

# Package ‘classyfireR’

November 18, 2019

**Type** Package

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

**Version** 0.3.0

**Date** 2019-11-18

**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, cli, purrr, dplyr, stringr, methods

**Suggests** testthat, covr

**License** GPL (>= 3)

**Encoding** UTF-8

**LazyData** true

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

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

**RoxygenNote** 7.0.0

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

**NeedsCompilation** no

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alternative_parents	<i>alternative_parents</i>
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**Description**

Get the alternative\_parents

**Usage**

```
alternative_parents(object)
```

```
## S4 method for signature 'ClassyFire'
alternative_parents(object)
```

**Arguments**

object            a ClassyFire S4 object

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chebi	<i>chebi</i>
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**Description**

Get the predicted ChEBI identifications

**Usage**

```
chebi(object)
```

```
## S4 method for signature 'ClassyFire'
chebi(object)
```

**Arguments**

object            a ClassyFire S4 object

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classification            *Accessor Methods for the ClassyFire S4 class*

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**Description**

Get the ClassyFire classification results

**Usage**

```
classification(object)

## S4 method for signature 'ClassyFire'
classification(object)
```

**Arguments**

object            a ClassyFire S4 object

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ClassyFire-class            *ClassyFire Class*

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**Description**

A S4 class to store the results from the ClassFire 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 identifications  
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

**Usage**

```
description(object)
```

```
## S4 method for signature 'ClassyFire'  
description(object)
```

**Arguments**

object            a ClassyFire S4 object

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descriptors	<i>descriptors</i>
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**Description**

Get the external descriptors

**Usage**

```
descriptors(object)
```

```
## S4 method for signature 'ClassyFire'  
descriptors(object)
```

**Arguments**

object            a ClassyFire S4 object

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direct_parent	<i>direct_parent</i>
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**Description**

Get the direct\_parent

**Usage**

```
direct_parent(object)
```

```
## S4 method for signature 'ClassyFire'  
direct_parent(object)
```

**Arguments**

object            a ClassyFire 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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meta	<i>meta</i>
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**Description**

Get the ClassyFire meta data

**Usage**

```
meta(object)

## S4 method for signature 'ClassyFire'
meta(object)
```

**Arguments**

object            a ClassyFire S4 object

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show,ClassyFire-method	<i>show-ClassyFire</i>
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**Description**

show-ClassyFire

**Usage**

```
## S4 method for signature 'ClassyFire'
show(object)
```

**Arguments**

object            a ClassyFire S4 object

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