Package 'uCAREChemSuiteCLI'

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Type Package

Title Resistome Predicter

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Description

This suite of packages is developed to predicts resistome for unknown chemical compounds. 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 profile of Escherichia coli and Pseudomonas aeruginosa for the drug class is fetched from the database.

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Encoding UTF-8

LazyData true

RoxygenNote 6.1.1

Imports ChemmineR, stats, utils, usethis

NeedsCompilation no

Repository CRAN

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R topics documented:

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", "Organism")
```

Arguments

sdf	input sdf file
Organism	Escherichia coli = 1, Pseudomonas aeruginosa = 2

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, "1")
}
```

`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", "Organism")
```

Arguments

`sdf`	input sdf file
`NearestNeighbor`	Nearest Neighbor = 1, 3
`Threshold`	Threshold = 0.25, 0.3, 0.35, 0.4
`Organism`	Escherichia coli = 1, Pseudomonas aeruginosa = 2

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", "1")
}
```

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