

Package ‘classyfireR’

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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, dplyr

License GPL (>= 3)

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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')
```

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)
```

```
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

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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