

# Package ‘classyfireR’

February 17, 2022

**Type** Package

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

**Version** 0.3.8

**Date** 2022-02-17

**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,  
RSQLite,  
tidyjson,  
tidyr

**Suggests** testthat,  
covr,  
knitr,  
rmarkdown,  
stringi

**License** GPL (>= 3)

**Encoding** UTF-8

**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:**

alternative_parents . . . . .	2
chebi . . . . .	3
classification . . . . .	3
ClassyFire-class . . . . .	4
description . . . . .	4
descriptors . . . . .	5
direct_parent . . . . .	5
get_classification . . . . .	6
get_query . . . . .	7
meta . . . . .	7
open_cache . . . . .	8
Query-class . . . . .	8
show,ClassyFire-method . . . . .	9
submit_query . . . . .	9
unclassified . . . . .	10
<b>Index</b>	<b>11</b>

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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

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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/'. The optional local cache function enables classification requests with less waiting time. Furthermore, there will be fewer traffic on the classyFire servers. For best high efficiency there is an option for creating a SQLite database to cache results.

**Usage**

```
get_classification(inchi_key, conn = NULL)
```

**Arguments**

inchi_key	a character string of a valid InChIKey
conn	a DBIConnection object, as produced by dbConnect

**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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open\_cache

*Open Cache*


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### Description

Creates a SQLite database for the local caching. This database includes already queried Inchikeys and the serialized classification object.

### Usage

```
open_cache(dbname = ":memory:")
```

### Arguments

dbname	The path to the database file. SQLite keeps each database instance in one single file. The name of the database is the file name, thus database names should be legal file names in the running platform. There are two exceptions: "" will create a temporary on-disk database. The file will be deleted when the connection is closed. ":memory:" or "file::memory:" will create a temporary in-memory database.
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### Value

conn a DBIConnection object, as produced by dbConnect

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Query-class

*ClassyFire Query Class*


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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**

<code>object</code>	a Query S4 object
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`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**

<code>label</code>	a string the label of the query.
<code>input</code>	a named list or vector of SMILES strings.
<code>type</code>	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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unclassified

*unclassified*

---

**Description**

Get the identifiers of any inputs that were not classified

**Usage**

```
unclassified(object)

## S4 method for signature 'Query'
unclassified(object)
```

**Arguments**

object            a Query S4 object

# Index

alternative\_parents, [2](#)  
alternative\_parents, ClassyFire-method  
    (alternative\_parents), [2](#)  
alternative\_parents, Query-method  
    (alternative\_parents), [2](#)  
  
chebi, [3](#)  
chebi, ClassyFire-method (chebi), [3](#)  
chebi, Query-method (chebi), [3](#)  
classification, [3](#)  
classification, ClassyFire-method  
    (classification), [3](#)  
classification, Query-method  
    (classification), [3](#)  
ClassyFire-class, [4](#)  
  
description, [4](#)  
description, ClassyFire-method  
    (description), [4](#)  
description, Query-method (description),  
    [4](#)  
descriptors, [5](#)  
descriptors, ClassyFire-method  
    (descriptors), [5](#)  
descriptors, Query-method (descriptors),  
    [5](#)  
direct\_parent, [5](#)  
direct\_parent, ClassyFire-method  
    (direct\_parent), [5](#)  
direct\_parent, Query-method  
    (direct\_parent), [5](#)  
  
get\_classification, [6](#)  
get\_query, [7](#)  
  
meta, [7](#)  
meta, ClassyFire-method (meta), [7](#)  
meta, Query-method (meta), [7](#)  
  
open\_cache, [8](#)  
  
Query-class, [8](#)  
  
show, ClassyFire-method, [9](#)  
show, Query-method  
    (show, ClassyFire-method), [9](#)  
submit\_query, [9](#)  
  
unclassified, [10](#)  
unclassified, Query-method  
    (unclassified), [10](#)