

# Package ‘classyfireR’

April 14, 2021

**Type** Package

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

**Version** 0.3.7

**Date** 2021-04-14

**Description** Access to the ClassyFire REST 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,  
knitr,  
rmarkdown

**License** GPL (>= 3)

**Encoding** UTF-8

**LazyData** true

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

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

**RoxygenNote** 7.1.1

**Roxygen** list(markdown = TRUE)

**Collate** 'allGenerics.R'  
          'allClasses.R'  
          'accessor-methods.R'  
          'get\_classification.R'  
          'internals.R'  
          'query.R'  
          'show-method.R'  
          'zzz.R'

**VignetteBuilder** knitr

**R topics documented:**

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alternative_parents	<i>alternative_parents</i>
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**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

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chebi

*chebi*

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**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

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ClassyFire-class	<i>ClassyFire Class</i>
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**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	<i>description</i>
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**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

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descriptors	<i>descriptors</i>
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**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

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direct_parent	<i>direct_parent</i>
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**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	<i>Get Entity Classification</i>
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**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	<i>Retrieves the classification results for a given query.</i>
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**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

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meta	<i>meta</i>
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**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

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Query-class	<i>ClassyFire Query Class</i>
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**Description**

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

**Slots**

meta a 'tibble' of the input SMILE, InChI Key and classification version used  
classification a tibbles of the ClassyFire classification results  
direct\_parent a tibbles the direct parent  
alternative\_parents a 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 identifications  
description a list of character vectors for the compound descriptions  
unclassified a character string of any input structures that failed the ClassyFire classification

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show, ClassyFire-method

*show-ClassyFire*

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**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.*

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**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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