

Package ‘fmcsR’

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Type Package

Title Mismatch Tolerant Maximum Common Substructure Searching

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Author Yan Wang, Tyler Backman, Kevin Horan, Thomas Girke

Maintainer Thomas Girke <thomas.girke@ucr.edu>

Description The fmcsR package introduces an efficient maximum common substructure (MCS) algorithms combined with a novel matching strategy that allows for atom and/or bond mismatches in the substructures shared among two small molecules. The resulting flexible MCSs (FMCSs) are often larger than strict MCSs, resulting in the identification of more common features in their source structures, as well as a higher sensitivity in finding compounds with weak structural similarities. The fmcsR package provides several utilities to use the FMCS algorithm for pairwise compound comparisons, structure similarity searching and clustering.

Depends R (>= 2.10.0), ChemmineR, methods

Suggests BiocStyle, knitr, knitcitations, knitrBootstrap, rmarkdown, codetools

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LazyLoad yes

URL <https://github.com/girke-lab/fmcsR>

biocViews Cheminformatics, BiomedicalInformatics, Pharmacogenetics, Pharmacogenomics, MicrotitrePlateAssay, CellBasedAssays, Visualization, Infrastructure, DataImport, Clustering, Proteomics, Metabolomics

Imports RUnit, methods, ChemmineR, BiocGenerics, parallel

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| | |
|---------------|-------------------------------|
| fmcsR-package | <i>A FMCS solver package.</i> |
|---------------|-------------------------------|

Description

The package consists of two main functions, `fmcs` which computes the flexible MCS between two SDF objects. And `fmcsBatch` runs the FMCS algorithm on a SDF set.

Details

Package: fmcsR
 Type: Package
 Version: 1.0
 Date: 2012-02-01

Author(s)

Yan Wang

Maintainer: Yan Wang <wangya@cs.ucr.edu>

Examples

```
library(fmcsR)
data(sdfsampl)
sdfset <- sdfsampl
result1 <- fmcs(sdfset[[1]], sdfset[[2]])
result2 <- fmcs(sdfset[[1]], sdfset[[2]], au=3)
result3 <- fmcs(sdfset[[1]], sdfset[[2]], bu=3)
result4 <- fmcs(sdfset[[1]], sdfset[[2]], au=1, bu=1)
result5 <- fmcs(sdfset[[1]], sdfset[[2]], matching.mode="aromatic")
result6 <- fmcs(sdfset[[1]], sdfset[[2]], au=2, bu=1, matching.mode="aromatic")

fmcsBatch(sdfset[[1]], sdfset[1:3])
fmcsBatch(sdfset[[1]], sdfset[1:3], au=2)
fmcsBatch(sdfset[[1]], sdfset[1:3], bu=1)
fmcsBatch(sdfset[[1]], sdfset[1:3], matching.mode="aromatic", au=1, bu=1)
```

 fmcs

Flexible MCS (FMCS) Finder

Description

R function to call the C++ implementation of the flexible common substructure (FMCS) algorithm. The FMCS algorithm provides an improved maximum common substructure (MCS) search method that allows atom and/or bond mismatches in the substructures shared among two small molecules. The resulting flexible MCSs (FMCSs) are often larger than strict MCSs, resulting in the identification of more common features in their source structures, as well as a higher sensitivity in detecting weak similarities among compounds.

Usage

```
fmcs(sdf1, sdf2, al = 0, au = 0, bl = 0, bu = 0, matching.mode =
  "static", fast = FALSE, timeout=60000)
```

Arguments

| | |
|---------------|--|
| sdf1 | Input query SDF object or SDFset object with a single molecule. |
| sdf2 | Input target SDF object SDFset object with a single molecule. |
| al | Lower bound for the number of atom mismatches. |
| au | Upper bound for the number of atom mismatches. |
| bl | Lower bound for the number of bond mismatches. |
| bu | Upper bound for the number of bond mismatches. |
| matching.mode | Three modes for bond matching are supported: "static", "aromatic", and "ring". |
| fast | If fast is set to TRUE, then the fast computing mode will be turned on. In this case, the algorithm will only return the size information about the source structures and their MCSs, while omitting all structural information. |
| timeout | The maximum amount of time to spend searching, in milliseconds. A value of 0 indicates no timeout. |

Details

...

Value

Returns object of class MCS

Author(s)

Yan Wang, Thomas Girke

References

Publication in preparation.

See Also

plotMCS, fmcsBatch, ?"MCS-class"

Examples

```
library(fmcsR)
data(sdfsampl)
sdfset <- sdfsampl
mcs1 <- fmcs(sdfset[[1]], sdfset[[2]])
mcsfast <- fmcs(sdfset[[1]], sdfset[[2]], fast=TRUE)
mcs2 <- fmcs(sdfset[[1]], sdfset[[2]], au=3)
mcs3 <- fmcs(sdfset[[1]], sdfset[[2]], bu=3)
mcs4 <- fmcs(sdfset[[1]], sdfset[[2]], au=1, bu=1)
mcs5 <- fmcs(sdfset[[1]], sdfset[[2]], matching.mode="aromatic")
mcs6 <- fmcs(sdfset[[1]], sdfset[[2]], au=2, bu=1, matching.mode="aromatic")

## Plot MCS objects
plotMCS(mcs6)

## Methods to return components of MCS objects
stats(mcs6)
mcs6[["stats"]]
mcs1(mcs6)
mcs6[["mcs1"]]
mcs2(mcs6)
mcs6[["mcs2"]]

## Constructor method from list
mylist <- list(stats=stats(mcs6), mcs1=mcs1(mcs6), mcs2=mcs2(mcs6))
mymcs <- as(mylist, "MCS")
```

`fmcsBatch`*FMCS Search Function*

Description

Compound search function that runs the FMCS algorithm for a query compound against a set of molecules stored in an SDFset container.

Usage

```
fmcsBatch(querySdf, sdfset, al = 0, au = 0, bl = 0, bu = 0,
matching.mode = "static", timeout=60000, numParallel=1)
```

Arguments

| | |
|----------------------------|--|
| <code>querySdf</code> | Input query SDF object or SDFset object of length one. |
| <code>sdfset</code> | Input target SDFset object. |
| <code>al</code> | Lower bound for the number of atom mismatches. |
| <code>au</code> | Upper bound for the number of atom mismatches. |
| <code>bl</code> | Lower bound for the number of bond mismatches. |
| <code>bu</code> | Upper bound for the number of bond mismatches. |
| <code>matching.mode</code> | Three matching mode are supported, "static", "aromatic", and "ring". |
| <code>timeout</code> | The maximum amount of time to spend on each pair of comparisons, in milliseconds. A value of 0 indicates no timeout. |
| <code>numParallel</code> | The number of comparisons to run in parallel, using local cores. |

Details

This function runs the FMCS algorithm in fast computing mode. Thus, it will only return the similarity scores and size information about the source structures and their MCSs, while omitting all structural information.

Value

Returns a matrix with compound IDs as row names and the following columns: Query_Size, Target_Size, MCS_Size, Tanimoto_Coefficient and Overlap_Coefficient. For details see vignette of this package.

Author(s)

Yan Wang, Thomas Girke

See Also

`plotMCS`, `fmcs`, `? "MCS-class"`

Examples

```
library(fmcsR)
data(sdfsampl)
sdfset <- sdfsampl
fmcsBatch(sdfset[[1]], sdfset[1:3])
fmcsBatch(sdfset[[1]], sdfset[1:3], au=2)
fmcsBatch(sdfset[[1]], sdfset[1:3], bu=1)
fmcsBatch(sdfset[[1]], sdfset[1:3], matching.mode="aromatic", au=1, bu=1)
```

fmcstest

SD file stored in SDFset object

Description

Sample compound structures stored in SDF format.

Usage

```
data(fmcstest)
```

Format

Object of class SDFset

Details

Object stores X molecules from a sample SD file.

Source

<ftp://ftp.ncbi.nih.gov/pubchem/>

References

SDF format definition: <http://www.symyx.com/downloads/public/ctfile/ctfile.jsp>

Examples

```
data(fmcstest)
sdfset <- fmcstest
view(sdfset)
```

MCS-class

Class "MCS"

Description

List-like container for storing results from `fmcs` function.

Objects from the Class

Objects can be created by calls of the form `new("MCS", ...)`.

Slots

`stats`: Object of class "numeric" ~~

`mcs1`: Object of class "SDFset" ~~

`mcs2`: Object of class "SDFset" ~~

Methods

`[[` signature(x = "MCS"): ...

`coerce` signature(from = "list", to = "MCS"): ...

`mcs1` signature(x = "MCS"): ...

`mcs2` signature(x = "MCS"): ...

`stats` signature(x = "MCS"): ...

Note

...

Author(s)

Yan Wang

References

...

See Also

Related classes: `SDF`, `SDFstr`

Examples

```
## Create MCS instance
showClass("MCS")
data(sdfsampl)
sdfset <- sdfsampl
mcs <- fmcs(sdfset[[1]], sdfset[[2]], au=2, bu=2)

## Methods to return components of MCS
stats(mcs)
mcs[["stats"]]
mcs1(mcs)
mcs[["mcs1"]]
mcs2(mcs)
mcs[["mcs2"]]

## Constructor method from list
mylist <- list(stats=stats(mcs), mcs1=mcs1(mcs), mcs2=mcs2(mcs))
mymcs <- as(mylist, "MCS")
```

mcs2sdfset

Return MCS object as SDFset

Description

Helper function to run `atomssubset` from `ChemmineR` library on MCS objects in order to obtain their results in SDFset format.

Usage

```
mcs2sdfset(x, ...)
```

Arguments

| | |
|-----|---|
| x | Object of class MCS |
| ... | Arguments to be passed to/from other methods. |

Details

Returns MCS data in form of a list containing two SDFset objects, one for the query and one for the target structure.

Value

List with two SDFset objects.

Note

...

Author(s)

Thomas Girke

References

...

See Also

fmcs

Examples

```
library(fmcsR)
data(sdfsampl)
sdfset <- sdfsampl
mcs <- fmcs(sdfset[[1]], sdfset[[2]], au=2, bu=1, matching.mode="aromatic")
mcs2sdfset(x=mcs, type="new")
mcs2sdfset(x=mcs, type="old")[[1]][[1]]
plot(mcs2sdfset(x=mcs, type="new")[[1]][[1]])
```

plotMCS

Plot MCS

Description

Convenience plotting function to visualize and compare MCSs generated by fmcs function.

Usage

```
plotMCS(x, mcs = 1, print = FALSE, ...)
```

Arguments

| | |
|-------|---|
| x | MCS object |
| mcs | Selection of MCS solution by position number, default is 1. |
| print | print=FALSE turns of printing behavior of class. |
| ... | Arguments to be passed to/from other methods. |

Details

The two structures, target and query, used to generate x with a call to fmcs are plotted next to each other, and the corresponding MCS substructures are highlighted in color.

Value

Prints summary of MCS to screen and plots their structures to graphics device.

Note

...

Author(s)

Yan Wang

References

...

See Also`sdf.visualize`**Examples**

```
library(fmcsR)
data(sdfsampl)
sdfset <- sdfsampl
mcs <- fmcs(sdfset[[1]], sdfset[[2]], au=2, bu=1, matching.mode="aromatic")
plotMCS(mcs, mcs=1)
```

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