

# Package ‘classyfireR’

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**Type** Package

**Title** R Interface to the ClassyFire RESTful API

**Version** 0.1.1

**Date** 2018-10-05

**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

**Suggests** testthat, covr, dplyr, purrr, tidyr

**License** GPL (>= 3)

**Encoding** UTF-8

**LazyData** true

**URL** <https://github.com/wilsonsom/classyfireR>

**BugReports** <https://github.com/wilsonsom/classyfireR/issues>

**RoxygenNote** 6.1.0

**Roxygen** list(markdown = TRUE)

**NeedsCompilation** no

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entity\_classification *Entity Classification*

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## 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)
library(tidyr)

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

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

classification_list <- map(classification_list, ~{select(.,-CHEMONT)})

spread_tibble <- purrr::map(classification_list, ~{
  spread(., Level, Classification)
}) %>% bind_rows() %>% data.frame()

rownames(spread_tibble) <- keys

classification_df <- data.frame(InChIKey = rownames(spread_tibble),
  Kingdom = spread_tibble$kingdom,
  SuperClass = spread_tibble$superclass,
  Class = spread_tibble$class,
  SubClass = spread_tibble$subclass)

print(classification_df)
```

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get\_status\_code

*Get Status Code*

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### Description

Retreive the status code of a new submission for entity classification

### 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

**Examples**

```
retrieve_classification(2813259)
```

---

`submit_classification`    *Submit InChI Code for Classification*

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**Description**

Submit and new entity for classification using the ClassyFire webserver

**Usage**

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

**Arguments**

`query`            a character 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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