Package 'ChemmineOB'

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Type Package

Title R interface to a subset of OpenBabel functionalities

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Imports BiocGenerics, zlibbioc

Description ChemmineOB provides an R interface to a subset of cheminformatics functionalities implemented by the OpelBabel C++ project. OpenBabel is an open source cheminformatics toolbox that includes utilities for structure format interconversions, descriptor calculations, compound similarity searching and more. ChemineOB aims to make a subset of these utilities available from within R. For non-developers, ChemineOB is primarily intended to be used from ChemmineR as an add-on package rather than used directly.

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Depends R (>= 2.15.1), methods

System Requirements OpenBabel (>= 2.3.1) with headers. http://openbabel.org

Enhances ChemmineR (>= 2.13.0)

URL http://manuals.bioinformatics.ucr.edu/home/chemminer

VignetteBuilder knitr

biocViews Cheminformatics

LinkingTo BH

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`convertFormat` *Convert Formats*

Description

Converts compound data from one format to another.

Usage

```
convertFormat(from, to, source)
```

Arguments

`from`	The format that `source` is in. This should be a string supported by OpenBabel.
`to`	The format to convert `source` to.
`source`	The initial compound format, as a string. The format of the string should be identical to the file format of the same name. Tabs and newlines may be represented with \t and \n, repsectivly.

Value

Returns the compound given in `source` in the format specified by `to`.

Author(s)

Kevin Horan

References

OpenBabel http://openbabel.org

See Also

`convertFormatFile`

Examples

```
sdfStr = convertFormat("SMI","SDF","CC(=O)OC1=CC=CC=C1C(=O)O\ttest_name")
```

convertFormatFile *Convert Format of Files*

Description

Convert a file from one format to another

Usage

```
convertFormatFile(from, to, fromFile, toFile)
```

Arguments

from	The format that fromFile is in. This should be a string supported by OpenBabel.
to	The format to convert toFile to.
fromFile	The name of the file to be converted
toFile	The name of the new file to be created or overwritten

Value

No value is returned. toFile will be created with the compound in the new format.

Author(s)

Kevin Horan

References

OpenBabel http://openbabel.org

See Also

convertFormat

Examples

```
## Not run:
convertFormatFile("SMI","SDF","test.smiles","test.sdf")

## End(Not run)
```

fingerprint_OB *Fingerprints from OpenBabel*

Description

Generates fingerprints using OpenBabel. The compound format can be specified as anything supported by OpenBabel. The fingerprint name can also be specified.

Usage

```
fingerprint_OB(obmolRefs, fingerprintName)
```

Arguments

obmolRefs	A list of OBMol references (of class '_p_OpenBabel__OBMol') representing the molecules to compute properites for. If you have your molecules in string format, you can create a list of OBMol references using the forEachMol function, see the example.
fingerprintName	The name of the fingerprint to generate. A list of available names can be found with "obabel -L fingerprints". Currently that list is: "FP2", "FP3", "FP4", and "MACCS".

Value

A matrix of binary values is returned. There is a row for each compound. The length of a row is determined by the fingerprint specified.

Author(s)

Kevin Horan

Examples

```
molRefs = forEachMol("SMILES","C1CCCCC1\ttest-compound-name",identity)
fingerprint_OB(molRefs,"FP3")
```

forEachMol *For Each Mol*

Description

Reads in molecules from the given string in the given format and calls function `f` on each molecule. The results are then combinded using the `reduce` function, if given.

Usage

```
forEachMol(inFormat, inString, f, reduce)
```

Arguments

`inFormat`	Format of string in `source`. This can be any OpenBabel format such as "SDF" or "SMILES". A full list can be found by executing "obabel -L formats".
`inString`	The compounds to generate fingerprints for. The format should be exactly what would be in a file of the same format. Newlines can be represented with "\n".
`f`	A function taking one OBMol reference and possibly returning a result.
`reduce`	This function will be passed to the `Reduce` function along with the results of all the `f` calls. This can be used to combine the results.

Value

The result will be a List of return values from the `f` function if not `reduce` function was given. Otherwise it will be the result of the `reduce` function applied to the results of the `f` function.

Author(s)

Kevin Horan

Examples

```
molRefs = forEachMol("SMILES","C1CCCCC1\ttest-compound-name",
                        identity,c)
```

OB-classes *Classes from OB*

Description

These are methods generated by SWIG for R. These should not generally be used outside of ChemmineOB, they are listed here to quite some warnings.

prop_OB *Properties from OpenBabel*

Description

Generates the following descriptors: "cansmi", "cansmiNS", "formula", "HBA1", "HBA2", "HBD", "InChI", "InChIKey", "logP", "MR", "MW", "nF", "s", "smarts", "title", "TPSA".

Usage

```
prop_OB(obmolRefs)
```

Arguments

obmolRefs	A list of OBMol references (of class '_p_OpenBabel__OBMol') representing the molecules to compute properites for. If you have your molecules in string format, you can create a list of OBMol references using the forEachMol function, see the example.

Value

Returns a data frame with the following OpenBabel descriptors: "cansmi", "cansmiNS", "formula", "HBA1", "HBA2", "HBD", "InChI", "InChIKey", "logP", "MR", "MW", "nF", "s", "smarts", "title", "TPSA".

Author(s)

Kevin Horan

Examples

```
molRefs = forEachMol("SMILES","C1CCCCC1\ttest-compound-name",identity)
prop_OB(molRefs)
```

smartsSearch_OB *SMARTS Search*

Description

Returns the number of matches found for each compound given.

Usage

```
smartsSearch_OB(obmolRefs, smartsPattern, uniqueMatches = TRUE)
```

Arguments

obmolRefs	A list of OBMol references (of class '_p_OpenBabel__OBMol') representing the molecules to compute properites for. If you have your molecules in string format, you can create a list of OBMol references using the forEachMol function, see the example.
smartsPattern	Any valid SMARTS pattern.
uniqueMatches	Should only unique matches be counted?

Value

A vector of counts.

Author(s)

Kevin Horan

Examples

```
molRefs = forEachMol("SMILES","C1CCCCC1\ttest-compound-name",identity)
smartsSearch_OB(molRefs,"[CH3X4]")
```

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