Package 'classyfireR'

March 27, 2018

Type Package

Title R Interface to the ClassyFire API

Version 0.0.99

Description Access the ClassyFire REST API.

Depends magrittr

Imports httr, jsonlite, tibble, crayon, clisymbols

Suggests testthat, covr

License GPL (>= 3)

Encoding UTF-8

LazyData true

RoxygenNote 6.0.1

Roxygen list(markdown = TRUE)

NeedsCompilation no

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R topics documented:

`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

```
entity_classification('BRMWTNUJHUMWMS-LURJTMIESA-N')

entity_classification('MDHYEMXUFSJLGV-UHFFFAOYSA-N')
```

`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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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

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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