Package 'ChemmineOB'

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Type Package

Title R interface to a subset of OpenBabel functionalities

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Suggests ChemmineR, BiocStyle

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)

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

Enhances ChemmineR (>= 2.13.0)

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

R topics documented:

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(format, source, fingerprintName)
```

Arguments

`format`	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".
`source`	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".
`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

```
fingerprint_OB("SMILES","C1CCCCC1\ttest-compound-name","FP3")
```

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(from, source)
```

Arguments

from	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".
source	The compounds to generate descriptors for. The format should be exactly what would be in a file of the same format. Newlines can be represented with "\n".

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

```
prop_OB("SMILES","C1CCCCC1\ttest-compound-name")
```

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