification code

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