

Package ‘uCAREChemSuiteCLI’

June 7, 2018

Type Package

Title Resistome Predictor

Version 0.1.2

Date 2018-05-29

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Description Predicts Escherichia coli's resistome for candidate drug. It utilizes two algorithms viz. deterministic model and stochastic model (manuscript under preparation) for the prediction of drug class. Once the drug class is predicted, the resistome is fetched from the database for the predicted class.

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Encoding UTF-8

LazyData true

RoxygenNote 6.0.1

Imports ChemmineR, stats, utils, usethis

NeedsCompilation no

Repository CRAN

Date/Publication 2018-06-07 16:15:15 UTC

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drug.class.deterministic
drug.class.deterministic

Description

Takes structure data file (SDF) of candidate drug and predicts its drug class using deterministic model.

Usage

```
drug.class.deterministic("sdf")
```

Arguments

sdf input sdf file

Details

uCAREChemSuiteCLI

Value

predicted drug class of the candidate drug by deterministic model

Examples

```
{  
example.class.deterministic<- system.file('extdata/example.sdf', package="uCAREChemSuiteCLI")  
drug.class.deterministic(example.class.deterministic)  
}
```

drug.class.stochastic *drug.class.stochastic*

Description

Takes structure data file (SDF) of candidate drug, Nearest Neighbor value and threshold similarity score to predict its drug class using stochastic model.

Usage

```
drug.class.stochastic("sdf", "NearestNeighbor", "Threshold")
```

Arguments

| | |
|-----------------|----------------------------------|
| sdf | input sdf file |
| NearestNeighbor | Nearest Neighbor = 1, 3 |
| Threshold | Threshold = 0.25, 0.3, 0.35, 0.4 |

Details

uCAREChemSuiteCLI

Value

Predicted drug class of the candidate drug using Nearest Neighbor algorithm

Examples

```
{  
  example.class.stochastic<- system.file('extdata/example.sdf', package="uCAREChemSuiteCLI")  
  drug.class.stochastic(example.class.stochastic,"3","0.25")  
}
```

`drug.resistome.deterministic`
drug.resistome.deterministic

Description

Takes structure data file (SDF) of candidate drug to predicts its resistome using deterministic model.

Usage

```
drug.resistome.deterministic("sdf")
```

Arguments

| | |
|-----|----------------|
| sdf | input sdf file |
|-----|----------------|

Details

uCAREChemSuiteCLI

Value

Predicted resistome of the candidate drug using deterministic model

Examples

```
{
  example.resistome.deterministic<- system.file('extdata/example.sdf', package="uCAREChemSuiteCLI")
  drug.resistome.deterministic(example.resistome.deterministic)
}
```

```
drug.resistome.stochastic
      drug.resistome.stochastic
```

Description

Takes structure data file (SDF) of candidate drug to predict its resistome using stochastic model.

Usage

```
drug.resistome.stochastic("sdf", "NearestNeighbor", "Threshold")
```

Arguments

| | |
|-----------------|----------------------------------|
| sdf | input sdf file |
| NearestNeighbor | Nearest Neighbor = 1, |
| Threshold | Threshold = 0.25, 0.3, 0.35, 0.4 |

Details

uCAREChemSuiteCLI

Value

Predicted resistome of the candidate drug using Nearest Neighbor algorithm

Examples

```
{
  example.resistome.stochastic<- system.file('extdata/example.sdf', package="uCAREChemSuiteCLI")
  drug.resistome.stochastic(example.resistome.stochastic, "3", "0.25")
}
```

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