

Package ‘rcdk’

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Title rcdk - Interface to the CDK Libraries

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Imports rJava, rcdklibs (>= 1.5.8), methods, png, iterators

Suggests xtable, RUnit

License LGPL

LazyLoad yes

Description This package allows the user to access functionality in the CDK, a Java framework for cheminformatics. This allows the user to load molecules, evaluate fingerprints, calculate molecular descriptors and so on. In addition the CDK API allows the user to view structures in 2D.

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NeedsCompilation no

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Atoms

Operations on atoms

Description

get.symbol returns the chemical symbol for an atom.

get.point3d returns the 3D coordinates of the atom

get.point2d returns the 2D coordinates of the atom

get.atomic.number returns the atomic number of the atom

get.hydrogen.count returns the number of implicit H's on the atom. Depending on where the molecule was read from this may be NULL or an integer greater than or equal to 0

get.charge returns the partial charge on the atom. If charges have not been set the return value is NULL, otherwise the appropriate charge.

`get.formal.charge` is returns the formal charge on the atom. By default the formal charge will be 0 (i.e., NULL is never returned)

`is.aromatic` returns TRUE if the atom is aromatic, FALSE otherwise

`is.aliphatic` returns TRUE if the atom is part of an aliphatic chain, FALSE otherwise

`is.in.ring` returns TRUE if the atom is in a ring, FALSE otherwise

`get.atom.index` returns the index of the atom in the molecule (starting from 0)

`get.connected.atoms` returns a list of atoms that are connected to the specified atom

Usage

```
get.symbol(atom)
get.point3d(atom)
get.point2d(atom)
get.atomic.number(atom)
get.hydrogen.count(atom)
get.charge(atom)
get.formal.charge(atom)
get.connected.atoms(atom, mol)
get.atom.index(atom, mol)
is.aromatic(atom)
is.aliphatic(atom)
is.in.ring(atom)
```

Arguments

| | |
|-------------------|---|
| <code>atom</code> | A <code>jobjRef</code> representing an <code>IAtom</code> object |
| <code>mol</code> | A <code>jobjRef</code> representing an <code>IAtomContainer</code> object |

Value

In the case of `get.point3d` the return value is a 3-element vector containing the X, Y and Z coordinates of the atom. If the atom does not have 3D coordinates, it returns a vector of the form `c(NA,NA,NA)`. Similarly for `get.point2d`, in which case the return vector is of length 2.

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

See Also

[get.atoms](#)

bpdata *Boiling Point Data*

Description

Structures and associated boiling points for 277 molecules, primarily alkanes and substituted alkanes.

Usage

bpdata

Format

A data.frame with two columns:

| | | | |
|------|--------|-----------|----------------------------|
| [,1] | SMILES | character | Structure in SMILES format |
| [,2] | BP | numeric | Boiling point in Kelvin |

The names of the molecules are used as the row names

References

Goll, E.S. and Jurs, P.C.; "Prediction of the Normal Boiling Points of Organic Compounds From Molecular Structures with a Computational Neural Network Model", *J. Chem. Inf. Comput. Sci.*, 1999, 39, 974-983.

cdk.version *Get Current CDK Version*

Description

Returns a string containing the version of the CDK used in this package

Usage

cdk.version()

Value

A string representing the CDK version

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

| | |
|------------------|---|
| cdkFormula-class | <i>Class cdkFormula, a class for handling molecular formula</i> |
|------------------|---|

Description

This class handles molecular formulae. It provides extra information such as the IMolecularFormula Java object, elements contained and number of them.

Objects from the Class

Objects can be created using new constructor and filled with a specific mass and window accuracy.

Note

No notes yet.

Author(s)

Miguel Rojas-Cherto (<miguelrojasch@yahoo.es>)

References

A parallel effort to expand the Chemistry Development Kit: <http://cdk.sourceforge.net>

See Also

[get.formula](#), [set.charge.formula](#), [get.isotopes.pattern](#), [isvalid.formula](#),

| | |
|----------------|---|
| do.aromaticity | <i>Perform Aromaticity Detection, atom typing or isotopic configuration</i> |
|----------------|---|

Description

These methods can be used to perform aromaticity detection, atom typing or isotopic configuration on a molecule object. In general, when molecules are loaded via [load.molecules](#) these are performed by default. If molecules are obtained via [parse.smiles](#) these operations are not performed and so the user should call one or both of these methods to correctly configure a molecule.

Usage

```
do.aromaticity(molecule)
do.typing(molecule)
do.isotopes(molecule)
```

Arguments

molecule The molecule on which the operation is to be performed. Should of class jobjRef with a jclass attribute of IAtomContainer

Value

No return value. If the operations fail an exception is thrown and an error message is printed

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

See Also

[load.molecules](#), [parse.smiles](#)

eval.atomic.desc *Evaluate an Atomic Descriptor*

Description

The CDK implements a number of descriptors divided into three main groups - atomic, molecular and bond. This method evaluates the specified atomic descriptor(s) for a molecule

Usage

```
eval.atomic.desc(molecule, which.desc, verbose=FALSE)
```

Arguments

molecule A reference to a CDK IAtomContainer object
which.desc The fully qualified class name of the descriptor to evaluate or a vector such names
verbose If TRUE, progress will be written to the screen, otherwise the function performs silently

Value

A data.frame is returned.

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

See Also

[get.atomic.desc.names](#) [get.desc.names](#) [eval.desc](#)

| | |
|-----------|--|
| eval.desc | <i>Evaluate a Molecular Descriptor</i> |
|-----------|--|

Description

The CDK implements a number of descriptors divided into three main groups - atomic, molecular and bond. This method evaluates the specified molecular descriptor(s) for a molecule

Usage

```
eval.desc(molecules, which.desc, verbose=FALSE)
```

Arguments

| | |
|------------|---|
| molecules | A single IAtomContainer object or a list of references to CDK IAtomContainer objects |
| which.desc | The fully qualified class name of the descriptor to evaluate or a vector such names |
| verbose | If TRUE, progress will be written to the screen, otherwise the function performs silently |

Value

A data.frame is returned. For a single molecule it will have one row, for multiple molecules it will have the number of rows equal to the number of molecules

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

See Also

[get.desc.names](#) [get.desc.categories](#)

Examples

```
smiles <- c('CCC', 'c1ccccc1', 'CC(=O)C')
mols <- sapply(smiles, parse.smiles)

dnames <- get.desc.names('topological')
descs <- eval.desc(mols, dnames, verbose=TRUE)
```

generate.2d.coordinates

Generate 2D Coordinates from Connectivity Information

Description

This function will generate reasonable 2D coordinates based purely on connectivity information.

Usage

```
generate.2d.coordinates(molecule)
```

Arguments

molecule An IAtomContainer object that can be obtained by loading them from disk or drawing them in the editor.

Value

Returns the input molecule with 2D coordinates added.

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

generate.formula

Generate a cdkFormula object.

Description

This function generate a list of cdkFormula objects given a mass.

Usage

```
generate.formula(mass, window=0.01, elements=list(c("C",0,50),c("H",0,50),
                                                c("N",0,50),c("O",0,50),
                                                c("S",0,50)),
                validation=FALSE, charge=0.0)
```

Arguments

mass The mass value from which to be generate the formulas.,
 window The window accuracy in the same units as mass.,
 elements Elements to take into account.,
 validation TRUE, if the method should only generate valid formulas. If FALSE, nonsensical formulae may be generated which must be filtered out by the user,
 charge The charge value of the formula.

Value

Objects of class MassToFormulaTool, from the IMolecularFormula package

Author(s)

Miguel Rojas-Cherto (<miguelrojasch@yahoo.es>)

See Also

[get.formula](#), [set.charge.formula](#), [get.isotopes.pattern](#), [isvalid.formula](#)

Examples

```
mfSet <- generate.formula(18.03383, charge=1,
                          elements=list(c("C", 0, 50), c("H", 0, 50), c("N", 0, 50)))
for (i in mfSet) {
  print(i)
}
```

get.atomic.desc.names *Get the names of the available atomic descriptors*

Description

The CDK implements a number of descriptors divided into three main groups - atomic, molecular and bond. This method returns the names of the available atomic descriptors.

Usage

```
get.atomic.desc.names(type = "all")
```

Arguments

| | |
|------|---|
| type | A string which can be one of "all", "topological", "geometrical", "hybrid", "constitutional", "electronic", allowing you to choose atomic descriptors of specific categories. The keyword "all" will return all available descriptors |
|------|---|

Value

A vector of fully qualified descriptor names.

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

See Also

[eval.atomic.desc](#) [get.desc.names](#) [eval.desc](#)

| | |
|-----------|--|
| get.atoms | <i>Get the atoms from a molecule or bond</i> |
|-----------|--|

Description

This function returns a list containing IAtom objects from a molecule or a bond.

Usage

```
get.atoms(object)
get.atom.count(molecule)
```

Arguments

| | |
|----------|---|
| object | A jobjRef representing an IAtomContainer, IMolecule or IBond object |
| molecule | A jobjRef representing an IAtomContainer |

Value

A list containing jobjRef's to a CDK IAtom object or else the number of atoms in the molecule

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

See Also

[get.bonds](#), [get.point3d](#), [get.symbol](#)

| | |
|-----------|--------------------------------------|
| get.bonds | <i>Get the bonds from a molecule</i> |
|-----------|--------------------------------------|

Description

This function returns a list containing IABond objects from a molecule

Usage

```
get.bonds(molecule)
```

Arguments

| | |
|----------|---|
| molecule | A jobjRef representing an IAtomContainer, IMolecule |
|----------|---|

Value

A list containing jobjRef's to a CDK IBond object

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

See Also

[get.atoms](#), [get.connected.atom](#),

`get.connected.atom` *Get the atom connected to an atom in a bond*

Description

This function returns the atom that is connected to a specified in a specified bond. Note that this function assumes 2-atom bonds, mainly because the CDK does not currently support other types of bonds

Usage

```
get.connected.atom(bond, atom)
```

Arguments

| | |
|-------------------|--|
| <code>bond</code> | A <code>jObjRef</code> representing an <code>IBond</code> object |
| <code>atom</code> | A <code>jObjRef</code> representing an <code>IAtom</code> object |

Value

A `jObjRef` representing an `IAtom` object

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

See Also

[get.atoms](#)

get.desc.categories *Get Descriptor Class Names*

Description

This function returns the broad descriptor categories that are available. Examples include topological, geometrical and so on. You can use a specific category to avoid calculating all descriptors for a set of molecules and saves you having to select individual descriptors by hand.

Usage

```
get.desc.categories()
```

Value

A character vector of descriptor category names

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

See Also

[eval.desc](#), [get.desc.names](#)

get.desc.names *Get Descriptor Class Names*

Description

The CDK implements a number of descriptors divided into three main groups - atomic, molecular and bond. Currently the package will only evaluate molecular descriptors. This function returns the class names of the available descriptors, which can then be used to calculate descriptors for a specific molecule.

By default all available descriptor class names are returned. However it is possible to specify that a subset of the descriptors should be considered. The subset is specified by keyword and can be one of: topological, geometrical, hybrid, constitutional, protein, electronic.

Usage

```
get.desc.names(type = "all")
```

Arguments

type Indicates which subset of molecular descriptors should be considered

Value

A character vector of descriptor class names

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

See Also

[eval.desc](#), [get.desc.categories](#)

get.fingerprint *Evaluate Fingerprints*

Description

This function evaluates fingerprints of a specified type for a set of molecules or a single molecule. Depending on the nature of the fingerprint, parameters can be specified. Currently five different fingerprints can be specified:

- standard - Considers paths of a given length. The default is but can be changed. These are hashed fingerprints, with a default length of 1024
- extended - Similar to the standard type, but takes rings and atomic properties into account into account
- graph - Similar to the standard type by simply considers connectivity
- hybridization - Similar to the standard type, but only consider hybridization state
- maccs - The popular 166 bit MACCS keys described by MDL
- estate - 79 bit fingerprints corresponding to the E-State atom types described by Hall and Kier
- pubchem - 881 bit fingerprints defined by PubChem
- kr - 4860 bit fingerprint defined by Klekota and Roth
- shortestpath - A fingerprint based on the shortest paths between pairs of atoms and takes into account ring systems, charges etc.
- signature - A feature,count type of fingerprint, similar in nature to circular fingerprints, but based on the signature descriptor
- circular - An implementation of the ECFP6 fingerprint

Depending on whether the input is a single IAtomContainer object, a list or single vector is returned. Each element of the list is an S4 object of class [fingerprint-class](#) or [featvec-class](#), which can be manipulated with the fingerprint package.

Usage

```
get.fingerprint(molecule, type = 'standard',  
                fp.mode = 'bit', depth=6, size=1024, verbose=FALSE)
```

Arguments

| | |
|----------|---|
| molecule | An IAtomContainer object that can be obtained by loading them from disk or drawing them in the editor. |
| type | The type of fingerprint. See description for possible values. The default is the standard binary fingerprint. |
| fp.mode | The type of fingerprint to return. Possible values are 'bit', 'raw', and 'count'. The 'raw' mode will return a feavec-class type of fingerprint, representing fragments and their count of occurrence in the molecule. The 'count' mode is similar, except that it returns hash values of fragments and their count of occurrence. While any of these values can be specified, a given fingerprint implementation may not implement all of them, and in those cases the return value is NULL. |
| depth | The search depth. This argument is ignored for the 'pubchem', 'maccs', 'kr' and 'estate' fingerprints |
| size | The length of the fingerprint bit string. This argument is ignored for the 'pubchem', 'maccs', 'kr', 'signature', 'circular' and 'estate' fingerprints |
| verbose | If TRUE, exceptions, if they occur, will be printed |

Value

Objects of class `fingerprint-class` or `feavec-class`, from the fingerprint package. If there is a problem during fingerprint calculation, NULL is returned.

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

References

Faulon et al, **The Signature Molecular Descriptor. 1. Using Extended Valence Sequences in QSAR and QSPR studies**, *J. Chem. Inf. Comput. Sci.*, 2003, 43, 707-720.

See Also

[load.molecules](#)

Examples

```
## get some molecules
sp <- get.smiles.parser()
smiles <- c('CCC', 'CCN', 'CCN(C)(C)', 'c1ccccc1Cc1ccccc1', 'C1CCC1CC(CN(C)(C))CC(=O)CC')
mols <- parse.smiles(smiles)

## get a single fingerprint using the standard
## (hashed, path based) fingerprinter
fp <- get.fingerprint(mols[[1]])

## get MACCS keys for all the molecules
```

```
fps <- lapply(mols, get.fingerprint, type='maccs')  
  
## get Signature fingerprint  
## feature, count fingerprint  
fps <- lapply(mols, get.fingerprint, type='signature', fp.mode='raw')
```

get.formula

Get the formula object from a formula character.

Description

This function returns a formula object containing mass, string character and isotopes when is given a character/string formula.

Usage

```
get.formula(mf, charge=0)
```

Arguments

mf A string containing the formula of the molecular formula of chemical object.
charge The charge of the molecular formula.

Value

Objects of class `cdkFormula`, from the `IMolecularFormula` package

Author(s)

Miguel Rojas-Cherto (<miguelrojasch@yahoo.es>)

References

A parallel effort to expand the Chemistry Development Kit: <http://cdk.sourceforge.net>

See Also

[set.charge.formula](#), [get.isotopes.pattern](#), [isvalid.formula](#), [generate.formula](#)

Examples

```
formula <- get.formula('NH4', charge = 1)  
formula
```

get.isotopes.pattern *Generate the isotope pattern.*

Description

This function get the isotope pattern given a cdkFormula object. It modifies as the IMolecularFormula Java object as the its mass.

Usage

```
get.isotopes.pattern(formula,minAbund=0.1)
```

Arguments

| | |
|----------|--|
| formula | A cdkFormula object. |
| minAbund | Minimal abundance of the isotopes to be added in the combinatorial search. |

Value

Objects of class IsotopePatternGenerator, from the IMolecularFormula package

Author(s)

Miguel Rojas-Cherto (<miguelrojasch@yahoo.es>)

References

A parallel effort to expand the Chemistry Development Kit: <http://cdk.sourceforge.net>

See Also

[get.formula](#), [set.charge.formula](#), [isvalid.formula](#), [generate.formula](#)

get.mol2formula *Parser a molecule to formula object.*

Description

This function convert a molecule object to a formula object.

Usage

```
get.mol2formula(molecule, charge=0)
```


Arguments

molecule The molecule to be parsed.,
charge The charge characterizing the molecule.,

Value

Objects of class MolecularFormulaManipulator, from the IMolecularFormulaManipulator package

Author(s)

Miguel Rojas-Cherto (<miguelrojasch@yahoo.es>)

See Also

[set.charge.formula](#), [get.isotopes.pattern](#), [isvalid.formula](#)

Examples

```
molecule <- parse.smiles("N")[[1]]  
convert.implicit.to.explicit(molecule)  
formula <- get.mol2formula(molecule, charge=0)
```

get.murcko.fragments *Molecule Fragmentation Methods*

Description

A variety of methods for fragmenting molecules are available ranging from exhaustive, rings to more specific methods such as Murcko frameworks. Fragmenting a collection of molecules can be a useful for a variety of analyses. In addition fragment based analysis can be a useful and faster alternative to traditional clustering of the whole collection, especially when it is large.

Note that exhaustive fragmentation of large molecules (with many single bonds) can become time consuming.

Usage

```
get.murcko.fragments(mols, min.frag.size = 6, as.smiles = TRUE, single.framework = FALSE)  
get.exhaustive.fragments(mols, min.frag.size = 6, as.smiles = TRUE)
```

Arguments

| | |
|------------------|--|
| mols | A molecule object or list of molecule objects. Each object should have a jclass of IAtomContainer |
| min.frag.size | The size of the smallest fragments to be considered |
| as.smiles | If TRUE, the fragments are returned as SMILES strings, otherwise as IAtomContainer objects |
| single.framework | If TRUE, then a single framework (i.e., the framework consisting of the union of all ring systems and linkers) is returned for each molecule. Otherwise, all combinations of ring systems and linkers are returned |

Value

get.murcko.fragments returns a list with each element being a list with two elements: rings and frameworks. Each of these elements is either a character vector of SMILES strings or a list of IAtomContainer objects. get.exhaustive.fragments returns a list of length equal to the number of input molecules. Each element is a character vector of SMILES strings or a list of IAtomContainer objects.

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

See Also

[load.molecules](#), [parse.smiles](#),

Examples

```
mol <- parse.smiles('c1ccc(cc1)CN(c2cc(ccc2[N+](=O)[O-])c3c(nc(nc3CC)N)N)C')[[1]]
mf1 <- get.murcko.fragments(mol, as.smiles=TRUE, single.framework=TRUE)
mf1 <- get.murcko.fragments(mol, as.smiles=TRUE, single.framework=FALSE)
```

get.properties

Get All Property Values of a Molecule

Description

Returns a list of all the properties of a molecule. The names of the list are set to the property names

Usage

```
get.properties(molecule)
```

Arguments

| | |
|----------|--|
| molecule | A Java object of class IAtomContainer or IMolecule |
|----------|--|

Value

A list of the property values, with names equal to the property names. NULL property values are returned as NA

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

See Also

[get.property](#), [set.property](#), [remove.property](#)

Examples

```
smiles <- 'c1ccccc1'
mol <- parse.smiles(smiles)[[1]]
set.property(mol, 'prop1', 23.45)
set.property(mol, 'prop2', 'inactive')
get.properties(mol)
```

get.property

Get the Value of a Molecule Property

Description

This function retrieves the value of a keyed property that has previously been set on the molecule.

The `get.title` function is simply a wrapper around `get.property` that directly provides access to the molecule title.

Usage

```
get.property(molecule, key)
get.title(molecule)
```

Arguments

| | |
|----------|---------------------------------------|
| molecule | A Java object of class IAtomContainer |
| key | A string naming the property |

Value

The value of the property is the key is found else NA. For `get.title`, the title of the molecule if available otherwise NA

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

See Also

[get.properties](#), [set.property](#), [remove.property](#)

Examples

```
smiles <- 'c1ccccc1'
mol <- parse.smiles(smiles)[[1]]
set.property(mol, 'prop1', 23.45)
set.property(mol, 'prop2', 'inactive')
get.property(mol, 'prop1')
```

get.smiles

Get the SMILES for a Molecule

Description

The function will generate a SMILES representation of an IAtomContainer object. The default parameters of the CDK SMILES generator are used. This can mean that for large ring systems the method may fail. See CDK Javadocs for more information

Usage

```
get.smiles(molecule, type = 'generic', aromatic = FALSE, atomClasses = FALSE)
```

Arguments

| | |
|-------------|---|
| molecule | A Java object of class IAtomContainer |
| type | The type of SMILES to output. Possible values are <ol style="list-style-type: none">1. generic - non-canonical SMILES string, different atom ordering produces different SMILES. No isotope or stereochemistry encoded.2. unique - canonical SMILES string, different atom ordering produces the same* SMILES. No isotope or stereochemistry encoded.3. isomeric - non-canonical SMILES string, different atom ordering produces different SMILES. Isotope and stereochemistry is encoded.4. absolute - canonical SMILES string, different atom ordering produces the same SMILES. Isotope and stereochemistry is encoded. |
| aromatic | If TRUE aromatic SMILES are generated. The default is to output Kekule form |
| atomClasses | If TRUE include atom classes. See CDK docs for more details |

Value

An R character object containing the SMILES

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

Examples

```
sp <- get.smiles.parser()
smiles <- c('CCC', 'CCN', 'CCN(C)(C)', 'c1ccccc1Cc1ccccc1', 'C1CCC1CC(CN(C)(C))CC(=O)CC')
mols <- parse.smiles(smiles)
```

get.smiles.parser *Get a SMILES Parser*

Description

This function returns a reference to a SMILES parser object. If you are parsing multiple SMILES strings, it is preferable to create your own parser and supply it to `parse.smiles` rather than forcing that function to instantiate a new parser for each call

Usage

```
get.smiles.parser()
```

Value

A jobjRef to a CDK SmilesParser object

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

See Also

[get.smiles](#), [get.smiles.parser](#), [view.molecule.2d](#)

get.total.charge *Get the Total Charges for the Molecule*

Description

`get.total.charge` returns the summed partial charges for a molecule and `get.total.formal.charge` returns the summed formal charges. Currently, if one or more partial charges are unset, the function simply returns the sum of formal charges (via `get.total.formal.charge`). This is slightly different from how the CDK evaluates the total charge of a molecule (via `AtomContainerManipulator.getTotalCharge()`), but is in line with how OEChem determines net charge on a molecule.

In general, you will want to use the `get.total.charge` function.

Usage

```
get.total.charge(molecule)
get.total.formal.charge(molecule)
```

Arguments

molecule A Java object of class IAtomContainer

Value

A double value indicating the total partial charge or total formal charge

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

`get.total.hydrogen.count`

Get the Total Hydrogen Count for a Molecule

Description

The function will return the summed implicit hydrogens of all atoms in the specified AtomContainer

Usage

```
get.total.hydrogen.count(molecule)
```

Arguments

molecule A Java object of class IAtomContainer

Value

An integer value indicating the number of implicit hydrogens

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

`get.tpsa`*Commonly Used Molecular Descriptors*

Description

These methods will return the value for the corresponding descriptors. While they can always be evaluated using [eval.desc](#), they are common enough that separate functions are provided.

Usage

```
get.tpsa(molecule)
get.alogp(molecule)
get.xlogp(molecule)
get.volume(molecule)
```

Arguments

`molecule` A `jObjRef` representing an `IAtomContainer` object

Details

It's important to note that ALogP and XLogP assumes that the molecule has explicit hydrogens. If the molecule is read from an SD file, explicit H's are usually present. On the other hand, if the molecule is obtained from a SMILES, explicit hydrogens must be added.

The molecular volume is calculated using a group contribution method rather than the an analytical method. This allows to avoid the use of 3D structures.

Value

Single numeric value representing TPSA, ALogP, XLogP or molecular volume.

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

See Also

[eval.desc](#)

| | |
|---------|---|
| hasNext | <i>Does This Iterator Have A Next Element</i> |
|---------|---|

Description

hasNext is a generic function that indicates if the iterator has another element.

Usage

```
hasNext(obj, ...)
```

```
## S3 method for class 'iloader.molecules'  
hasNext(obj, ...)
```

Arguments

| | |
|-----|--|
| obj | an iterator object. |
| ... | additional arguments that are ignored. |

Value

Logical value indicating whether the iterator has a next element. In the context of reading a structure file, this indicates whether there are more molecules to read

See Also

[iloader.molecules](#)

| | |
|--------------|---|
| is.connected | <i>Get the Largest Component in a Disconnected Molecule</i> |
|--------------|---|

Description

These methods allow one to check whether a molecule is fully connected or else retrieve the largest disconnected component

Usage

```
get.largest.component(mol)  
is.connected(mol)
```

Arguments

| | |
|-----|---|
| mol | A <code>jObjRef</code> representing an <code>IAtomContainer</code> object |
|-----|---|

Value

For `get.largest.component`, if the input molecule has more than one disconnected component, the largest is returned. Otherwise, the molecule itself is returned.

For `is.connected`, TRUE if the molecule is fully connected, FALSE otherwise

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

Examples

```
m <- parse.smiles("CC.CCCCC.CCCC")[[1]]
largest <- get.largest.component(m)
length(get.atoms(largest)) == 6
```

| | |
|-----------------|--------------------------------------|
| isvalid.formula | <i>Validate a cdkFormula object.</i> |
|-----------------|--------------------------------------|

Description

This function validates a `cdkFormula` object. At the moment is using the nitrogen Rule and RDBE Rule.

Usage

```
isvalid.formula(formula, rule = c("nitrogen", "RDBE"))
```

Arguments

| | |
|---------|---|
| formula | A <code>cdkFormula</code> object. |
| rule | The rules to be applied: nitrogen and RDBE. |

Value

Objects of class `MolecularFormulaChecker`, from the `IMolecularFormula` package

Author(s)

Miguel Rojas-Cherto (<miguelrojasch@yahoo.es>)

References

A parallel effort to expand the Chemistry Development Kit: <http://cdk.sourceforge.net>

See Also

[get.formula](#), [set.charge.formula](#), [get.isotopes.pattern](#), [generate.formula](#)

Examples

```
formula <- get.formula('NH4', charge = 0)
isvalid.formula(formula, rule = c("nitrogen", "RDBE"))
```

| | |
|----------------|--|
| load.molecules | <i>Load Molecular Structures From Disk</i> |
|----------------|--|

Description

The CDK can read a variety of molecular structure formats. This function encapsulates the calls to the CDK API to load a structure given its filename

Usage

```
load.molecules(molfiles=NA, aromaticity = TRUE, typing = TRUE, isotopes = TRUE,
               verbose=FALSE)
iload.molecules(molfile, type="smi", aromaticity = TRUE, typing = TRUE, isotopes = TRUE,
                skip=TRUE)
```

Arguments

| | |
|-------------|---|
| molfiles | A character vector of filenames. Note that the full path to the files should be provided. URL's can also be used as paths. In such a case, the URL should start with "http://" |
| molfile | A string containing the filename to load. Must be a local file |
| type | Indicates whether the input file is SMILES or SDF. Valid values are "smi" or "sdf" |
| aromaticity | If TRUE then aromaticity detection is performed on all loaded molecules. If this fails for a given molecule, then the molecule is set to NA in the return list |
| typing | If TRUE then atom typing is performed on all loaded molecules. The assigned types will be CDK internal types. If this fails for a given molecule, then the molecule is set to NA in the return list |
| isotopes | If TRUE then atoms are configured with isotopic masses |
| verbose | If TRUE, output (such as file download progress) will be bountiful |
| skip | If TRUE, then the reader will continue reading even when faced with an invalid molecule. If FALSE, the reader will stop at the fist invalid molecule |

Details

Note that if molecules are read in from formats that do not have rules for handling implicit hydrogens (such as MDL MOL), the molecule will not have implicit or explicit hydrogens. To add explicit hydrogens, make sure that the molecule has been typed (this is TRUE by default for this function) and then call `convert.implicit.to.explicit`. On the other hand for a format such as SMILES, implicit or explicit hydrogens will be present.

Value

`load.molecules` returns a list of CDK Molecule objects, which can be used in other rcdk functions.

`iload.molecules` is an iterating version of the loader and is applicable for large SMILES or SDF files. In contrast to `load.molecules` this does not load all the molecules into memory at one go, and as a result lets you process arbitrarily large structure files.

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

See Also

[view.molecule.2d](#), [convert.implicit.to.explicit](#)

Examples

```
## Not run:

## load a single file
amol <- load.molecules('foo.sdf')

## load multiple files
mols <- load.molecules(c('mol1.sdf', 'mol2.smi',
                        'https://github.com/rajarshi/cdkr/blob/master/data/set2/dhfr00008.sdf?raw=true'))

## iterate over a large file
moliter <- iload.molecules("big.sdf", type="sdf")
while(hasNext(moliter)) {
  mol <- nextElem(moliter)
  print(get.property(mol, "cdk:Title"))
}

## End(Not run)
```

matches

Perform Substructure Searching & MCS Detection

Description

These functions perform substructure searches of a query, specified in SMILES or SMARTS forms, over one or more target molecules and maximum common substructure searches for pairs of molecules.

Usage

```
matches(query, target, return.matches=FALSE)
is.subgraph(query, target)
get.mcs(mol1, mol2, as.molecule = TRUE)
```

Arguments

| | |
|----------------|--|
| query | A SMILES or SMARTS string |
| target | A single IAtomContainer object or a list of IAtomContainer objects |
| mol1 | An IAtomContainer |
| mol2 | An IAtomContainer |
| return.matches | If TRUE the lists of atom indices that correspond to the matching substructure are returned |
| as.molecule | If TRUE the MCS is returned as a new IAtomContainer object. Otherwise a atom index mapping between the two molecules is returned as a 2D array of integers |

Details

For the case of `is.subgraph`, the query molecule must be a single `IAtomContainer` or a valid SMILES string. Note that this method can be significantly faster than `matches`, but is limited by the fact that SMARTS patterns cannot be specified. This uses the "TurboSubStructure" SMSD method and so only searches for the first substructure match.

For MCS detection, the default SMSD algorithm is employed and the best scoring MCS is returned by default. Furthermore, one can obtain the resultant MCS either as an `IAtomContainer` in which the atoms and bonds are clones of the corresponding matching atoms and bonds in one of the molecule. Or else as a 2D array of dimensions $N \times 2$ of atom index mappings. Here N is the size of the MCS and the first column represents the atom index from the first molecule and the second column the atom index from the second molecule.

Note that since the CDK SMARTS matcher internally will perform aromaticity perception and atom typing, the target molecules need not have these operations done on them beforehand for `matches` method. However, if `is.subgraph` or `get.mcs` is being used, the molecules should have aromaticity detected and atom typing performed explicitly.

If the atom indices of the matching substructures (in the target molecule) are desired, use the `matches` function directly.

Value

For `matches` with `return.matches = FALSE`, a boolean vector where each element is TRUE or FALSE depending on whether the corresponding element in targets contains the query or not. If `return.matches = TRUE`, the return value is a list of lists. The number of elements of the top level list equals the number of matches. Each element is a list of two elements, named "match" and "mapping". The first element is TRUE if the query matched the target. If so, the second element is a list of numeric vectors, giving the atom indices (0-indexed) of the target atoms that matched the query. If there was no match for this target molecule, this element will be NULL.

For `is.subgraph`, a boolean vector, where each element is TRUE or FALSE depending on whether the corresponding element in targets contains the query or not.

For `get.mcs` an `IAtomContainer` object or a 2D array of atom index mappings between the two molecules.

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

See Also

[load.molecules](#), [get.smiles](#), [do.aromaticity](#), [do.typing](#), [do.isotopes](#)

Examples

```
smiles <- c('CCC', 'c1ccccc1', 'C(C)(C=O)C(CCNC)C1CC1C(=O)')
mols <- sapply(smiles, parse.smiles)
query <- '#6]=0'
doesMatch <- matches(query, mols)

## get mappings
mappings <- matches("CCC", mols, TRUE)
```

Molecule

Operations on molecules

Description

Various functions to perform operations on molecules.

`get.exact.mass` returns the exact mass of a molecule

`get.natural.mass` returns the natural exact mass of a molecule

`convert.implicit.explicit` converts implicit hydrogens to explicit hydrogens. This function does not return any value but rather modifies the molecule object passed to it

`is.neutral` returns TRUE if all atoms in the molecule have a formal charge of 0, otherwise FALSE

Usage

```
get.exact.mass(molecule)
get.natural.mass(molecule)
convert.implicit.to.explicit(molecule)
is.neutral(molecule)
```

Arguments

`molecule` A `jObjRef` representing an `IAtomContainer` or `IMolecule` object

Details

In some cases, a molecule may not have any hydrogens (such as when read in from an MDL MOL file that did not have hydrogens). In such cases, `convert.implicit.to.explicit` will add implicit hydrogens and then convert them to explicit ones. In addition, for such cases, make sure that the molecule has been typed beforehand.

Value

exact.mass returns a numeric
get.natural.mass returns a numeric
convert.implicit.to.explicit has no return value
is.neutral returns a boolean.

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

See Also

[get.atoms](#), [do.typing](#)

Examples

```
m <- parse.smiles('c1ccccc1')[[1]]

## Need to configure the molecule
do.aromaticity(m)
do.typing(m)
do.isotopes(m)

get.exact.mass(m)
get.natural.mass(m)

convert.implicit.to.explicit(m)
get.natural.mass(m)
do.isotopes(m) # Configure isotopes of newly added hydrogens
get.exact.mass(m)

is.neutral(m)
```

parse.smiles

Parse a Vector of SMILES Strings

Description

This function parses a vector of SMILES strings to generate a list of IAtomContainer objects. Note that the resultant molecule will not have any 2D or 3D coordinates.

Note that the molecules obtained from this method will not have any aromaticity perception, atom typing or isotopic configuration done on them. This is in contrast to the [load.molecules](#) method. Thus, you should perform these steps manually on the molecules.

Usage

```
parse.smiles(smiles, kekulise=TRUE)
```

Arguments

| | |
|----------|--|
| smiles | A SMILES string |
| kekulise | If set to FALSE disables electron checking and allows for parsing of incorrect SMILES. If a SMILES does not parse by default, try setting this to FALSE - though the resultant molecule may not have consistent bonding. As an example, <chem>c4ccc2c(cc1=Nc3ncccc3(Cn12))c4</chem> will not be parsed by default because it is missing a nitrogen. With this argument set to FALSE it will parse successfully, but this is a hack to handle an incorrect SMILES |

Value

A list of jobjRefs to their corresponding CDK IAtomContainer objects. If a SMILES string could not be parsed, NA is returned instead.

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

See Also

[load.molecules](#), [get.smiles](#), [get.smiles.parser](#), [view.molecule.2d](#), [do.aromaticity](#), [do.typing](#), [do.isotopes](#)

Examples

```
smiles <- c('CCC', 'c1ccccc1', 'C(C)(C=O)C(CCNC)C1CC1C(=O)')
mol <- parse.smiles(smiles[1])
mols <- parse.smiles(smiles)
```

| | |
|------------------|---|
| remove.hydrogens | <i>Remove Hydrogens from a Molecule</i> |
|------------------|---|

Description

This function generate a new IAtomContainer object in which the hydrogens have been removed. This can be useful for descriptor calculations.

Usage

```
remove.hydrogens(molecule)
```

Arguments

| | |
|----------|---------------------------------------|
| molecule | A Java object of class IAtomContainer |
|----------|---------------------------------------|

Value

A jobref that refers to a IAtomContainer object

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

remove.property *Remove A Property From a Molecule*

Description

This function removes a keyed property from a molecule object. This deletes the key and its value from the molecule

Usage

```
remove.property(molecule, key)
```

Arguments

| | |
|----------|---------------------------------------|
| molecule | A Java object of class IAtomContainer |
| key | A string naming the property |

Value

None

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

See Also

[get.property](#), [set.property](#)

set.charge.formula *Set the charge to a cdkFormula object.*

Description

This function set the charge to a cdkFormula object. It modifies as the IMolecularFormula Java object as the its mass.

Usage

```
set.charge.formula(formula, charge=-1)
```


Arguments

| | |
|---------|---------------------------------|
| formula | A cdkFormula object. |
| charge | The value of the charge to set. |

Value

Returns the formula object with the specified charge

Author(s)

Miguel Rojas-Cherto (<miguelrojasch@yahoo.es>)

References

A parallel effort to expand the Chemistry Development Kit: <http://cdk.sourceforge.net>

See Also

[get.formula](#), [get.isotopes.pattern](#), [invalid.formula](#), [generate.formula](#)

set.property

Set A Property On A Molecule

Description

This function allows one to add a keyed property to a molecule. The key must be a string, but the value can be string, numeric or even an arbitrary Java object (of class `jobjRef`)

Usage

```
set.property(molecule, key, value)
```

Arguments

| | |
|----------|--|
| molecule | A Java object of class <code>IAtomContainer</code> |
| key | A string naming the property |
| value | The value of the property. This can be character, integer, double or of class <code>jobjRef</code> |

Value

None

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

See Also

[get.property](#), [get.properties](#), [remove.property](#)

Examples

```
smiles <- 'c1ccccc1'
mol <- parse.smiles(smiles)[[1]]
set.property(mol, 'prop1', 23.45)
set.property(mol, 'prop2', 'inactive')
get.properties(mol)
```

view.molecule.2d

View and Copy 2D Structure Diagrams

Description

The CDK is capable of generating 2D structure diagrams. These methods allow one to view 2D structure diagrams. Depending on the method called a Swing JFrame is displayed which allows resizing of the image or a raster image (derived from a PNG byte stream) is returned, which can be viewed using [rasterImage](#). It is also possible to copy a 2D depiction to the system clipboard, which can then be pasted into various external applications.

Usage

```
view.molecule.2d(molecule, ncol = 4, cellx = 200, celly = 200)
view.image.2d(molecule, width = 200, height = 200)
copy.image.to.clipboard(molecule, width = 200, height = 200)
```

Arguments

| | |
|----------|---|
| molecule | If a single molecule is to be viewed this should be a reference to a IAtomContainer object. If multiple molecules are to be viewed this should be a list of such objects. If a character is specified then it is taken as the name of a file and the molecules are loaded from the file |
| ncol | The number of columns if a grid is desired |
| cellx | The width of the grid cells |
| celly | The height of the grid cells |
| width | The width of the image |
| height | The height of the image |

Details

For the case of `view.molecule.2d`, if a `jobjRef` is passed it should be a reference to an `IAtomContainer` object. In case the first argument is of class character it is assumed to be a file and is loaded by the function.

This function can be used to view a single molecule or multiple molecules. If a list of molecule objects is supplied the molecules are displayed as a grid of 2D viewers. In case a file is specified, it will display a single molecule or multiple molecules depending on how many molecules are loaded.

For `view.image.2d`, the image can be viewed via [rasterImage](#).

`copy.image.to.clipboard` copies the 2D depiction to the system clipboard in PNG format. You can then paste into other applications.

Due to event handling issues, the depiction will show on OS X, but the window will be unresponsive. Also copying images to the clipboard will not work. As a result, on OS X we make use of a standalone helper that is run via the system command. Currently, this is supported for the `view.molecule.2d` method (for a single molecule) and the `copy.image.to.clipboard` method. In the future, other view methods will also be accessible via this mechanism. While this allows OS X users to view molecules, it is slow due to invoking a new process.

The depictions will work fine (i.e., no need to shell out) on Linux and Windows.

Value

`view.molecule.2d` and `copy.image.to.clipboard` do not return anything. `view.image.2d` returns an array of the dimensions height x width x channels, from the original PNG version of the 2D depiction.

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

See Also

[view.table](#), [rasterImage](#), [link{readPNG}](#)

Examples

```
m <- parse.smiles('c1cccc1C(=O)NC')[[1]]
## Not run:
img <- view.image.2d(m, 100,100)
plot(1:10, 1:10, pch=19)
rasterImage(img, 0,8, 2,10)

## End(Not run)
```

view.table

*View 2D Structures With Data***Description**

The CDK is capable of generating 2D structure diagrams. This function can be used to view a set of molecules along with some associated data. The format of the output is a table, where the first column are the 2D images of the molecules, followed by the data columns.

Usage

```
view.table(molecules, dat, cellx = 200, celly = 200)
```

Arguments

| | |
|-----------|--|
| molecules | A list of jobRef objects that represent IAtomContainer |
| dat | A data.frame containing numeric or character columns. If columns are named they will be used in the data table. If not, names are autogenerated. The number of rows of the data.frame should be equal to the number of molecules |
| cellx | Initial width of the table cells |
| celly | Initial height of the table cells |

Details

Due to event handling issues, the depiction will show on OS X, but the window will be unresponsive. The depictions will work fine on Linux and Windows.

Value

Nothing

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

See Also

[view.molecule.2d](#)

Examples

```
smiles <- c('CCC', 'CCN', 'CCN(C)(C)',
           'c1ccccc1Cc1ccccc1',
           'C1CCC1CC(CN(C)(C))CC(=O)CC')
mols <- parse.smiles(smiles)
dframe <- data.frame(x = runif(4),
                    toxicity = factor(c('Toxic', 'Toxic', 'Nontoxic', 'Nontoxic')),
                    solubility = c('yes', 'yes', 'no', 'yes'))
## Not run: view.table(mols[1:4], dframe)
```

| | |
|-----------------|--------------------------------|
| write.molecules | <i>Write Molecules To Disk</i> |
|-----------------|--------------------------------|

Description

This function writes one or more molecules to an SD file on disk, which can be of the single- or multi-molecule variety. In addition, if the molecule has keyed properties, they can also be written out as SD tags.

Usage

```
write.molecules(mols, filename, together=TRUE, write.props=FALSE)
```

Arguments

| | |
|-------------|---|
| mols | A list of Java objects of class IAtomContainer |
| filename | The name of the SD file to write. Note that if together is FALSE then this argument is taken as a prefix for the name of the individual files |
| together | If TRUE then all the molecules are written to a single SD file. If FALSE each molecule is written to an individual file |
| write.props | Should keyed properties be included in the SD file output |

Details

This function can be used to write a single SD file containing multiple molecules. In case individual SD files are desired the together argument can be set to FALSE. In this case, the value of filename is used as a prefix, to which a numeric identifier and the suffix of ".sdf" is appended. In case, a single molecule is to be written to disk, simply specify the filename and use the default value of together

Value

The value of the property

Author(s)

Rajarshi Guha (<rajarshi.guha@gmail.com>)

See Also

[load.molecules](#), [set.property](#), [get.property](#), [remove.property](#)

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