

# Package ‘ChemmineR’

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**Type** Package

**Title** Cheminformatics Toolkit for R

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**Description** ChemmineR is a cheminformatics package for analyzing drug-like small molecule data in R. Its latest version contains functions for efficient processing of large numbers of molecules, physicochemical/structural property predictions, structural similarity searching, classification and clustering of compound libraries with a wide spectrum of algorithms. In addition, it offers visualization functions for compound clustering results and chemical structures.

**License** Artistic-2.0

**Depends** R (>= 2.10.0), methods

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

**Imports** rjson, graphics, stats, RCurl, DBI, digest, BiocGenerics, Rcpp (>= 0.11.0), ggplot2, grid, gridExtra, png, base64enc, DT, rsvg, jsonlite, stringi

**Suggests** RSQLite, scatterplot3d, gplots, fmcsR, snow, RPostgreSQL, BiocStyle, knitr, knitcitations, knitrBootstrap, ChemmineDrugs, png, rmarkdown, BiocManager, bibtex

**Enhances** ChemmineOB

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

**VignetteBuilder** knitr

**LinkingTo** Rcpp, BH

**SystemRequirements** GNU make

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## R topics documented:

|                              |    |
|------------------------------|----|
| addDescriptorType . . . . .  | 5  |
| addNewFeatures . . . . .     | 5  |
| ap . . . . .                 | 6  |
| AP-class . . . . .           | 8  |
| apfp . . . . .               | 9  |
| apset . . . . .              | 10 |
| APset-class . . . . .        | 11 |
| apset2descdb . . . . .       | 12 |
| atomblock . . . . .          | 14 |
| atomcount . . . . .          | 15 |
| atomprop . . . . .           | 17 |
| atomssubset . . . . .        | 17 |
| batchByIndex . . . . .       | 19 |
| bondblock . . . . .          | 20 |
| bonds . . . . .              | 21 |
| browseJob . . . . .          | 22 |
| bufferLines . . . . .        | 23 |
| bufferResultSet . . . . .    | 24 |
| byCluster . . . . .          | 25 |
| canonicalize . . . . .       | 26 |
| canonicalNumbering . . . . . | 27 |
| cid . . . . .                | 28 |
| cluster.sizestat . . . . .   | 29 |
| cluster.visualize . . . . .  | 30 |
| cmp.cluster . . . . .        | 32 |
| cmp.duplicated . . . . .     | 34 |
| cmp.parse . . . . .          | 36 |
| cmp.parse1 . . . . .         | 37 |
| cmp.search . . . . .         | 38 |
| cmp.similarity . . . . .     | 40 |
| conMA . . . . .              | 42 |
| connections . . . . .        | 43 |
| datablock . . . . .          | 44 |
| datablock2ma . . . . .       | 45 |
| db.explain . . . . .         | 46 |
| db.subset . . . . .          | 47 |
| dbTransaction . . . . .      | 48 |
| desc2fp . . . . .            | 49 |
| draw_sdf . . . . .           | 50 |
| exactMassOB . . . . .        | 52 |

|                     |     |
|---------------------|-----|
| ExtSDF-class        | 53  |
| findCompounds       | 54  |
| findCompoundsByName | 55  |
| fingerprintOB       | 56  |
| fold                | 57  |
| foldCount           | 57  |
| FP-class            | 58  |
| fp2bit              | 59  |
| FPset-class         | 61  |
| fpSim               | 62  |
| fptype              | 65  |
| fromNNMatrix        | 65  |
| genAPDescriptors    | 66  |
| generate3DCoords    | 67  |
| genParameters       | 68  |
| getAllCompoundIds   | 69  |
| getAtomAttr         | 70  |
| getBondAttr         | 71  |
| getCompoundFeatures | 71  |
| getCompoundNames    | 73  |
| getCompounds        | 74  |
| getIds-deprecated   | 75  |
| grepSDFset          | 76  |
| groups              | 77  |
| header              | 78  |
| initDb              | 79  |
| jarvisPatrick       | 80  |
| jarvisPatrick_c     | 82  |
| jobToken-class      | 83  |
| largestComponent    | 84  |
| launchCMTool        | 84  |
| listCMTools         | 86  |
| listFeatures        | 87  |
| loadSdf             | 88  |
| makeUnique          | 90  |
| maximallyDissimilar | 91  |
| nearestNeighbors    | 92  |
| numBits             | 93  |
| obmol               | 94  |
| openBabelPlot       | 95  |
| parBatchByIndex     | 96  |
| plotStruc           | 97  |
| propOB              | 99  |
| pubchemCidToSDF     | 100 |
| pubchemFPencoding   | 101 |
| pubchemInchi2cid    | 101 |
| pubchemInchikey2sdf | 102 |
| pubchemName2CID     | 103 |

|                         |     |
|-------------------------|-----|
| pubchemSDFSearch        | 104 |
| pubchemSmilesSearch     | 105 |
| read.AP                 | 106 |
| read.SDFindex           | 107 |
| read.SDFset             | 109 |
| read.SDFstr             | 110 |
| read.SMIset             | 111 |
| regenerateCoords        | 112 |
| result                  | 113 |
| rings                   | 114 |
| SDF-class               | 116 |
| sdf.subset              | 118 |
| sdf.visualize           | 119 |
| sdf2ap                  | 120 |
| SDF2apcmp               | 121 |
| sdf2list                | 122 |
| sdf2smiles              | 123 |
| sdf2str                 | 124 |
| SDFDataTable            | 125 |
| sdfid                   | 126 |
| sdfsamples              | 127 |
| SDFset-class            | 128 |
| SDFset2list             | 130 |
| SDFset2SDF              | 132 |
| SDFstr-class            | 133 |
| sdfstr2list             | 134 |
| sdfStream               | 135 |
| searchSim-deprecated    | 137 |
| searchString-deprecated | 138 |
| selectInBatches         | 139 |
| setPriorities           | 140 |
| smartsSearchOB          | 141 |
| SMI-class               | 142 |
| smiles2sdf              | 143 |
| smisamples              | 144 |
| SMIset-class            | 145 |
| status                  | 146 |
| toolDetails             | 147 |
| trimNeighbors           | 148 |
| validSDF                | 149 |
| view                    | 150 |
| write.SDF               | 151 |
| write.SDFsplit          | 152 |
| write.SMI               | 153 |

---

|                   |                            |
|-------------------|----------------------------|
| addDescriptorType | <i>Add Descriptor Type</i> |
|-------------------|----------------------------|

---

**Description**

Add a new descriptor type to the database. Normally descriptor types are added as needed, but if you are doing a parrallel data load you must pre-load the descriptor type to prevent duplicate defintion errors.

**Usage**

```
addDescriptorType(conn, descriptorType)
```

**Arguments**

|                |                                 |
|----------------|---------------------------------|
| conn           | Any database connection object. |
| descriptorType | The name of the descriptor.     |

**Value**

No return value.

**Author(s)**

Kevin Horan

**Examples**

```
## Not run:  
conn = initDb(...)  
addDescriptor(conn, "fp")  
  
## End(Not run)
```

---

|                |                         |
|----------------|-------------------------|
| addNewFeatures | <i>Add New Features</i> |
|----------------|-------------------------|

---

**Description**

Adds new features to a database without adding any data. Note that if you are loading new data anyway, it is much more efficient to use the loadSdf function and include the new features then. This function will have to read all compounds out of the database first.

**Usage**

```
addNewFeatures(conn, featureGenerator)
```

### Arguments

`conn` A database connection object, such as is returned by [initDb](#).  
`featureGenerator` A function which returns a data frame containing the new features. It may also contain features which are already in the database, these will simply be ignored. See the description of `fct` in [loadSdf](#) for details.

### Value

No value is returned.

### Author(s)

Kevin Horan

### See Also

[loadSdf](#)

### Examples

```
#create and initialize a new SQLite database
conn = initDb("test.db")

data(sdfsampl)

#just load the data with no features or descriptors
ids=loadSdf(conn,sdfsampl)
  addNewFeatures(conn, function(sdfset)
data.frame(MW = MW(sdfset),
            rings(sdfset,type="count",upper=6, arom=TRUE))
)

unlink("test.db")
```

---

ap

*Return atom pair component of AP/APset*

---

### Description

Returns atom pair component of objects of class AP or APset as list of vectors.

### Usage

`ap(x)`

**Arguments**

x                    Object of class AP and APset

**Details**

...

**Value**

List                with one to many of following components:  
numeric            atom pairs

**Author(s)**

Thomas Girke

**References**

Chen X and Reynolds CH (2002). "Performance of similarity measures in 2D fragment-based similarity searching: comparison of structural descriptors and similarity coefficients", J Chem Inf Comput Sci.

**See Also**

Functions: SDF2apcmp, apset2descdb, cmp.search, cmp.similarity

**Examples**

```
## Instance of SDFset class
data(sdfsampl)
sdfset <- sdfsampl[1:50]
sdf <- sdfset[[1]]

## Compute atom pair library
ap <- sdf2ap(sdf)
(apset <- sdf2ap(sdfset))
view(apset[1:4])

## Return main components of APset object
cid(apset[1:4]) # compound IDs
ap(apset[1:4]) # atom pair descriptors

## Return atom pairs in human readable format
db.explain(apset[1])
```

---

AP-class

Class "AP"

---

### Description

Container for storing the atom pair descriptors of a single compound as numeric vector. The atom pairs are used as structural similarity measures and for compound similarity searching.

### Objects from the Class

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

### Slots

AP: Object of class "numeric"

### Methods

**ap** signature(x = "AP"): returns atom pairs as numeric vector

**coerce** signature(from = "APset", to = "AP"): as(apset, "AP")

**show** signature(object = "AP"): prints summary of AP

### Author(s)

Thomas Girke

### References

Chen X and Reynolds CH (2002). "Performance of similarity measures in 2D fragment-based similarity searching: comparison of structural descriptors and similarity coefficients", J Chem Inf Comput Sci.

### See Also

Related classes: SDF, SDFset, SDFstr, APset.

Functions: SDF2apcmp, apset2descdb, cmp.search, cmp.similarity

### Examples

```
showClass("AP")

## Instance of SDFset class
data(sdfsampl)
sdfset <- sdfsampl[1:50]
sdf <- sdfsampl[[1]]

## Compute atom pair library
ap <- sdf2ap(sdf)
```



```
(apset <- sdf2ap(sdfset))
view(apset[1:4])

## Return main components of APset object
cid(apset[1:4]) # compound IDs
ap(apset[1:4]) # atom pair descriptors

## Return atom pairs in human readable format
db.explain(apset[1])

## Coerce APset to other objects
apset2descdb(apset) # returns old list-style AP database
tmp <- as(apset, "list") # returns list
as(tmp, "APset") # convert list back to APset

## Compound similarity searching with APset
cmp.search(apset, apset[1], type=3, cutoff=0.2)
plot(sdfset[names(cmp.search(apset, apset[6], type=2, cutoff=0.4))])

## Identify compounds with identical AP sets
cmp.duplicated(apset, type=2)

## Structure similarity clustering
cmp.cluster(db=apset, cutoff = c(0.65, 0.5))[1:20,]
```

---

apfp

*Frequent Atom Pairs*

---

## Description

Ranked set of 4096 most frequent atom pairs observed in the compound collection from DrugBank with a MW < 1000. Their atom pairs were generated with the `sdf2ap` function. The provided data frame is sorted row-wise by atom pair frequency and only the 4096 most frequent atom pairs are included. This data set can be used as predefined atom pair selection when computing atom pair fingerprints with the `desc2fp` function.

## Usage

```
data(apfp)
```

## Format

Object of class `data.frame`. First column contains atom pair (AP) IDs and the second column their frequency in DrugBank compounds.

## Details

Object stores 4096 most frequent atom pairs generated from DrugBank compounds.

**Source**

DrugBank: <http://www.drugbank.ca/>

**References**

Chen X and Reynolds CH (2002). "Performance of similarity measures in 2D fragment-based similarity searching: comparison of structural descriptors and similarity coefficients", J Chem Inf Comput Sci.

**Examples**

```
data(apfp)
apfp[1:4,]
```

---

apset

*Atom pairs stored in APset object*

---

**Description**

Atom pairs for 100 molecules stored in sdfsample.

**Usage**

```
data(apset)
```

**Format**

Object of class apset

**Details**

Object stores atom pairs of 100 molecules.

**Source**

```
apset <- sdf2ap(sdfsample)
```

**References**

Chen X and Reynolds CH (2002). "Performance of similarity measures in 2D fragment-based similarity searching: comparison of structural descriptors and similarity coefficients", J Chem Inf Comput Sci.

**Examples**

```
data(apset)
apset[1:4]
view(apset[1:4])
```

---

APset-class

Class "APset"

---

### Description

List-like container for storing the atom pair descriptors of a many compounds as objects of class AP. This container is used for structure similarity searching of compounds.

### Objects from the Class

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

### Slots

AP: Object of class "list"

ID: Object of class "character"

### Methods

[ signature(x = "APset"): subsetting of class with bracket operator

[[ signature(x = "APset"): returns single component as AP object

[<- signature(x = "APset"): replacement method for single AP component

[<- signature(x = "APset"): replacement method for several AP components

**ap** signature(x = "APset"): returns atom pair list from AP slot

**c** signature(x = "APset"): concatenates two APset containers

**cid** signature(x = "APset"): returns all compound identifiers from ID slot

**cid<-** signature(x = "APset"): replacement method for compound identifiers in ID slot

**coerce** signature(from = "APset", to = "AP"): as(apset, "AP")

**coerce** signature(from = "APset", to = "list"): as(apset, "list")

**coerce** signature(from = "list", to = "APset"): as(list, "APset")

**length** signature(x = "APset"): returns number of entries stored in object

**show** signature(object = "APset"): prints summary of APset

**view** signature(x = "APset"): prints extended summary of APset

### Author(s)

Thomas Girke

### References

Chen X and Reynolds CH (2002). "Performance of similarity measures in 2D fragment-based similarity searching: comparison of structural descriptors and similarity coefficients", in J Chem Inf Comput Sci.

**See Also**

Related classes: SDF, SDFset, SDFstr, AP, FPset, FP.

Functions: SDF2apcmp, apset2descdb, cmp.search, cmp.similarity

**Examples**

```
showClass("APset")

## Instance of SDFset class
data(sdfsampl)
sdfset <- sdfsampl[1:50]
sdf <- sdfsampl[[1]]

## Compute atom pair library
ap <- sdf2ap(sdf)
(apset <- sdf2ap(sdfset))
view(apset[1:4])

## Return main components of APset object
cid(apset[1:4]) # compound IDs
ap(apset[1:4]) # atom pair descriptors

## Return atom pairs in human readable format
db.explain(apset[1])

## Coerce APset to other objects
apset2descdb(apset) # returns old list-style AP database
tmp <- as(apset, "list") # returns list
as(tmp, "APset") # convert list back to APset

## Compound similarity searching with APset
cmp.search(apset, apset[1], type=3, cutoff=0.2)
plot(sdfset[names(cmp.search(apset, apset[6], type=2, cutoff=0.4))])

## Identify compounds with identical AP sets
cmp.duplicated(apset, type=2)

## Structure similarity clustering
cmp.cluster(db=apset, cutoff = c(0.65, 0.5))[1:20,]
```

---

apset2descdb

APset to list-style AP database

---

**Description**

Coerces APset to old list-style descriptor database used by search/cluster functions.

**Usage**

```
apset2descdb(apset)
```

**Arguments**

apset            Object of class apset

**Details**

...

**Value**

|         |   |
|---------|---|
| list    | with following components   |
| descdb  | list of atom pair sets  |
| cids    | compound IDs  |
| sdfsegs | start/end coordinates for each molecule in SD file; only populated when <code>cmp.parse</code> is used for import |
| source  | path/name of SD file  |
| type    | import method   |

**Author(s)**

Thomas Girke

**References**

Chen X and Reynolds CH (2002). "Performance of similarity measures in 2D fragment-based similarity searching: comparison of structural descriptors and similarity coefficients", J Chem Inf Comput Sci.

**See Also**

Functions: `SDF2apcmp`, `sdf2ap`, `cmp.search`, `cmp.similarity`

**Examples**

```
## Instance of SDFset class
data(sdfsampl)
sdfset <- sdfsampl[1:50]
sdf <- sdfsampl[[1]]

## Compute atom pair library
ap <- sdf2ap(sdf)
(apset <- sdf2ap(sdfset))
view(apset[1:4])

## Return main components of APset object
cid(apset[1:4]) # compound IDs
```

```
ap(apset[1:4]) # atom pair descriptors

## Return atom pairs in human readable format
db.explain(apset[1])

## Coerce APset to other objects
apset2descdb(apset) # returns old list-style AP database
tmp <- as(apset, "list") # returns list
as(tmp, "APset") # convert list back to APset

## Compound similarity searching with APset
cmp.search(apset, apset[1], type=3, cutoff=0.2)
plot(sdfset[names(cmp.search(apset, apset[6], type=2, cutoff=0.4))])

## Identify compounds with identical AP sets
cmp.duplicated(apset, type=2)

## Structure similarity clustering
cmp.cluster(db=apset, cutoff = c(0.65, 0.5))[1:20,]
```

---

atomblock

*Return atom block*

---

## Description

Returns atom block(s) from an object of class SDF or SDFset.

## Usage

```
atomblock(x)
```

## Arguments

x                    object of class SDF or SDFset

## Details

...

## Value

matrix if SDF is provided or list of matrices if SDFset is provided

## Author(s)

Thomas Girke

## References

...

**See Also**

header, atomcount, bondblock, datablock, cid, sdfid

**Examples**

```
## SDF/SDFset instances
data(sdfsample)
sdfset <- sdfsample
sdf <- sdfset[[1]]

## Extract atome block
atomblock(sdf)
atomblock(sdfset[1:4])

## Replacement methods
sdfset[[1]][[2]][1,1] <- 999
sdfset[[1]]
atomblock(sdfset)[1:2] <- atomblock(sdfset)[3:4]
atomblock(sdfset[[1]]) == atomblock(sdfset[[3]])
view(sdfset[1:2])
```

---

atomcount

*Molecular property functions*

---

**Description**

Functions to compute molecular properties: weight, formula, atom frequencies, etc.

**Usage**

```
atomcount(x, addH = FALSE, ...)
```

```
atomcountMA(x, ...)
```

```
MW(x, mw=atomprop, ...)
```

```
MF(x, ...)
```

**Arguments**

|      |  |
|------|--|
| x    | object of class SDFset or SDF  |
| mw   | data.frame with atomic weights; imported by default with data(atomprop); supports custom data sets                   |
| addH | 'addH = TRUE' should be passed on to any of these function to add hydrogens that are often not specified in SD files |
| ...  | Arguments to be passed to/from other methods.  |

**Details**

...

**Value**

|              |             |
|--------------|-------------|
| named vector | MW and MF   |
| list         | atomcount   |
| matrix       | atomcountMA |

**Author(s)**

Thomas Girke

**References**Standard atomic weights (2005) from: <http://iupac.org/publications/pac/78/11/2051/>**See Also**

Functions: datablock, datablocktag

**Examples**

```
## Instance of SDFset class
data(sdfsampl)
sdfset <- sdfsampl

## Compute properties; to consider missing hydrogens, set 'addH = TRUE'
MW(sdfset[1:4], addH = FALSE)
MF(sdfset[1:4], addH = FALSE)
atomcount(sdfset[1:4], addH = FALSE)
propma <- atomcountMA(sdfset[1:4], addH = FALSE)
boxplot(propma, main="Atom Frequency")

## Example for injecting a custom matrix/data frame into the data block of an
## SDFset and then writing it to an SD file
props <- data.frame(MF=MF(sdfset), MW=MW(sdfset), atomcountMA(sdfset))
datablock(sdfset) <- props
view(sdfset[1:4])
# write.SDF(sdfset[1:4], file="sub.sdf", sig=TRUE, cid=TRUE)
```



---

|          |                                |
|----------|--------------------------------|
| atomprop | <i>Standard atomic weights</i> |
|----------|--------------------------------|

---

**Description**

Data frame with atom names, symbols, standard atomic weights, group number and period number.

**Usage**

```
data(atomprop)
```

**Format**

The format is a data frame with 117 rows and 6 columns.

**Source**

Columns 1 to 4 from: <http://iupac.org/publications/pac/78/11/2051/> Columns 5 to 6 from: [http://en.wikipedia.org/wiki/List\\_of\\_elements](http://en.wikipedia.org/wiki/List_of_elements)

**References**

Pure Appl. Chem., 2006, Vol. 78, No. 11, pp. 2051-2066

**Examples**

```
data(atomprop)
atomprop[1:4,]
```

---

|             |   |
|-------------|---|
| atomssubset | <i>Subset SDF/SDFset Objects by Atom Index to Obtain Substructure</i> |
|-------------|---|

---

**Description**

Function to obtain a substructure from SDF/SDFset objects by providing a row index for the atom block in an SDF referencing the atoms of interest. The function subsets both the atom and bond block(s) accordingly.

**Usage**

```
atomssubset(x, atomrows, type="new", datablock = FALSE)
```

**Arguments**

|           |   |
|-----------|---|
| x         | object of class SDFset or SDF   |
| atomrows  | The argument atomrows can be assigned a numeric index referencing the atoms in the atom block of x. If x is of class SDF, the index needs to be provided as vector. If x is of class SDFset, the same number of index vectors as molecules stored in x need to be passed on in a list with component names identical to the component (molecule) names stored in x. |
| type      | The argument type="new" assigns new atom numbers to a subsetted SDF, while type="old" maintains the numbering of the source SDF.  |
| datablock | By default the data block(s) in SDF/SDFset objects are removed after atom subsetting. The setting datablock=TRUE will maintain the data block information in the subsetted result.  |

**Details**

...

**Value**

object of class SDF or SDFset

**Author(s)**

Thomas Girke

**References**

...

**See Also**

...

**Examples**

```
## Instance of SDFset class
data(sdfsampl)
sdfset <- sdfsampl

## Subset one or more molecules with atom index(es) to obtain substructure(s)
atomssubset(sdfset[[1]], atomrows=1:18)
indexlist <- list(1:18, 1:12)
names(indexlist) <- cid(sdfset[1:2])
atomssubset(sdfset[1:2], atomrows=indexlist)
```

---

|              |                       |
|--------------|-----------------------|
| batchByIndex | <i>Batch by Index</i> |
|--------------|-----------------------|

---

### Description

When doing a select where the condition is a large number of ids it is not always possible to include them in a single SQL statement. This function will break the list of ids into chunks and allow the indexProcessor to deal with just a small number of ids.

### Usage

```
batchByIndex(allIndices, indexProcessor, batchSize = 1e+05)
```

### Arguments

|                |  |
|----------------|--|
| allIndices     | A vector of values that will be broken into batches and passed as an argument to the indexProcessor function.  |
| indexProcessor | A function that takes one batch of indices. It is called once for each batch. The return value from this function is ignored. To accumulate results you can write to a global variable using the "<<-" operator. |
| batchSize      | The size of each batch. The last batch may be smaller than this value.   |

### Value

No value is returned.

### Author(s)

Kevin Horan

### See Also

[parBatchByIndex](#)

### Examples

```
## Not run:
result=NA
indices = 1:10000

#run a query on each batch of indexes, appending each result to
# "result" as we go.
batchByIndex(indices, function(indexBatch){
df = dbGetQuery(dbConnection, generateQuery(indexBatch))
result <<- if(is.na(result)) df else rbind(result,df)
},1000)

## End(Not run)
```

---

|           |                          |
|-----------|--------------------------|
| bondblock | <i>Return bond block</i> |
|-----------|--------------------------|

---

**Description**

Returns bond block(s) from an object of class SDF or SDFset.

**Usage**

```
bondblock(x)
```

**Arguments**

x                    object of class SDF or SDFset

**Details**

...

**Value**

matrix if SDF is provided or list of matrices if SDFset is provided

**Author(s)**

Thomas Girke

**References**

...

**See Also**

header, atomcount, atomblock, datablock, cid, sdfid

**Examples**

```
## SDF/SDFset instances
data(sdfsampl)
sdfset <- sdfsampl
sdf <- sdfset[[1]]

## Extract bond block
bondblock(sdf)
bondblock(sdfset[1:4])

## Replacement methods
```

```
sdfset[[1]][[3]][1,1] <- 999
sdfset[[1]]
bondblock(sdfset)[1:2] <- bondblock(sdfset)[3:4]
bondblock(sdfset[[1]]) == bondblock(sdfset[[3]])
view(sdfset[1:2])
```

---

bonds

*Bonds, charges and missing hydrogens*

---

### Description

Returns information about bonds, charges and missing hydrogens in SDF and SDFset objects.

### Usage

```
bonds(x, type = "bonds")
```

### Arguments

|      |   |
|------|---|
| x    | SDF or SDFset containers  |
| type | If type="bonds" (default), a data.frame is returned with columns: atom (atom labels), Nbondcount (observed bond count), Nbondrule (bond count according to position in periodic table) and charge (charge of each atom).<br>If type="charge", all charged atoms are returned and if type="addNH", the number of missing hydrogens are returned for each molecule. |

### Details

It is used by many other functions (e.g. MW, MF, atomcount, atomcuntMA and plot) to correct for missing hydrogens that are often not specified in SD files.

### Value

If x is of class SDF, then a single data.frame or vector is returned. If x is of class SDFset, then a list of data.frames or vecotors is returned that has the same length and order as x.

### Author(s)

Thomas Girke

### References

...

### See Also

Functions: conMA  
Class: SDF and SDFset

## Examples

```
## Instances of SDFset class
data(sdfsamples)
sdfset <- sdfsamples

## Returns data frames with bonds and charges
bonds(sdfset[1:2], type="bonds")

## Returns charged atoms in each molecule
bonds(sdfset[1:2], type="charge")

## Returns the number of missing hydrogens in each molecule
bonds(sdfset[1:2], type="addNH")
```

---

browseJob

*Open ChemMine Tools Job in Web Browser*

---

## Description

Launches a web browser to view the results of a ChemMine Tools web job with an interactive online viewer. Note that this reassigns the job to the current logged in user within the browser, so it becomes no longer accessible by the `result` and `status` functions. Any results should be saved within R before launching a browser.

## Usage

```
browseJob(object)
```

## Arguments

`object`            A `jobToken` job as returned by the function `launchCMTool`

## Value

Returns an URL string which can be used to access the job results. The function also attempts to open the url with the `browseURL` function. As this URL can only be used once, the returned string is only useful if the `browseURL` function fails to open a browser.

## Author(s)

Tyler William H Backman

## References

See ChemMine Tools at <http://chemmine.ucr.edu>.

**See Also**

Functions: toolDetails, listCMTools, launchCMTool, result, status

**Examples**

```
## Not run:
## list available tools
listCMTools()

## get detailed instructions on using a tool
toolDetails("Fingerprint Search")

## download compound 2244 from PubChem
job1 <- launchCMTool("pubchemID2SDF", 2244)

## check job status and download result
status(job1)
result1 <- result(job1)

## open job in web browser
browseJob(job1)

## End(Not run)
```

---

bufferLines

*Buffer File Input*

---

**Description**

Buffer the input of files to increase efficiency

**Usage**

```
bufferLines(fh, batchSize, lineProcessor)
```

**Arguments**

|               |  |
|---------------|--|
| fh            | file handle  |
| batchSize     | How many lines to read in each batch                               |
| lineProcessor | Each batch of lines will be passed to this function for processing |

**Value**

No return value

**Author(s)**

Kevin Horan

**Examples**

```
## Not run:
fh = file("filename")
bufferLines(fh,100,function(lines) {
  message("found ",length(lines)," lines")
})

## End(Not run)
```

---

bufferResultSet      *Buffer Query Results*

---

**Description**

Allow query results to be processed in batches for efficiency.

**Usage**

```
bufferResultSet(rs, rsProcessor, batchSize = 1000,closeRS=FALSE)
```

**Arguments**

|             |  |
|-------------|--|
| rs          | A DBIResult object, usually from dbSendQuery.                              |
| rsProcessor | Each batch will be passed as a data frame to this function for processing. |
| batchSize   | The number of rows to read in each batch                                   |
| closeRS     | Should the result set be closed by this function when it is done?          |

**Value**

No value.

**Author(s)**

Kevin Horan

**Examples**

```
##-- ==> Define data, use random,
##--or do help(data=index) for the standard data sets.

## The function is currently defined as
function(rs, rsProcessor, batchSize = 1000)
{
  while (TRUE) {
    chunk = fetch(rs, n = batchSize)
    if (dim(chunk)[1] == 0)
      break
    rsProcessor(chunk)
  }
}
```



```
    }  
  }
```

---

`byCluster`*By Cluster*

---

**Description**

Re-organize a vector valued clustering into an list which groups cluster members together

**Usage**

```
byCluster(clustering, excludeSingletons = TRUE)
```

**Arguments**

`clustering` A named vector in which the names are cluster members and the values are cluster labels. This is format output by `jarvisPatrick`.

`excludeSingletons` If true only clusters with more than 1 member will be in the output, otherwise all clusters will be used.

**Value**

A list with a slot for each cluster. Each slot of the list is a vector containing the cluster members.

**Author(s)**

Kevin Horan

**See Also**

[jarvisPatrick](#)

**Examples**

```
data(apset)  
cl = jarvisPatrick(nearestNeighbors(apset,cutoff=0.6),k=2)  
print(byCluster(cl))
```

---

|              |                     |
|--------------|---------------------|
| canonicalize | <i>Canonicalize</i> |
|--------------|---------------------|

---

**Description**

Canonicalizes the atom numbering of a compound. The implementation of this function is in Open Babel and requires the ChemmineOB package to function.

**Usage**

```
canonicalize(sdf)
```

**Arguments**

sdf            Any sdfset object.

**Value**

A new SDFset in which all compounds have been canonicalized

**Author(s)**

Kevin Horan

**References**

[http://openbabel.org/api/2.3/canonical\\_code\\_algorithm.shtml](http://openbabel.org/api/2.3/canonical_code_algorithm.shtml)

**See Also**

[canonicalNumbering](#)

**Examples**

```
## Not run:  
data(sdfsamples)  
canonicalSdf = canonicalize(sdfsamples[1])  
  
## End(Not run)
```

---

|                    |                            |
|--------------------|----------------------------|
| canonicalNumbering | <i>Canonical Numbering</i> |
|--------------------|----------------------------|

---

**Description**

Computes a re-arrangement required to transform the atom numbering of the given compound into the canonical atom numbering. This function uses the `OBGraphSym` and `CanonicalLabels` classes of Open Babel to compute the re-arrangement.

**Usage**

```
canonicalNumbering(sdf)
```

**Arguments**

sdf            Any sdfset object.

**Value**

A list of vectors of index values. Each item in the list corresponds to one of the given compounds. The values of a list item are the re-arrangement of the atoms. For example, if the value in item 1, column 1 is 25, that means that atom number 1 in the original compound should become atom number 25 in the canonical version of that compound.

**Author(s)**

Kevin Horan

**References**

[http://openbabel.org/api/2.3/canonical\\_code\\_algorithm.shtml](http://openbabel.org/api/2.3/canonical_code_algorithm.shtml)

**See Also**

[canonicalize](#)

**Examples**

```
## Not run:  
data(sdfsamples)  
labels = canonicalNumbering(sdfsamples[1])  
  
## End(Not run)
```

---

|     |                            |
|-----|----------------------------|
| cid | <i>Return compound IDs</i> |
|-----|----------------------------|

---

**Description**

Returns the compound identifiers from the ID slot of an SDFset object.

**Usage**

```
cid(x)
```

**Arguments**

x                    object of class SDFset or APset

**Details**

...

**Value**

character vector

**Author(s)**

Thomas Girke

**References**

...

**See Also**

atomblock, atomcount, bondblock, datablock, header, sdfid

**Examples**

```
## SDFset/APset instances
data(sdfsampl)
sdfset <- sdfsampl
apset <- sdf2ap(sdfset[1:4])

## Extract compound IDs from SDFset/APset
cid(sdfset[1:4])
cid(apset[1:4])

## Extract IDs defined in SD file
sdfid(sdfset[1:4])
```

```
## Assigning compound IDs and keeping them unique
unique_ids <- makeUnique(sdfid(sdfset))
cid(sdfset) <- unique_ids
cid(sdfset[1:4])

## Replacement Method
cid(sdfset) <- as.character(1:100)
```

---

cluster.sizestat      *generate statistics on sizes of clusters*

---

### Description

'cluster.sizestat' is used to do simple statistics on sizes of clusters generated by 'cmp.cluster'. It will return a dataframe which maps a cluster size to the number of clusters with that size. It is often used along with 'cluster.visualize'.

### Usage

```
cluster.sizestat(cls, cluster.result=1)
```

### Arguments

`cls`                    The clustering result returned by 'cmp.cluster'

`cluster.result`    If multiple cutoff values are used in clustering process, this argument tells which cutoff value is to be considered here.

### Details

'cluster.sizestat' depends on the format that is returned by 'cmp.cluster' - it will treat the first column as the indices, and the second column as the cluster sizes of effective clustering. Because of this, when multiple cutoffs are used when 'cmp.cluster' is called, 'cluster.sizestat' will only consider the clustering result of the first cutoff. If you want to work on an alternative cutoff, you have to manually reorder/remove columns.

### Value

Returns a data frame of two columns.

`cluster size`      This column lists cluster sizes

`count`              This column lists number of clusters of a cluster size

### Author(s)

Y. Eddie Cao

**See Also**

[cmp.cluster](#), [cluster.visualize](#)

**Examples**

```
## Load sample SD file
# data(sdfsampl); sdfset <- sdfsampl

## Generate atom pair descriptor database for searching
# apset <- sdf2ap(sdfset)

## Loads same atom pair sample data set provided by library
data(apset)

## Binning clustering using variable similarity cutoffs.
cluster <- cmp.cluster(db=apset, cutoff = c(0.65, 0.5))

## Statistics on sizes of clusters
cluster.sizestat(cluster[,c(1,2,3)])
cluster.sizestat(cluster[,c(1,4,5)])
```

---

`cluster.visualize`      *visualize clustering result using multi-dimensional scaling*

---

**Description**

'cluster.visualize' takes clustering result returned by 'cmp.cluster' and generate multi-dimensional scaling plot for visualization purpose.

**Usage**

```
cluster.visualize(db, cls, size.cutoff, distmat=NULL, color.vector=NULL, non.interactive="", cluster.
```

**Arguments**

|                              |   |
|------------------------------|---|
| <code>db</code>              | The descriptor database, in the format returned by 'cmp.parse'.   |
| <code>cls</code>             | The clustering result returned by 'cmp.cluster'.  |
| <code>size.cutoff</code>     | The cutoff size for clusters considered in this visualization. Clusters of size smaller than the cutoff will not be considered.   |
| <code>distmat</code>         | A distance matrix that corresponds to the 'db'. If not provided, it will be computed on-the-fly in an efficient manner.   |
| <code>color.vector</code>    | Colors to be used in the plot. If the number of colors in the vector is not enough for the plot, colors will be reused. If not provided, color will be generated and randomly sampled from 'rainbow'. |
| <code>non.interactive</code> | If provided, will enable the non-interactive mode, and the plot will be in an eps file named after this value.  |

|                                  |  |
|----------------------------------|--|
| <code>cluster.result</code>      | Used to select the clustering result if multiple clustering results are present in 'cls'.  |
| <code>dimensions</code>          | Dimensionality to be used in visualization. See details.   |
| <code>quiet</code>               | Whether to suppress the progress bar.  |
| <code>highlight.compounds</code> | A vector of compound IDs, corresponding to compounds to be highlighted in the plot. A highlighted compound is represented as a filled circle.            |
| <code>highlight.color</code>     | Color used for highlighted compounds. If not set, a highlighted compounds will have the same color as that used for other compounds in the same cluster. |
| <code>...</code>                 | Further arguments will be passed to 'cmp.similarity' to calculate similarity matrix.   |

## Details

'cluster.visualize' internally calls the 'cmdscale' function to generate a set of points in 2-D for the compounds in selected clusters. Note that for compounds in clusters smaller than the cutoff size, they will not be considered in this calculation - their entries in 'dismat' will be discarded if 'dismat' is provided, and distances involving them will not be computed if 'dismat' is not provided.

To determine the value for 'size.cutoff', you can use 'cluster.sizestat' to see the size distribution of clusters.

Because 'cmp.cluster' function allows you to perform multiple clustering processes simultaneously with different cutoff values, the 'cls' parameter may point to a data frame containing multiple clustering results. The user can use 'cluster.result' to specify which result to use. By default, this is set to 1, and the first clustering result will be used in visualization. Whatever the value is, in interactive mode (described below), all clustering result will be displayed when a compound is selected in the interactive plot.

If the colors provided in 'color.vector' are not enough to distinguish clusters by colors, the function will silently reuse the colors, resulting multiple clusters colored in the same color. We suggest you use 'cluster.sizestat' to see how many clusters will be selected using your 'size.cutoff', or simply provide no 'color.vector'.

If 'non.interative' is not set, the final plot is interactive. You will be able to select points by clicking them. When you click on any point, information about the compound represented by that point will be displayed. This includes the cluster ID, cluster size, compound index in the SDF and compound name if any. You can then perform another selection. To exit this process, right click on X11 device or press ESC in non-X11 device (Quartz and Windows).

By default, 'dimensions' is set to 2, and the built-in 'plot' function will be used for plotting. If you need to do 3-Dimensional plotting, set 'dimensions' to 3, and pass the returned value to 3D plot utilities, such as 'scatterplot3d' or 'rggobi'. This package does not perform 3D plot on its own.

## Value

This function returns a data frame of MDS coordinates and clustering result. This value can be passed to 3D plot utilities such as 'scatterplot3d' and 'rggobi'.

The last column of the output gives whether the compounds have been clicked in the interactive mode.

**Author(s)**

Y. Eddie Cao

**See Also**[cmp.parse](#), [cmp.cluster](#), [cluster.sizestat](#)**Examples**

```
## Load sample SD file
# data(sdfsampl); sdfset <- sdfsampl

## Generate atom pair descriptor database for searching
# apset <- sdf2ap(sdfset)

## Loads same atom pair sample data set provided by library
data(apset)
db <- apset

## cluster db with 2 cutoffs
clusters <- cmp.cluster(db, cutoff=c(0.5, 0.4))

## Return size stats
sizestat <- cluster.sizestat(clusters)

## Visualize results, using a cutoff of 3, write to file 'test.eps'
coord <- cluster.visualize(db, clusters, 2, non.interactive="test.eps")

## Not run:
## visualize it in interactive mode, using a cutoff of 3 and the 2nd clustering result
coord <- cluster.visualize(db, clusters, cluster.result=2, 3)

## 3D visualization with scatterplot3d
coord <- cluster.visualize(db, clusters, 3, dimensions=3)
library(scatterplot3d)
scatterplot3d(coord)

## End(Not run)
```

---

`cmp.cluster`*cluster compounds using a descriptor database*

---

**Description**

'cmp.cluster' uses structural compound descriptors and clusters the compounds based on their pairwise distances. `cmp.cluster` uses single linkage to measure distance between clusters when it merges clusters. It accepts both a single cutoff and a cutoff vector. By using a cutoff vector, it can generate results similar to hierarchical clustering after tree cutting.



## Usage

```
cmp.cluster(db, cutoff, is.similarity = TRUE, save.distances = FALSE,  
           use.distances = NULL, quiet = FALSE, ...)
```

## Arguments

|                |  |
|----------------|--|
| db             | The descriptor database, in the format returned by 'cmp.parse'.  |
| cutoff         | The clustering cutoff. Can be a single value or a vector. The cutoff gives the maximum distance between two compounds in order to group them in the same cluster.          |
| is.similarity  | Set when the cutoff supplied is a similarity cutoff. This cutoff is the minimum similarity value between two compounds such that they will be grouped in the same cluster. |
| save.distances | whether to save distance for future clustering. See details below.   |
| use.distances  | Supply pre-computed distance matrix.   |
| quiet          | Whether to suppress the progress information.  |
| ...            | Further arguments to be passed to <code>cmp.similarity</code> .  |

## Details

`cmp.cluster` will compute distances on the fly if `use.distances` is not set. Furthermore, if `save.distances` is not set, the distance values computed will never be stored and any distance between two compounds is guaranteed not to be computed twice. Using this method, `cmp.cluster` can deal with large databases when a distance matrix in memory is not feasible. The speed of the clustering function should be slowed when using a transient distance calculation.

When `save.distances` is set, `cmp.cluster` will be forced to compute the distance matrix and save it in memory before the clustering. This is useful when additional clusterings are required in the future without re-computed the distance matrix. Set `save.distances` to `TRUE` if you only want to force the clustering to use this 2-step approach; otherwise, set it to the filename under which you want the distance matrix to be saved. After you save it, when you need to reuse the distance matrix, you can 'load' it, and supply it to `cmp.cluster` via the `use.distances` argument.

`cmp.cluster` supports a vector of several cutoffs. When you have multiple cutoffs, `cmp.cluster` still guarantees that pairwise distances will never be recomputed, and no copy of distances is kept in memory. It is guaranteed to be as fast as calling `cmp.cluster` with a single cutoff that results in the longest processing time, plus some small overhead linear in processing time.

## Value

Returns a `data.frame`. Besides a variable giving compound ID, each of the other variables in the data frame will either give the cluster IDs of compounds under some clustering cutoff, or the size of clusters that the compounds belong to. When `N` cutoffs are given, in total  $2*N+1$  variables will be generated, with `N` of them giving the cluster ID of each compound under each of the `N` cutoffs, and the other `N` of them giving the cluster size under each of the `N` cutoffs. The rows are sorted by cluster sizes.

**Author(s)**

Y. Eddie Cao, Li-Chang Cheng

**See Also**

[cmp.parse1](#), [cmp.parse](#), [cmp.search](#), [cmp.similarity](#)

**Examples**

```
## Load sample SD file
# data(sdfsampl); sdfset <- sdfsampl

## Generate atom pair descriptor database for searching
# apset <- sdf2ap(sdfset)

## Loads atom pair and atom pair fingerprint samples provided by library
data(apset)
db <- apset
fpset <- desc2fp(apset)

## Clustering of 'APset' object with multiple cutoffs
clusters <- cmp.cluster(db=apset, cutoff=c(0.5, 0.85))

## Clustering of 'FPset' object with multiple cutoffs. This method allows to call
## various similarity methods provided by the fpSim function.
clusters2 <- cmp.cluster(fpset, cutoff=c(0.5, 0.7), method="Tversky")

## Saves the distance matrix before clustering:
clusters <- cmp.cluster(db, cutoff=0.65, save.distances="distmat.rda")
# Later one reload the matrix and pass it the clustering function.
load("distmat.rda")
clusters <- cmp.cluster(db, cutoff=0.60, use.distances=distmat)
```

---

cmp.duplicated      *quickly detect compound duplication in a descriptor database*

---

**Description**

'cmp.duplicated' detects duplicated compounds from a descriptor database generated by 'cmp.parse'. Two compounds are said to duplicate each other when their descriptors are the same.

**Usage**

```
cmp.duplicated(db, sort = FALSE, type=1)
```

**Arguments**

|      |   |
|------|---|
| db   | The descriptor database, in the format returned by 'cmp.parse'. |
| sort | Whether to sort the descriptors for a compound. See details.    |
| type | Returns results as vector (type=1) or data frame (type=2).      |

## Details

'cmp.duplicated' will take the descriptors in the descriptor database, concatenate all descriptors for the same compound into a string, and use this string as the identification of a compound. If two compounds share the same identification string, they are said to duplicate each other.

'cmp.duplicated' assume the the database passed in as argument to follow the format generated by 'cmp.parse'. That is, 'db' is a list, 'db\$descdb' is a list, and each entry of 'db\$descdb' is an array of numeric values that give descriptors for one compound.

By default, 'cmp.duplicated' will assume the descriptors for a compound is already sorted. That is each entry in 'db\$descdb' is a sorted array. This is true for database generated by 'cmp.parse'. If you generate the database using some other tools, you might want to enable sorting.

## Value

Returns a logic array, telling whether a compound in the database is a duplication of a compound appearing before this one. For example, if the i-th element of the array is TRUE, it means that the i-th compound in the database is a duplication of a compound listed before this compound in the database.

The returned array can be used to remove duplication. Simply use it to index the descriptor database.

If you are interested in what compound is duplicated, you can do a search in the database with cutoff set to 1.

## Author(s)

Y. Eddie Cao

## See Also

[cmp.parse](#), [cmp.search](#)

## Examples

```
## Load sample SD file
# data(sdfsampl); sdfset <- sdfsampl

## Generate atom pair descriptor database for searching
# apset <- sdf2ap(sdfset)

## Loads same atom pair sample data set provided by library
data(apset)
db <- apset

## Manually create a duplication (here compound 1 and 10)
db[10] <- db[1]

## Find duplication
dup <- cmp.duplicated(db)
dup
cid(db[dup])
```

```
## Remove all duplications  
db <- db[!dup]
```

---

`cmp.parse`*Parse an SDF file and compute descriptors for all compounds*

---

## Description

'cmp.parse' will take a SDF file, parse all the compounds encoded, compute their atom-pair descriptors, and return the descriptors as a list. The list contains two names, 'descdb' and 'cids'. 'descdb' is a vector of descriptors, and 'cids' is a list of names of compounds found in the SDF file. The returned list is usually used to a database, against which similarity search can be performed using the 'search' function. These two functions will parse all compounds in the SDF file. To parse a single compound, use 'cmp.parse1' instead.

## Usage

```
cmp.parse(filename)
```

## Arguments

filename            The file name of the SDF file

## Details

The 'filename' can be a local file or an URL. It is interactive, and will display the parsing progress. Since the parsing will also compute of atom-pair descriptors, it is time consuming. You will be reminded to save the parsing result for future use at the end of parsing.

'type' is either set to the default value 'normal' or 'file-backed'. When set to 'file-backed', the parsing work will be delegated to a separate package called 'ChemmineRpp', and the database will be stored in a file instead of in the primary memory. Therefore, 'file-backed' mode can handle larger compound libraries. In 'file-backed' mode, 'dbname' will be used to name the database file. A suffix '.cdb' will be appended to the given name.

The type of the database is transparent to other part of the package. For example, calling 'cmp.search' against a database in 'file-backed' mode will cause the package to load the descriptors from the database file progressively.

## Value

Return a list that can be used as the database against which similarity search can be performed. The 'search' and 'cmp.cluster' functions both expect a database returned by 'cmp.parse'.

descdb            A vector containing the descriptors for all the compounds.

cids              Compound ID information found in the SDF file. It is the first line of SDF of a compound.

**Author(s)**

Y. Eddie Cao, Li-Chang Cheng

**References**

Chen X and Reynolds CH (2002). "Performance of similarity measures in 2D fragment-based similarity searching: comparison of structural descriptors and similarity coefficients", in *J Chem Inf Comput Sci*.

**See Also**

[cmp.parse1](#), [cmp.search](#), [cmp.cluster](#), [cmp.similarity](#)

**Examples**

```
## Load sample SD file
# data(sdfsamples); sdfset <- sdfsamples

## Generate atom pair descriptor database for searching
# apset <- sdf2ap(sdfset)

## Loads same atom pair sample data set provided by library
data(apset)
db <- apset
# (optionally) save the db for future use
save(db, file="db.rda", compress=TRUE)
# ...
# later, in a separate session, you can load it back:
load("db.rda")
```

---

cmp.parse1

*Parsing an SDF file and calculate the descriptor for one compound*

---

**Description**

Read SDF information from an SDF file or connection, parse the first compound, and calculate the descriptor for that compound. The returned descriptor can be added to database returned by 'cmp.parse' or be used as the query structure when calling 'search'. This function will only parse one compound and return only the descriptor. To parse all compounds in an SDF file, use 'cmp.parse'.

**Usage**

```
cmp.parse1(filename)
```

**Arguments**

filename      The file name of the SDF file or a URL or a connection.

## Details

'cmp.parse1' can take a file name or a URL or a connection. When a connection is used, the current line must be the first line of SDF of the compound to be parsed. 'cmp.parse1' will skip the header and parse from the 4th line. Therefore, the compound ID information will be skipped. After the parsing is done, if 'filename' is a connection, it will then point to the line after the connection table of SDF. You can use some other procedure to parse the annotation block.

## Value

Return the descriptor, which is encoded as a vector.

## Author(s)

Y. Eddie Cao, Li-Chang Cheng

## References

Chen X and Reynolds CH (2002). "Performance of similarity measures in 2D fragment-based similarity searching: comparison of structural descriptors and similarity coefficients", in *J Chem Inf Comput Sci*.

## See Also

[cmp.parse](#), [cmp.search](#), [cmp.cluster](#), [cmp.similarity](#)

## Examples

```
# load an SDF file from web and parse it
## Not run: structure <- cmp.parse1("http://bioweb.ucr.edu/ChemMineV2/compound/Aurora/b32:NNQS2MBRHAZI===/sdf")
```

---

|            |   |
|------------|---|
| cmp.search | <i>Search a descriptor database for compounds similar to query compound</i> |
|------------|---|

---

## Description

Given descriptor of a query compound and a database of compound descriptors, search for compounds that are similar to the query compound. User can limit the output by supplying a cutoff similarity score or a cutoff that limits the number of returned compounds. The function can also return the scores together with the compounds.

## Usage

```
cmp.search(db, query, type=1, cutoff = 0.5, return.score = FALSE, quiet = FALSE,
mode = 1, visualize = FALSE, visualize.browse = TRUE, visualize.query = NULL)
```

**Arguments**

|                  |  |
|------------------|--|
| db               | The compound descriptor database returned by 'cmp.parse'.  |
| query            | The query descriptor, which is usually returned by 'cmp.parse1'.   |
| type             | Returns results in form of position indices (type=1), named vector with compound IDs (type=2) or data frame (type=3).  |
| cutoff           | The cutoff similarity (when cutoff <= 1) or the number of maximum compounds to be returned (when cutoff > 1).  |
| return.score     | Whether to return similarity scores. If set to TRUE, a data frame will be returned; otherwise, only the compounds' indices in the database will be returned in the order of decreasing scores. |
| quiet            | Whether to disable progress information.   |
| mode             | Mode used when computing similarity scores. This value is passed to 'cmp.similarity'.  |
| visualize        |  |
| visualize.browse |  |
| visualize.query  |  |

**Details**

'cmp.search' will go through all the compound descriptors in the database and calculate the similarity between the query compound and compounds in the database. When cutoff similarity score is set, compounds having a similarity score higher than the cutoff will be returned. When maximum number of compounds to return is set to N via 'cutoff', the compounds having the highest N similarity scores will be returned.

**Value**

When 'return.score' is set to FALSE, a vector of matching compounds' indices in the database will be returned. Otherwise, a data frame will be returned:

|        |   |
|--------|---|
| ids    | The indices of matching compounds in the database.                          |
| scores | The similarity scores between the matching compounds and the query compound |

**Author(s)**

Y. Eddie Cao, Li-Chang Cheng

**References**

Chen X and Reynolds CH (2002). "Performance of similarity measures in 2D fragment-based similarity searching: comparison of structural descriptors and similarity coefficients", in *J Chem Inf Comput Sci*.

**See Also**

[cmp.parse1](#), [cmp.parse](#), [cmp.search](#), [cmp.cluster](#), [cmp.similarity](#), [sdf.visualize](#)

## Examples

```
## Load sample SD file
# data(sdfsampl); sdfset <- sdfsampl

## Generate atom pair descriptor database for searching
# apset <- sdf2ap(sdfset)

## Loads same atom pair sample data set provided by library
data(apset)
db <- apset
query <- db[1]

## Optimally, save the db for future use
save(db, file="db.rda", compress=TRUE)

## Search for similar compounds using similarity cutoff
cmp.search(db, query, cutoff=0.2, type=1) # returns index
cmp.search(db, query, cutoff=0.2, type=2) # returns named vector
cmp.search(db, query, cutoff=0.2, type=3) # returns data frame

## in the next session, you may use load a saved db and do the search:
load("db.rda")
cmp.search(db, query, cutoff=3)
## you may also use the loaded db to do clustering:
cmp.cluster(db, cutoff=0.35)
```

---

cmp.similarity

*Compute similarity between two compounds using their descriptors*

---

## Description

Given descriptors for two compounds, 'cmp.similarity' returns the similarity measure between the two compounds.

## Usage

```
cmp.similarity(a, b, mode = 1, worst = 0)
```

## Arguments

|       |  |
|-------|--|
| a     | Descriptor of the first compound.  |
| b     | Descriptor of the second compound.   |
| mode  | Mode used when computing the distance. See details below.  |
| worst | The worst value you are expecting. If 'cmp.similarity' finds the upper bound of similarity is worse than it, it will return a 0 and potentially save some computation. |



## Details

'cmp.similarity' uses descriptor information generated by 'cmp.parse' and 'cmp.parse1'. Basically, a descriptor is a vector of numbers. The vector actually represents the set of descriptors of structural fragment. Similarity measurement uses Tanimoto coefficient.

'cmp.similarity' supports 3 different modes. In mode 1, normal Tanimoto coefficient is used. In mode 2, it uses the size of descriptor intersection over the size of the smaller descriptor, mainly to deal with compounds that vary a lot in size. In mode 3, it is similar to mode 2, except that it raises the similarity to the power 3 to penalize small values. When mode is 0, 'cmp.similarity' will select mode 1 or mode 3, based on the size differences between the two descriptors.

When 'cmp.similarity' is used in searching compounds with a threshold similarity value, or in clustering with a cutoff distance, the threshold similarity and cutoff distance can be used to decide a 'worse' value. 'cmp.similarity' can compute an upper bound of similarity easier, and by comparing this upper bound to the 'worst' value, it can potentially skip the real computation if it finds the similarity will be below the 'worst' value and will be useless to the caller.

## Value

Return a numeric value between 0 and 1 which gives the similarity between the two compounds.

## Author(s)

Y. Eddie Cao, Li-Chang Cheng

## References

Chen X and Reynolds CH (2002). "Performance of similarity measures in 2D fragment-based similarity searching: comparison of structural descriptors and similarity coefficients", in *J Chem Inf Comput Sci*.

Peter Willett (1998). "Chemical Similarity Searching", in *J. Chem. Inf. Comput. Sci*.

## See Also

[cmp.parse1](#), [cmp.parse](#), [cmp.search](#), [cmp.cluster](#)

## Examples

```
## Load sample SD file
# data(sdfsampl); sdfset <- sdfsampl

## Generate atom pair descriptor database for searching
# apset <- sdf2ap(sdfset)

## Loads same atom pair sample data set provided by library
data(apset)

## Compute similarities among two compounds
cmp.similarity(apset[1], apset[2])

## Search apset database with a query compound
cmp.search(apset, apset[1], type=3, cutoff = 0.3)
```

---

conMA

*Bond Matrices*

---

### Description

Creates a bond matrix from SDF and SDFset objects. The matrix contains the atom labels in the row and column titles and the bond types are given in the data part as follows: 0 is no connection, 1 is a single bond, 2 is a double bond and 3 is a triple bond.

### Usage

```
conMA(x, exclude = "none")
```

### Arguments

|         |   |
|---------|---|
| x       | SDF or SDFset containers  |
| exclude | if exclude="none", then all atoms will be considered in the resulting connection table; if exclude=c("H"), then the H atoms will be excluded. Any number of atom labels to be excluded can be passed on to this argument in form of a character vector. |

### Details

...

### Value

If x is of class SDF, then a single bond matrix is returned. If x is of class SDFset, then a list of matrices is returned that has the same length as x.

### Author(s)

Thomas Girke

### References

...

### See Also

Functions: bonds

Class: SDF and SDFset

## Examples

```
## Instances of SDFset class
data(sdfsamples)
sdfset <- sdfsamples

## Create bond matrix for first two molecules in sdfset
conMA(sdfset[1:2], exclude=c("H"))

## Return bond matrix for first molecule and plot its structure with atom numbering
conMA(sdfset[[1]], exclude=c("H"))
plot(sdfset[1], atomnum = TRUE, noHbonds=FALSE, no_print_atoms = "", atomcex=0.8)

## Return number of non-H bonds for each atom
rowSums(conMA(sdfset[[1]], exclude=c("H")))
```

---

connections

*Database Connections*

---

## Description

Get a connection to one of the pre-build compound databases. The DrugBank database is distributed in the ChemmineDrugs package.

The DUD database will be downloaded the first time it is called. It will download a 1.8GB zipped file which will expand to about 9GB. A directory to store the database in can be passed to the DUD() function.

## Usage

```
DUD(destinationDir=".")
```

```
DrugBank()
```

## Arguments

`destinationDir` The directory to store the downloaded DUD database in.

## Value

A connection object to either the DUD or DrugBank database. This object must be passed to other functions which make use of the connection.

## Author(s)

Kevin Horan

## Examples

```
dbConn = DrugBank()
```

---

|           |                          |
|-----------|--------------------------|
| datablock | <i>Return data block</i> |
|-----------|--------------------------|

---

**Description**

Returns data block(s) from an object of class SDF or SDFset.

**Usage**

```
datablock(x)
```

```
datablocktag(x, tag)
```

**Arguments**

|     |  |
|-----|--|
| x   | object of class SDF or SDFset  |
| tag | numeric position (index) or character name of entry in data block vector |

**Details**

...

**Value**

named character vector if SDF is provided or list of named character vectors if SDFset is provided

**Author(s)**

Thomas Girke

**References**

...

**See Also**

atomblock, atomcount, bondblock, header, cid, sdfid

**Examples**

```
## SDF/SDFset instances
data(sdfsampl)
sdfset <- sdfsampl
sdf <- sdfset[[1]]

## Extract data block
datablock(sdf)
datablock(sdfset[1:4])
```

```

datablocktag(sdfset, tag="PUBCHEM_OPENEYE_CAN_SMILES")

## Replacement methods
sdfset[[1]][[1]][1] <- "test"
sdfset[[1]]
datablock(sdfset)[1] <- datablock(sdfset[2])
view(sdfset[1:2])

## Example for injecting a custom matrix/data frame into the data block of an
## SDFset and then writing it to an SD file
props <- data.frame(MF=MF(sdfset), MW=MW(sdfset), atomcountMA(sdfset))
datablock(sdfset) <- props
view(sdfset[1:4])
# write.SDF(sdfset[1:4], file="sub.sdf", sig=TRUE, cid=TRUE)

```

---

datablock2ma

*SDF data blocks to matrix*


---

## Description

Convert data blocks in SDFset to character matrix with datablock2ma, then store its numeric columns as numeric matrix and its character columns as character matrix.

## Usage

```

datablock2ma(datablocklist, cleanup = "\\(.*", ...)

splitNumChar(blockmatrix)

```

## Arguments

|               |  |
|---------------|--|
| datablocklist | list of data block vectors; can be created with datablock(sdfset)  |
| blockmatrix   | matrix returned by datablock2ma  |
| cleanup       | character pattern to be used to clean up the name fields of the data block vectors; the exact pattern matches are replaced by nothing (deleted). |
| ...           | option to pass on additional arguments   |

## Details

...

## Value

|              |   |
|--------------|---|
| datablock2ma | character matrix  |
| splitNumChar | list with two components, a numeric matrix and a character matrix |

**Author(s)**

Thomas Girke

**References**

...

**See Also**

Classes: SDFset

**Examples**

```
## SDFset instance
data(sdfsampl)
sdfset <- sdfsampl

# Convert data block to matrix
blockmatrix <- datablock2ma(datablocklist=datablock(sdfset))
blockmatrix[1:4, 1:4]

# Split matrix to numeric matrix and character matrix
numchar <- splitNumChar(blockmatrix=blockmatrix)
names(numchar)
numchar[[1]][1:4,]
numchar[[2]][1:4,]
```

---

db.explain

*Explain an atom-pair descriptor or an array of atom-pair descriptors*

---

**Description**

'db.explain' will take an atom-pair descriptor in numeric or a set of such descriptors, and interpret what they represent in a more human readable way.

**Usage**

```
db.explain(desc)
```

**Arguments**

desc            The descriptor or the array/vector of descriptors

**Details**

'desc' can be a single numeric giving a single descriptor or can be any container data type, such as vector or array, such that 'length(desc)' returns 2 or larger.

**Value**

Return a character vector describing the descriptors.

**See Also**

[cmp.parse](#)

**Examples**

```
## Load sample SD file
# data(sdfsamples); sdfset <- sdfsamples

## Generate atom pair descriptor database for searching
# apset <- sdf2ap(sdfset)

## Loads same atom pair sample data set provided by library
data(apset)
db <- apset

## Return atom pairs of first compound in human readable format
db.explain(db[1])
```

---

|           |  |
|-----------|--|
| db.subset | <i>Subset a descriptor database and return a sub-database for the selected compounds</i> |
|-----------|--|

---

**Description**

'db.subset' will take a descriptor database generated by 'cmp.parse' and an array of indices, and return a new database for compounds corresponding to these indices. The returned value is a descriptor database as returned by the [cmp.parse](#) function.

**Usage**

```
db.subset(db, cmprs)
```

**Arguments**

|       |  |
|-------|--|
| db    | The database generated by 'cmp.parse'  |
| cmprs | An array of indices that correspond to a set of selected compounds from the database |

**Details**

'db.subset' creates a sub-database from 'db' by only including information that is relevant to compounds indexed by 'cmprs'.

**Value**

Return a descriptor database for the selected compounds. The format of the database is compatible with the one returned by [cmp.parse](#).

**See Also**

[cmp.parse](#), [sdf.subset](#)

**Examples**

```
## Note: this functionality has become obsolete since the introduction of the
## 'apset' S4 class.

## Load sample SD file
# data(sdfsamples); sdfset <- sdfsamples

## Generate atom pair descriptor database for searching
# apset <- sdf2ap(sdfset)

## Loads same atom pair sample data set provided by library
data(apset)
db <- apset
olddb <- apset2descdb(db)

## Create a sub-database for the 1st and 2nd compound in that SDF
db_sub <- db.subset(olddb, c(1, 2))
```

---

dbTransaction

*DB Transaction*

---

**Description**

Run any db statements inside a transaction. If any error is raised the transaction will be rolled back, otherwise it will be committed at the end.

**Usage**

```
dbTransaction(conn, expr)
```

**Arguments**

|      |   |
|------|---|
| conn | A database connection object, such as is returned by <a href="#">initDb</a> . |
| expr | Any block of code.  |

**Value**

The value of the given block of code will be returned upon successfully committing the transaction. Otherwise an error will be raised.



**Author(s)**

Kevin Horan

**Examples**

```
conn = initDb("test15.db")
dbTransaction(conn,{
# any db code here
})
```

---

desc2fp

*Fingerprints from descriptor vectors*

---

**Description**

Generates fingerprints from descriptor vectors such as atom pairs stored in APset or list containers. The obtained fingerprints can be used for structure similarity comparisons, searching and clustering. Due to their compact size, computations on fingerprints are often more time and memory efficient than on their much more complex atom pair counterparts.

**Usage**

```
desc2fp(x, descnames=1024, type = "FPset")
```

**Arguments**

|           |   |
|-----------|---|
| x         | Object of classe APset or list of vectors   |
| descnames | Descriptor set to consider for fingerprint encoding. If a single value from 1-4096 is provided then the function uses the corresponding number of the most frequent atom pairs stored in the apfp data set provided by the package. Alternatively, one can provide here any custom atom pair selection in form of a character vector. |
| type      | return fingerprint set as FPset, matrix or character vector   |

**Details**

...

**Value**

matrix or character vectors

**Author(s)**

Thomas Girke

## References

Chen X and Reynolds CH (2002). "Performance of similarity measures in 2D fragment-based similarity searching: comparison of structural descriptors and similarity coefficients", J Chem Inf Comput Sci.

## See Also

Functions: sdf2ap, SDF2apcmp, apset2descdb, cmp.search, cmp.similarity

Related classes: SDF, SDFset, SDFstr, APset.

## Examples

```
## Instance of SDFset class
data(sdfsampl)
sdfset <- sdfsampl[1:10]

## Compute atom pair library
apset <- sdf2ap(sdfset)

## Compute atom pair fingerprint matrix using internal atom pair
## selection containing 4096 most common atom pairs in DrugBank.
## For details see ?apfp. The following example uses from this
## set the 1024 most frequent atom pairs:
fpset <- desc2fp(x=apset, descnames=1024, type="FPset")

## Alternatively, one can provide any custom atom pair selection. Here
## 1024 most common ones in apset object.
fpset1024 <- names(rev(sort(table(unlist(as(apset, "list")))))[1:1024])
fpset2 <- desc2fp(x=apset, descnames=fpset1024, type="FPset")

## A more compact way of storing fingerprints is as character values
fpchar <- desc2fp(x=apset, descnames=1024, type="character")

## Convert character fingerprints back to FPset or matrix
fpset <- as(fpchar, "FPset")
fpma <- as.matrix(fpset)

## Similarity searching returning Tanimoto similarity coefficients
fpSim(x=fpset[1], y=fpset)

## Clustering example
simMAap <- sapply(cid(fpset), function(x) fpSim(x=fpset[x], fpset, sorted=FALSE))
hc <- hclust(as.dist(1-simMAap), method="single")
plot(as.dendrogram(hc), edgePar=list(col=4, lwd=2), horiz=TRUE)
```

**Description**

Draws an sdf object in the 2D plane using ggplot2 library. Permits customization of bond colors and atom colors.

**Usage**

```
draw_sdf(sdf, filename = "test.jpg", alpha_edge = 0.5, alpha_node = 1, numbered = FALSE, font_size = 5, r
```

**Arguments**

|                       |   |
|-----------------------|---|
| sdf                   | An instance of a SDF or list of SDFs  |
| filename              | Filename to save image to. Defaults to 'test.jpg'. If set to NULL, does not save image.   |
| alpha_edge            | alpha of bonds in your image. Defaults to 0.5. 0 is fully transparent, 1 is fully opaque.   |
| alpha_node            | alpha of atoms in your image. Defaults to 1.0.  |
| numbered              | If 1 or TRUE, displays numbering of atoms at their location. If 2, displays a second numbering style.   |
| font_size             | Controls size of text to be displayed at atom locations. Beware when plotting multiple SDFs in one image. Ggplot will still scale fonts as if text is being plotted in one image. |
| node_vertical_offset  | Upward shift of atom text. Upward shift is in SDF units, not ggplot units.  |
| bgcolor               | An rgb(r,g,b,alpha) or similar object. produces a background of the specified color.  |
| node_background_color | A common color as a text string (e.g. 'white', 'pink') or an rgb(r,g,b,alpha). Draws a filled circle of the color specified before drawing text over each node.                   |
| bgraster              | A readPNG object or a path to an object that can be understood using readPNG. Will be used as background.   |
| node_policy           | Mapping that defines how atom strings should be displayed. Simplest would be c('default'='black')   |
| edge_policy           | Mapping that defines how bonds should be displayed. Simplest is c('default'='black'), though this will display all Hydrogen bonds as well.  |
| bond_dist_offset      | Defines space between double or triple bonds, in SDF units.   |
| fmcsR_sdf             | A second SDF object to run fmcsR on.  |

**Details**

Requires ggplot2. Additional features require grid, gridExtra, fmcsR, or png. Most matrix operations vectorized.

**Value**

Returns a ggplot2 object. Calling draw\_sdf(...) rather than assigning it will result in R trying to print a ggplot2 object.

**Author(s)**

John A. Sharifi

**Examples**

```
library(ChemmineR) # if not already imported
data(sdfsamples)
draw_sdf(sdfsamples[[1]])
```

---

exactMassOB

*Exact Mass (Monoisotopic Mass)*

---

**Description**

Computes the exact mass of each compound given.

**Usage**

```
exactMassOB(sdfset)
```

**Arguments**

sdfset            Any SDFset object.

**Value**

A vector of mass values.

**Author(s)**

Kevin Horan

**Examples**

```
## Not run:
library(ChemmineR)
data(sdfsamples)
mass = exactMassOB(sdfsamples)

## End(Not run)
```

---

ExtSDF-class

Class "ExtSDF"

---

### Description

This is a subclass of SDF and thus inherits all the slots and methods from that class. It adds a list of extended attributes for atoms and bonds. These attributes can currently only be populated from a V3000 formatted SDF file.

### Objects from the Class

Objects can be created by calls of the form `new("ExtSDF", ...)`. The function `read.SDFset` will also return objects of this class if the argument `extendedAttributes` is set to "TRUE".

### Slots

`extendedAtomAttributes`: Object of class "list"

`extendedBondAttributes`: Object of class "list"

### Methods

**getAtomAttr** signature(`x = "ExtSDF"`, `atomId`, `tag`): Returns the value of the given tag on the given atom number

**getBondAttr** signature(`x = "ExtSDF"`, `bondId`, `tag`): Returns the value of the given tag on the given bond number

**show** signature(`object = "ExtSDF"`): prints summary of SDF as well as any defined extended attributes for the atoms or bonds

### Author(s)

Kevin Horan

### References

SDF V3000 format definition: <http://www.symyx.com/downloads/public/ctfile/ctfile.jsp>

### See Also

Related classes: SDF, SDFset, SDFstr, AP, APset

### Examples

```
showClass("ExtSDF")
```

---

`findCompounds`*Find Compounds in Database*

---

### Description

Searches the SQL database using features computed at load time. Each feature used should be specified in the `featureNames` parameter. Then a set of filters can be given to search for specific compounds.

### Usage

```
findCompounds(conn, featureNames, tests)
```

### Arguments

|                           |   |
|---------------------------|---|
| <code>conn</code>         | A database connection object, such as is returned by <a href="#">initDb</a> .   |
| <code>featureNames</code> | A list of all feature names used in any test.   |
| <code>tests</code>        | A vector of filters that must all be true for a compound to be returned. For example: <code>c("MW &lt;= 400", "RINGS &gt; 3")</code> would return all compounds with a molecular weight of 400 or less and a more than 3 rings, assuming these features exist in the database. The syntax for each test is " <code>&lt;feature name&gt; &lt;SQL operator&gt; &lt;value&gt;</code> ". These tests will simply be concatenated together with "AND " in-between them and tacked on the end of a WHERE clause of an SQL statement. So any SQL that will work in that context is fine. |

### Value

Returns a list of compound ids. The actual compounds can be fetched with [getCompounds](#).

### Author(s)

Kevin Horan

### See Also

[getCompounds](#)

### Examples

```
#create and initialize a new SQLite database
conn = initDb("test1.db")

data(sdfsampl)

#load data and compute 3 features: molecular weight, with the MW function,
# and counts for RINGS and AROMATIC, as computed by rings, which returns a data frame itself.
ids=loadSdf(conn,sdfsampl,
  function(sdfset)
```

```
data.frame(MW = MW(sdfset), rings(sdfset,type="count",upper=6, arom=TRUE))
)
#search for compounds with molecular weight less than 200
lightIds = findCompounds(conn,"MW",c("MW < 200"))
MW(getCompounds(conn,lightIds)) # should find one compound with weight 140
unlink("test1.db")
```

---

findCompoundsByName     *Find compound by name*

---

## Description

Find the ids of compounds given the names.

## Usage

```
findCompoundsByName(conn, names, keepOrder = FALSE, allowMissing = FALSE)
```

## Arguments

|              |   |
|--------------|---|
| conn         | A database connection object, such as is returned by <a href="#">initDb</a> .   |
| names        | A list of names of compounds to search for. The names are those that would be returned by <a href="#">sdfid</a> . An error will be raised if any names are not found.                                     |
| keepOrder    | If true, the order of the output compound ids will be the same as the input names. This imposes a performance hit that can be significant for large datasets, thus it should be left FALSE unless needed. |
| allowMissing | When this is false an error will be raised when names queried were not found in the database. If true, just those that are found will be returned with no error or warning.                               |

## Value

Returns the compound ids for compounds with the given name. The output order is not guaranteed unless keepOrder is set to TRUE. An error will be raised if any name cannot be found.

## Author(s)

Kevin Horan

## Examples

```
#create and initialize a new SQLite database
conn = initDb("test4.db")

data(sdfsampl)

#just load the data with no features or descriptors
```

```
ids=loadSdf(conn,sdfsamplE)

# find id of compound 650003
findCompoundsByName(conn,c("650003"))
unlink("test4.db")
```

---

fingerprintOB

*Fingerprints from OpenBabel*

---

## Description

Generates fingerprints from SDFsets using OpenBabel. The name of the fingerprint can also be set and can be anything available through OpenBabel. You can see what this list is by executing "obabel -L fingerprints". Results are returned as an FPset.

## Usage

```
fingerprintOB(sdfSet, fingerprintName)
```

## Arguments

|                 |  |
|-----------------|--|
| sdfSet          | Input compounds to generate fingerprints for.  |
| fingerprintName | The name of the fingerprint in Open Babel. A list of available names can be found by executing "obabel -L fingerprints". Currently that list is: "FP2", "FP3", "FP4", and "MACCS". |

## Value

An FPset with an element for each given compound.

## Author(s)

Kevin Horan

## Examples

```
## Not run:
data(sdfsamplE)
fpset = fingerprintOB(sdfsamplE)

## End(Not run)
```



---

|      |             |
|------|-------------|
| fold | <i>Fold</i> |
|------|-------------|

---

**Description**

Fold a fingerprint. This takes the second half of the fingerprints and combines with the first half with a logical 'OR' operation. The result is a fingerprint with half as many bits.

**Usage**

```
fold(x, count = 1, bits = NULL)
```

**Arguments**

|       |   |
|-------|---|
| x     | The fingerprint(s) to fold. This can be either an FP or an FPset object.  |
| count | The number of times to fold this fingerprint. Folding will stop early if the fingerprint is reduced down to 1 bit before reaching the requested fold count. |
| bits  | Fold this fingerprint until it is bits bits long. An exception will be thrown if bits is not reachable.   |

**Value**

The new, folded, fingerprint.

**Author(s)**

Kevin Horan

**Examples**

```
fp = new("FP",fp=c(1,0,1,1, 0,0,1,0))
foldedFp = fold(fp,bits=4)
```

---

|           |                  |
|-----------|------------------|
| foldCount | <i>foldCount</i> |
|-----------|------------------|

---

**Description**

Returns the number of times this fingerprint has been folded.

**Usage**

```
foldCount(x)
```

**Arguments**

|   |                                  |
|---|----------------------------------|
| x | Either an FP or an FPset object. |
|---|----------------------------------|

**Value**

Returns the number of times this fingerprint has been folded.

**Author(s)**

Kevin Horan

**Examples**

```
fp = new("FP", fp=c(1,0,1,1, 0,0,1,0))
foldedFp=fold(fp)
fc = foldCount(foldedFp) # == 1
```

---

FP-class

*Class "FP"*

---

**Description**

Container for storing the fingerprint of a single compound. The FPset class is used for storing the fingerprints of many compounds.

**Objects from the Class**

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

**Slots**

**fp**: Object of class "numeric"  
**foldCount**: Object of class "numeric"  
**type**: Object of class "character"

**Methods**

**as.character** signature(x = "FP"): returns fingerprint as character string  
**as.numeric** signature(x = "FP"): returns fingerprint as numeric vector  
**as.vector** signature(x = "FP"): returns fingerprint as numeric vector  
**coerce** signature(from = "FPset", to = "FP"): coerce FPset component to list with many FP objects  
**coerce** signature(from = "numeric", to = "FP"): construct FP object from numeric vector  
**show** signature(object = "FP"): prints summary of FP  
**c** signature(x = "FP"): concatenates any number of FP objects  
**fold** signature(x = "FP"): fold fingerprint in half  
**foldCount** signature(x = "FP"): number of times this object has been folded  
**fpType** signature(x = "FP"): the type of this fingerprint  
**numBits** signature(x = "FP"): the number of bits in this fingerprint

**Author(s)**

Thomas Girke

**References**

Chen X and Reynolds CH (2002). "Performance of similarity measures in 2D fragment-based similarity searching: comparison of structural descriptors and similarity coefficients", in J Chem Inf Comput Sci.

**See Also**

Related classes: SDF, SDFset, SDFstr, AP, APset, FPset.

**Examples**

```
showClass("FP")

## Instance of FP class
data(aset)
fpset <- desc2fp(aset)
(fp <- fpset[[1]])

## Class usage
fpc <- as.character(fp)
fpn <- as.numeric(fp)
as(fpn, "FP")
as(fpset[1:4], "FP")
```

---

fp2bit*Convert base 64 fingerprints to binary*

---

**Description**

The function converts the base 64 encoded PubChem fingerprints to a binary matrix or a character vector. If applied to a SDFset object, then its data block needs to contain the PubChem fingerprint information.

**Usage**

```
fp2bit(x, type = 3, fptag = "PUBCHEM_CACTVS_SUBSKEYS")
```

**Arguments**

|       |  |
|-------|--|
| x     | Object of class SDFset, matrix or character  |
| type  | If set to 1, the results are returned as binary matrix. If set to 2, the results are returned as character strings in a named <i>vector</i> . If set to 3 (default), the results are returned as FPset object. |
| fptag | Name tag in SDF data block where the PubChem fingerprints are stored. Default is set to "PUBCHEM_CACTVS_SUBSKEYS".   |

**Details**

...

**Value**

matrix, character or FPset

**Author(s)**

Thomas Girke

**References**See PubChem fingerprint specification at: [ftp://ftp.ncbi.nih.gov/pubchem/specifications/pubchem\\_fingerprints.txt](ftp://ftp.ncbi.nih.gov/pubchem/specifications/pubchem_fingerprints.txt)**See Also**

Functions: fpSim

**Examples**

```
## Load PubChem SDFset sample
data(sdfsamples); sdfset <- sdfsamples
cid(sdfset) <- sdfid(sdfset)

## Convert base 64 encoded fingerprints to FPset object
fpset <- fp2bit(sdfset)

## Pairwise compound structure comparisons
fpSim(fpset[1], fpset[2])

## Structure similarity searching: x is query and y is fingerprint database
fpSim(x=fpset[1], y=fpset, method="Tanimoto", cutoff=0, top="all")

## Compute fingerprint based Tanimoto similarity matrix
simMA <- sapply(cid(fpset), function(x) fpSim(x=fpset[x], fpset, sorted=FALSE))

## Hierarchical clustering with simMA as input
hc <- hclust(as.dist(1-simMA), method="single")

## Plot hierarchical clustering tree
plot(as.dendrogram(hc), edgePar=list(col=4, lwd=2), horiz=TRUE)
```

FPset-class

Class "FPset"

**Description**

Container for storing fingerprints of many compounds. This container is used for structure similarity searching of compounds.

**Objects from the Class**

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

**Slots**

**fpma**: Object of class "matrix" with compound identifiers stored in row names

**foldCount**: Object of class "numeric"

**type**: Object of class "character"

**Methods**

**[** signature(x = "FPset"): subsetting of class with bracket operator

**[[** signature(x = "FPset"): returns single component as FP object

**[<-** signature(x = "FPset"): replacement method for several components

**as.character** signature(x = "FPset"): returns content as named character vector

**as.matrix** signature(x = "FPset"): returns content as numeric matrix

**c** signature(x = "FPset"): concatenates any number of FPset containers

**cid** signature(x = "FPset"): returns all compound identifiers from row names

**cid<-** signature(x = "FPset"): replacement method for compound identifiers

**coerce** signature(from = "FPset", to = "FP"): as(fpset, "FP")

**coerce** signature(from = "matrix", to = "FPset"): as(fpma, "FPset")

**coerce** signature(from = "character", to = "FPset"): as(fpchar, "FPset")

**length** signature(x = "FPset"): returns number of entries stored in object

**show** signature(object = "FPset"): prints summary of FPset

**view** signature(x = "FPset"): prints extended summary of FPset

**fold** signature(x = "FPset"): fold fingerprint in half

**foldCount** signature(x = "FPset"): number of times this object has been folded

**fpype** signature(x = "FPset"): the type of these fingerprints

**numBits** signature(x = "FPset"): the number of bits in these fingerprints

**Author(s)**

Thomas Girke

## References

Chen X and Reynolds CH (2002). "Performance of similarity measures in 2D fragment-based similarity searching: comparison of structural descriptors and similarity coefficients", in J Chem Inf Comput Sci.

## See Also

Related classes: SDF, SDFset, SDFstr, AP, APset, FP.

## Examples

```
showClass("FPset")

## Instance of FPset class
data(apset)
(fpset <- desc2fp(apset))
view(fpset)

## Class usage
fpset[1:4] # behaves like a list
fpset[[1]] # returns FP object
length(fpset) # number of compounds
cid(fpset) # returns compound ids
fpset[1] <- 0 # replacement
cid(fpset) <- 1:length(fpset) # replaces compound ids
c(fpset[1:4], fpset[11:14]) # concatenation

## Coerce FPset from/to other objects
fpma <- as.matrix(fpset) # coerces to matrix
fpchar <- as.character(fpset) # coerces to character strings
as(fpma, "FPset")
as(fpchar, "FPset")

## Compound similarity searching with FPset
fpSim(x=fpset[1], y=fpset, method="Tanimoto", cutoff=0.4, top=4)
```

---

fpSim

*Fingerprint Search*

---

## Description

Search function for fingerprints, such as PubChem or atom pair fingerprints. Enables structure similarity comparisons, searching and clustering.

## Usage

```
fpSim(x, y, sorted=TRUE, method="Tanimoto",
      addone=1, cutoff=0, top="all", alpha=1, beta=1,
      parameters=NULL, scoreType="similarity")
```

**Arguments**

|            |  |
|------------|--|
| x          | Query molecule of class <code>numeric</code> , <code>FP</code> or <code>FPset</code> (of length one) containing binary fingerprint data. Both x and y need to have the same number of bits and should contain the same type of fingerprints.   |
| y          | Subject molecule(s) of class <code>numeric</code> , <code>matrix</code> , <code>FP</code> or <code>FPset</code> containing binary fingerprint data.  |
| sorted     | return results sorted or unsorted  |
| method     | Similarity coefficient to return. One can choose here from several predefined similarity measures: "Tanimoto" (default), "Euclidean", "Tversky" or "Dice". Alternatively, one can pass on any custom similarity function containing the arguments a, b, c and d. For instance, one can define <code>myfct &lt;- function(a, b, c, d) c/(alpha*a + beta*b + c)</code> and then pass on <code>method=myfct</code> . The variable 'c' is the number of "on-bits" common in both compounds, 'd' is the number of "off-bits" common in both compounds, and 'a' and 'b' are the number of "on-bits" that are unique in one or the other compound, respectively.<br><br>The predefined methods will run a C++ version of this function which is about twice as fast as the R version. When a custom similarity function is given however, it will fall back to using the R version. |
| addone     | Value to add to numerator and denominator of similarity coefficient to avoid division by zero when fingerprint(s) contain only "off-bits" (zeros). Note: if <code>addone &gt; 0</code> then fingerprints with no "on-bits" will receive the highest similarity score. Typically, this occurs only with extremely small molecules.  |
| cutoff     | allows to restrict results to hits above a similarity cutoff value; default <code>cutoff=0</code> returns results for all compounds in y.  |
| top        | allows to restrict number of subject molecules to return; default <code>top="all"</code> returns results for all compounds in y above cutoff value.  |
| alpha      | Only used when <code>method="Tversky"</code> . Allows to specify the weighting variable 'alpha' of the Tversky index: $c/(\alpha*a + \beta*b + c)$   |
| beta       | Only used when <code>method="Tversky"</code> . Allows to specify the weighting variable 'beta' of the Tversky index.   |
| parameters | Parameters for computing Z-scores, E-values, and p-values. Pass this data if you want these scores returned. This data can be generated with the <a href="#">genParameters</a> function.   |
| scoreType  | If using the <code>parameters</code> argument, this argument specified which type of score the <code>cutoff</code> and <code>sorted</code> arguments should be applied to. It should be one of "similarity" (default), "zscore", "evalue", or "pvalue".  |

**Value**

Returns numeric vector with similarity coefficients as values and compound identifiers as names.

**Author(s)**

Thomas Girke, Kevin Horan

## References

Tanimoto similarity coefficient: Tanimoto TT (1957) IBM Internal Report 17th Nov see also Jaccard P (1901) Bulletin del la Societe Vaudoisesdes Sciences Naturelles 37, 241-272.

PubChem fingerprint specification: [ftp://ftp.ncbi.nih.gov/pubchem/specifications/pubchem\\_fingerprints.txt](ftp://ftp.ncbi.nih.gov/pubchem/specifications/pubchem_fingerprints.txt)

## See Also

Functions: fp2bit

## Examples

```
## Load PubChem SDFset sample
data(sdfsampl); sdfset <- sdfsampl
cid(sdfset) <- sdfid(sdfset)

## Convert base 64 encoded fingerprints to character vector or binary matrix
fpset <- fp2bit(sdfset)

## Alternatively, one can use atom pair fingerprints
## Not run:
fpset <- desc2fp(sdf2ap(sdfset))

## End(Not run)

## Pairwise compound structure comparisons
fpSim(x=fpset[1], y=fpset[2], method="Tanimoto")

## Structure similarity searching: x is query and y is fingerprint database
fpSim(x=fpset[1], y=fpset)

## Controlling the output
fpSim(x=fpset[1], y=fpset, method="Tversky", cutoff=0.4, top=4, alpha=0.5, beta=1)

## Use custom distance function
myfct <- function(a, b, c, d) c/(a+b+c+d)
fpSim(x=fpset[1], y=fpset, method=myfct)

## Compute fingerprint-based Tanimoto similarity matrix
simMA <- sapply(cid(fpset), function(x) fpSim(x=fpset[x], fpset, sorted=FALSE))

## Hierarchical clustering with simMA as input
hc <- hclust(as.dist(1-simMA), method="single")

## Plot hierarchical clustering tree
plot(as.dendrogram(hc), edgePar=list(col=4, lwd=2), horiz=TRUE)
```



---

|        |               |
|--------|---------------|
| fptype | <i>fptype</i> |
|--------|---------------|

---

**Description**

Returns the type label of this fingerprint

**Usage**

```
fptype(x)
```

**Arguments**

x                    Either an FP or an FPset object.

**Value**

The type label of this fingerprint.

**Author(s)**

Kevin Horan

**Examples**

```
fp = new("FP",fp=c(1,0,1,1, 0,0,1,0),type="testFP")
type = fptype(fp) # == "testFP"
```

---

|              |                                     |
|--------------|-------------------------------------|
| fromNNMatrix | <i>From Nearest Neighbor Matrix</i> |
|--------------|-------------------------------------|

---

**Description**

Converts a nearest neighbor matrix into a list that can be used with the jarvisPatrick function.

**Usage**

```
fromNNMatrix(data, names = rownames(data))
```

**Arguments**

data                    A matrix containing integer valued indexes which represent items to be clustered. The index values contained in the matrix must be smaller than the number of rows in the matrix. Each row in the matrix represents one item and the columns are the nearest neighbors of that item.

names                    The names for each row. The rownames of data will be used if not given.

**Value**

A list containing the slots "indexes" and "names".

**Author(s)**

Kevin Horan

**See Also**

[jarvisPatrick](#)

**Examples**

```
data(apset)

nn = nearestNeighbors(apset,cutoff=0.6)
nnMatrix = nn$indexes

cl = jarvisPatrick(fromNNMatrix(nnMatrix),k=2)
```

---

genAPDescriptors

*Generate AP Descriptors*

---

**Description**

Generates Atom Pair descriptors using a fast C function.

**Usage**

```
genAPDescriptors(sdf,uniquePairs=TRUE)
```

**Arguments**

|             |   |
|-------------|---|
| sdf         | A single SDF object.  |
| uniquePairs | When the same atom pair occurs more than once in a single compound, should the names be unique or not? Setting this to true will take slightly longer to compute. |

**Value**

A vector of descriptors for the compound given. An AP object can be generated as shown in the example below.

**Author(s)**

Kevin Horan

**Examples**

```
library(ChemmineR)
data(sdfsamples)
sdf = sdfsamples[[2]]
ap = new("AP", AP=genAPDescriptors(sdf))
```

---

|                  |                           |
|------------------|---------------------------|
| generate3DCoords | <i>Generate 3D Coords</i> |
|------------------|---------------------------|

---

**Description**

Uses Open Babel to compute 3D coordinates given an SDFset with only 2D coordinates.

**Usage**

```
generate3DCoords(sdf)
```

**Arguments**

sdf            Any sdfset object.

**Value**

A new SDFset in which all compounds have 3D coordinates.

**Author(s)**

Kevin Horan

**Examples**

```
## Not run:
data(sdfsamples)
sdf3D = generate3DCoords(sdfsamples[1])

## End(Not run)
```

---

genParameters                      *Generate Parameters*

---

### Description

Generate statistics from a fingerprint database for use in calculating z-scores, E-values, and p-values later.

### Usage

```
genParameters(fpset, similarity = fpSim, sampleFraction = 1, ...)
```

### Arguments

|                |   |
|----------------|---|
| fpset          | The database of fingerprints. Needs to be in the format expected by the similarity function. For the default similarity function, this would be an FPset.           |
| similarity     | A function to compute the similarity between two fingerprints. The first argument should be a single query and the second argument should be a set of fingerprints. |
| sampleFraction | The fraction of all pairs to use for estimating parameters. See Details section.  |
| ...            | Extra parameters will be passed on to the similarity function.  |

### Details

A beta function will be fit to the distribution of similarity scores produced by the given similarity function. By default, all pairwise similarities will be computed. Since this can be expensive for large databases, one can also sample pairs to use. This can be done by setting `sampleFraction` to the fraction of all pairwise similarities to use. For example, for a database of 100 fingerprints, there are 10,000 pairs. Setting `sampleFraction` to 0.5 will result in only 5,000 pairs being used to estimate the parameters.

Parameters are conditioned on the number of set bits. This function therefore groups fingerprints by the number of set bits they have and then estimates parameters for each group. A set of global parameters is also estimated and returned for use in cases where there was not enough data to estimate the parameters for a particular number of set bits.

### Value

A data frame with the following columns:

|          |  |
|----------|--|
| count    | The number of similarities used to estimate these parameters |
| avg      | the mean   |
| variance | the variance   |
| alpha    | The alpha parameter of the Beta function                     |
| beta     | The beta parameter of the Beta function                      |

There will be a row for each possible count of 1 bits. So for a database of 1024 bit fingerprints, there will be 1025 rows for the possible values of 0-1024 bits. There will also be one additional row at the end with the global parameters. This can be used for cases where there are no parameters estimated for the current query 1-bit count.

**Author(s)**

Kevin Horan

**References**

Pierre Baldi and Ramzi Nasr, "When is Chemical Similarity Significant? The Statistical Distribution of Chemical Similarity Scores and Its Extreme Values" *Journal of Chemical Information and Modeling* 2010 50 (7), 1205-1222

**See Also**

[fpSim](#)

**Examples**

```
library(ChemmineR)
data(apset)
fpset=desc2fp(apset) #get a fingerprint database

params = genParameters(fpset)
scores = fpSim(fpset[[1]], fpset, parameters=params, top=10)
```

---

|                   |                             |
|-------------------|-----------------------------|
| getAllCompoundIds | <i>Get All Compound Ids</i> |
|-------------------|-----------------------------|

---

**Description**

Return a vector of every compound id in the given database.

**Usage**

```
getAllCompoundIds(conn)
```

**Arguments**

conn            A database connection object, such as is returned by [initDb](#).

**Value**

A vector of compound\_id numbers

**Author(s)**

Kevin Horan

**Examples**

```
#create and initialize a new SQLite database
conn = initDb("test1.db")

data(sdfsampl)

#load data
ids=loadSdf(conn,sdfsampl)
ids2=getAllCompoundIds(conn)
#ids == ids2

unlink("test1.db")
```

---

`getAtomAttr`*getAtomAttr*

---

**Description**

On V3000 formatted compounds, returns the value of the given tag on the given atom number.

**Usage**

```
getAtomAttr(x,atomId,tag)
```

**Arguments**

|        |   |
|--------|---|
| x      | An SDFset of ExtSDF objects. ExtSDF objects are created with read.SDFset with extendedAttributes=TRUE when reading V3000 sdf files. |
| atomId | The index of the atom to fetch the tag value from.  |
| tag    | The name of the tag to fetch the value of on the given atom.  |

**Value**

The value of the given tag on the given atom.

**Author(s)**

Kevin Horan

**Examples**

```
## Not run:
getAtomAttr(v3Sdfs,10,"CHG")

## End(Not run)
```

---

getBondAttr                      *getBondAttr*

---

**Description**

On V3000 formatted compounds, returns the value of the given tag on the given bond number.

**Usage**

```
getBondAttr(x, bondId, tag)
```

**Arguments**

|        |   |
|--------|---|
| x      | An SDFset of ExtSDF objects. ExtSDF objects are created with read.SDFset with extendedAttributes=TRUE when reading V3000 sdf files. |
| bondId | The index of the bond to fetch the tag value from.  |
| tag    | The name of the tag to fetch the value of on the given bond.  |

**Value**

The value of the given tag on the given bond.

**Author(s)**

Kevin Horan

**Examples**

```
## Not run:  
getBondAttr(v3Sdfs, 10, "CFG")  
  
## End(Not run)
```

---

getCompoundFeatures            *Get Compound Features*

---

**Description**

Get feature values for specific compounds.

**Usage**

```
getCompoundFeatures(conn, compoundIds, featureNames, filename = NA, keepOrder = FALSE, allowMissing = F
```

**Arguments**

|              |   |
|--------------|---|
| conn         | A database connection object, such as is returned by <code>initDb</code> .  |
| compoundIds  | A vector of <code>compound_id</code> numbers from this database. These are not compound names. Features will be fetched for each compound given here.   |
| featureNames | A vector of features to fetch the value for, for each given compound.   |
| filename     | If given, dump the results into a comma separated values (CSV) file instead of returning a data frame. This can avoid some potential memory limits when fetching large sets of data.                                |
| keepOrder    | Ensure that the output order of values matches the order in which the compound ids were given. This will make things a little slower, so should only be used where required.  |
| allowMissing | If false, raise an exception if a compound cannot be found, otherwise just silently ignore it and return data for whatever compound were found.   |
| batchSize    | The number of compounds to fetch in a single query. If you find your running out of memory you can try reducing this values, as well as try writing the result to a file using the <code>filename</code> parameter. |

**Value**

If `filename` is not given, returns a data frame with the `compound_id` and any given feature names. Each row represents one compound. If `filename` is given a filename then no value is returned, but the given file is created.

**Author(s)**

Kevin Horan

**Examples**

```
#create and initialize a new SQLite database
conn = initDb("test1.db")

data(sdfsampl)

#load data
ids=loadSdf(conn,sdfsampl,
  function(sdfset)
data.frame(MW = MW(sdfset), rings(sdfset,type="count",upper=6, arom=TRUE))
)

f = getCompoundFeatures(conn,ids,c("mw","rings"))

unlink("test1.db")
```



---

|                  |                           |
|------------------|---------------------------|
| getCompoundNames | <i>Get Compound Names</i> |
|------------------|---------------------------|

---

**Description**

Fetch the names of the given compound ids, if they exist

**Usage**

```
getCompoundNames(conn, compoundIds, keepOrder = FALSE, allowMissing = FALSE)
```

**Arguments**

|              |   |
|--------------|---|
| conn         | A database connection object, such as is returned by <code>initDb</code> .  |
| compoundIds  | A vector of compound ids.   |
| keepOrder    | If true, the order of the output compound ids will be the same as the input names. This imposes a performance hit that can be significant for large datasets, thus it should be left FALSE unless needed. |
| allowMissing | When this is false an error will be raised when compound ids queried were not found in the database. If true, just those that are found will be returned with no error or warning.                        |

**Value**

Returns a vector of compound names. The rownames will be the compound ids. Compound ids not found, or for which a name is not defined, will be represented as NA.

**Author(s)**

Kevin Horan

**Examples**

```
#create and initialize a new SQLite database
conn = initDb("test2.db")

data(sdfsampl)

#just load the data with no features or descriptors
ids=loadSdf(conn,sdfsampl)

  getCompoundNames(conn,ids[1:3])
unlink("test3.db")
```

---

getCompounds                      *Get Compounds From Database*

---

### Description

Create SDF objects from the given set of compound ids. Id numbers can be found using the find-Compounds function.

### Usage

```
getCompounds(conn,compoundIds,filename=NA, keepOrder = FALSE, allowMissing = FALSE)
```

### Arguments

|              |   |
|--------------|---|
| conn         | A database connection object, such as is returned by <a href="#">initDb</a> .   |
| compoundIds  | A vector of compound ids, as returned by <a href="#">loadSdf</a> or <a href="#">findCompounds</a> .   |
| filename     | If given, writes the compounds directly to the file named.  |
| keepOrder    | If true, the order of the output compound ids will be the same as the input names. This imposes a performance hit that can be significant for large datasets, thus it should be left FALSE unless needed. |
| allowMissing | When this is false an error will be raised when compound ids queried were not found in the database. If true, just those that are found will be returned with no error or warning.                        |

### Value

An SDFset with the requested compounds or nothing if filename was specified. A warning will be raised if not all compounds could be found.

### Author(s)

Kevin Horan

### See Also

[loadSdf](#) [findCompounds](#).

### Examples

```
#create and initialize a new SQLite database
conn = initDb("test3.db")

data(sdfsampl)

#just load the data with no features or descriptors
ids=loadSdf(conn,sdfsampl)
```

```
#returns a SDFset with 3 compounds
getCompounds(conn, ids[1:3])

unlink("test3.db")
```

---

getIds-deprecated      *Import Compounds from PubChem*

---

### Description

Accepts one or more PubChem compound ids and downloads the corresponding compounds from PubChem Power User Gateway (PUG) returning results in an SDFset container. The ChemMine Tools web service is used as an intermediate, to translate queries from plain HTTP POST to a PUG SOAP query.

### Usage

```
getIds(cids)
```

### Arguments

cids                    A numeric object which contains one or more PubChem cids

### Value

SDFset                for details see ?"SDFset-class"

### Author(s)

Tyler Backman

### References

PubChem PUG SOAP: [http://pubchem.ncbi.nlm.nih.gov/pug\\_soap/pug\\_soap\\_help.html](http://pubchem.ncbi.nlm.nih.gov/pug_soap/pug_soap_help.html)

Chemmine web service: <http://chemmine.ucr.edu>

PubChem help: [http://pubchem.ncbi.nlm.nih.gov/search/help\\_search.html](http://pubchem.ncbi.nlm.nih.gov/search/help_search.html)

### Examples

```
## Not run:
## fetch 2 compounds from PubChem
compounds <- getIds(c(111,123))
## End(Not run)
```

---

grepSDFset                      *String search in SDFset*

---

### Description

Convenience grep function for string searching in SDFset containers.

### Usage

```
grepSDFset(pattern, x, field = "datablock", mode = "subset", ignore.case = TRUE, ...)
```

### Arguments

|             |   |
|-------------|---|
| pattern     | search pattern  |
| x           | SDFset  |
| field       | delimits search to specific section in SDF; can be header, atomblock, bondblock or datablock  |
| mode        | if mode = "index", then the match positions are returned as vector; if mode = "subset", a list with SDF components is returned where every entry has at least one query match |
| ignore.case | TRUE turns off case sensitivity   |
| ...         | option to pass on additional arguments  |

### Details

...

### Value

|         |  |
|---------|--|
| numeric | index vector where the name field contains the component positions in the SDFset and the values the row positions in each sub-component. |
| list    | if mode = "subset"   |

### Author(s)

Thomas Girke

### References

...

### See Also

Class: SDFset

**Examples**

```
## Instances of SDFset class
data(sdfsamples)
sdfset <- sdfsamples

## String Searching in SDFset
q <- grepSDFset("65000", sdfset, field="datablock", mode="subset")
as(q, "SDFset")
grepSDFset("65000", sdfset, field="datablock", mode="index")
```

---

groups

*Enumeration of Functional Groups and Atom Neighbors*

---

**Description**

Returns frequency information of functional groups in molecules provided as SDF or SDFset objects. Alternatively, the function can return for each atom its atom/bond neighbor information.

**Usage**

```
groups(x, groups = "fctgroup", type = "countMA")
```

**Arguments**

|        |   |
|--------|---|
| x      | SDF or SDFset containers  |
| groups | if groups="fctgroup", frequencies of functional groups are returned; if groups="neighbors", atom/bond neighbor information is returned.   |
| type   | if type="all", then the complete neighbor information is generated for each atom in a molecule; if type="count", the neighbors are enumerated in a list and if type="countMA", then the counts of atom neighbors or functional groups are returned in a frequency matrix. |

**Details**

At this point this function is in an experimental stage.

**Value**

...

**Author(s)**

Thomas Girke

**References**

...

**See Also**

...

**Examples**

```
## Instances of SDFset class
data(sdfsampl)
sdfset <- sdfsampl

## Enumerate functional groups
groups(sdfset[1:20], groups="fctgroup", type="countMA")

## Report atom/bond neighbors
groups(sdfset[1:4], groups="neighbors", type="countMA")
groups(sdfset[1:4], groups="neighbors", type="count")
groups(sdfset[1:4], groups="neighbors", type="all")
```

---

header

*Return header block*

---

**Description**

Returns header block(s) from an object of class SDF or SDFset.

**Usage**

```
header(x)
```

**Arguments**

x                    object of class SDF or SDFset

**Details**

...

**Value**

named character vector if SDF is provided or list of named character vectors if SDFset is provided

**Author(s)**

Thomas Girke

**References**

...

**See Also**

atomblock, atomcount, bondblock, datablock, cid, sdfid

**Examples**

```
## SDF/SDFset instances
data(sdfsampl)
sdfset <- sdfsampl
sdf <- sdfset[[1]]

## Extract header block
header(sdf)
header(sdfset[1:4])

## Replacement methods
sdfset[[1]][[1]][1] <- "test"
sdfset[[1]]
header(sdfset)[1] <- header(sdfset[2])
view(sdfset[1:2])
```

---

initDb

*Initialize SQL Database*

---

**Description**

This will ensure that the database connection given is ready for use. If it does not find the tables it needs, it will try to create them.

**Usage**

```
initDb(handle)
```

**Arguments**

handle            This can be either a filename, in which case we assume it is the name of an SQLite database and use RSQLite to connect to it, or else any DBI Connection.

**Value**

Returns a connection object that can be used with other database oriented functions.

**Author(s)**

Kevin Horan

**See Also**

RSQLite

## Examples

```
#create and initialize a new SQLite database
conn = initDb("test.db")
```

---

 jarvisPatrick

*Jarvis-Patrick Clustering*


---

## Description

Function to perform Jarvis-Patrick clustering. The algorithm requires a nearest neighbor table, which consists of neighbors for each item in the dataset. This information is then used to join items into clusters with the following requirements: (a) they are contained in each other's neighbor list (b) they share at least 'k' nearest neighbors. The nearest neighbor table can be computed with [nearestNeighbors](#). For standard Jarvis-Patrick clustering, this function takes the number of neighbors to keep for each item. It also has the option of passing a cutoff similarity value instead of the number of neighbors. In this mode, all neighbors which meet the cutoff criteria will be included in the table. This is a setting that is not part of the original Jarvis-Patrick algorithm. It allows to generate tighter clusters and to minimize some limitations of this method, such as joining completely unrelated items when clustering small data sets. Other extensions, such as the linkage parameter, can also help improve the clustering quality.

## Usage

```
jarvisPatrick(nnm, k, mode="a1a2b", linkage="single")
```

## Arguments

|         |  |
|---------|--|
| nnm     | A nearest neighbor table, as produced by <a href="#">nearestNeighbors</a> .  |
| k       | Minimum number of nearest neighbors two rows (items) in the nearest neighbor table need to have in common to join them into the same cluster.  |
| mode    | If mode = "a1a2b" (default), the clustering is run with both requirements (a) and (b); if mode = "a1b" then (a) is relaxed to a unidirectional requirement; and if mode = "b" then only requirement (b) is used. The size of the clusters generated by the different methods increases in this order: "a1a2b" < "a1b" < "b". The run time of method "a1a2b" follows a close to linear relationship, while it is nearly quadratic for the much more exhaustive method "b". Only methods "a1a2b" and "a1b" are suitable for clustering very large data sets (e.g. >50,000 items) in a reasonable amount of time. |
| linkage | Can be one of "single", "average", or "complete", for single linkage, average linkage and complete linkage merge requirements, respectively. In the context of Jarvis-Patrick, average linkage means that at least half of the pairs between the clusters under consideration must pass the merge requirement. Similarly, for complete linkage, all pairs must pass the merge requirement. Single linkage is the normal case for Jarvis-Patrick and just means that at least one pair must meet the requirement.   |



**Details**

...

**Value**

Depending on the setting under the `type` argument, the function returns the clustering result in a named vector or a nearest neighbor table as `matrix`.

**Note**

...

**Author(s)**

Thomas Girke

**References**

Jarvis RA, Patrick EA (1973) Clustering Using a Similarity Measure Based on Shared Near Neighbors. IEEE Transactions on Computers, C22, 1025-1034. URLs: [http://davide.eynard.it/teaching/2012\\_PAMI/JP.pdf](http://davide.eynard.it/teaching/2012_PAMI/JP.pdf), <http://www.btluke.com/jpclust.html>, <http://www.daylight.com/dayhtml/doc/cluster/index.pdf>

**See Also**

Functions: `cmp.cluster` [trimNeighbors](#) [nearestNeighbors](#)

**Examples**

```
## Load/create sample APset and FPset
data(apset)
fpset <- desc2fp(apset)

## Standard Jarvis-Patrick clustering on APset/FPset objects
jarvisPatrick(nearestNeighbors(apset,numNbrs=6), k=5, mode="a1a2b")
jarvisPatrick(nearestNeighbors(fpset,numNbrs=6), k=5, mode="a1a2b")

## Jarvis-Patrick clustering only with requirement (b)
jarvisPatrick(nearestNeighbors(fpset,numNbrs=6), k=5, mode="b")

## Modified Jarvis-Patrick clustering with minimum similarity 'cutoff'
## value (here Tanimoto coefficient)
jarvisPatrick(nearestNeighbors(fpset,cutoff=0.6, method="Tanimoto"), k=2 )

## Output nearest neighbor table (matrix)
nmm <- nearestNeighbors(fpset,numNbrs=6)

## Perform clustering on precomputed nearest neighbor table
jarvisPatrick(nmm, k=5)
```

---

`jarvisPatrick_c`*Jarvis Patrick Clustering in C code*

---

### Description

This not meant to be used directly, use `jarvisPatrick` instead. It is exposed so other libraries can make use of it.

### Usage

```
jarvisPatrick_c(neighbors,minNbrs,fast=TRUE,bothDirections=FALSE,linkage = "single")
```

### Arguments

|                             |  |
|-----------------------------|--|
| <code>neighbors</code>      | A matrix of integers. Non integer matrices will be coerced. Each row represents one element, indexed 1 to N. The values in row i should be the index value of the neighbors of i. Thus, each value should itself be a valid row index.   |
| <code>minNbrs</code>        | The minimum number of common neighbors needed for two elements to be merged.   |
| <code>fast</code>           | If true, only the neighbors given in each row are checked to see if they share <code>minNbrs</code> neighbors in common. If false, all pairs of elements are compared. For a matrix of size $N \times M$ , the first method yields a running time of $O(NM)$ , while the second yields a running time of $O(N^2)$ .  |
| <code>bothDirections</code> | If true, two elements must contain each other in their neighbor list in order to be merged. If false and <code>fast</code> is true, then only one element must contain the other as a neighbor. If false and <code>fast</code> is false, then neither element must contain the other as a neighbor, though in all cases there must still be at least <code>minNbrs</code> neighbors in common. |
| <code>linkage</code>        | See <code>jarvisPatrick</code> for details.  |

### Value

A cluster array with no names.

### Author(s)

Kevin Horan

---

|                |                  |
|----------------|------------------|
| jobToken-class | Class "jobToken" |
|----------------|------------------|

---

### Description

Container for storing a reference to a remote job ran on the ChemMine Tools web server.

### Objects from the Class

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

### Slots

`tool_name`: Object of class "character"

`jobId`: Object of class "character"

### Methods

`show signature(object = "jobToken")`: check the status of a launched job

### Author(s)

Tyler William H Backman

### References

See ChemMine Tools at <http://chemmine.ucr.edu>.

### See Also

Functions: `launchCMTool`, `toolDetails`, `listCMTools`, `result`, `browseJob`, `status`

### Examples

```
showClass("jobToken")
## Not run:
## launch a job on the server and obtain jobToken back
job1 <- launchCMTool("pubchemID2SDF", 2244)

## check status of the job
status(job1)

## obtain results
result1 <- result(job1)
result1

## End(Not run)
```

---

|                  |                          |
|------------------|--------------------------|
| largestComponent | <i>Largest Component</i> |
|------------------|--------------------------|

---

**Description**

If a single compound in an SDF file contains more than one disconnected component, this function will return an SDF with only the largest component, removing all other components. This will be applied to each SDF in the given SDFset.

**Usage**

```
largestComponent(sdfSet)
```

**Arguments**

sdfSet            any SDFset object.

**Value**

a new SDFset containing only single component compounds.

**Author(s)**

Kevin Horan

**Examples**

```
## Not run:  
sdf = smiles2sdf(c("C1.CCC1C2CC3C4C5(CC(C2C5O)N3C1O)C6=CC=CC=C6N4C TEST"))  
lg = largestComponent(sdf)  
  
## End(Not run)
```

---

|              |  |
|--------------|--|
| launchCMTool | <i>Launch a Tool on ChemMine Tools</i> |
|--------------|--|

---

**Description**

Accepts a tool name (string), input options, and input data to launch a remote web tool on the ChemMine Tools website.

**Usage**

```
launchCMTool(tool_name, input = "", ...)
```

**Arguments**

tool\_name      A tool name matching verbatim an existing tool name as listed by listCMTools.  
input            Input data in the format required for this tool as listed by listCMTools.  
...              Additional options as mentioned by running toolDetails on the tool specified.

**Details**

By running the function toolDetails on a tool of choice, you can see a pre-generated example function call for this tool.

**Value**

jobToken        for details see "?jobToken-class"

**Author(s)**

Tyler William H Backman

**References**

See ChemMine Tools at <http://chemmine.ucr.edu>.

**See Also**

Functions: toolDetails, listCMTools, result, browseJob, status

**Examples**

```
## Not run:  
## list available tools  
listCMTools()  
  
## get detailed instructions on using a tool  
toolDetails("Fingerprint Search")  
  
## download compound 2244 from PubChem  
job1 <- launchCMTool("pubchemID2SDF", 2244)  
  
## check job status and download result  
status(job1)  
result1 <- result(job1)  
  
## End(Not run)
```

---

`listCMTools`*List all available ChemMine Tools*

---

**Description**

Connects to the ChemMine Tools web service and obtains a list of all available tools, and their input and output formats.

**Usage**

```
listCMTools()
```

**Value**

`data.frame` A four column `data.frame` which describes a tool on each row

**Author(s)**

Tyler William H Backman

**References**

See ChemMine Tools at <http://chemmine.ucr.edu>.

**See Also**

Functions: `toolDetails`, `launchCMTool`, `result`, `browseJob`, `status`

**Examples**

```
## Not run:
## list available tools
listCMTools()

## get detailed instructions on using a tool
toolDetails("Fingerprint Search")

## download compound 2244 from PubChem
job1 <- launchCMTool("pubchemID2SDF", 2244)

## check job status and download result
status(job1)
result1 <- result(job1)

## End(Not run)
```

---

|              |                      |
|--------------|----------------------|
| listFeatures | <i>List Features</i> |
|--------------|----------------------|

---

### Description

List the available features in the given database. These features can be used in the [findCompounds](#) function.

### Usage

```
listFeatures(conn)
```

### Arguments

|      |                     |
|------|---------------------|
| conn | Database connection |
|------|---------------------|

### Value

A vector of character feature names.

### Author(s)

Kevin Horan

### See Also

[findCompounds](#)

### Examples

```
#create and initialize a new SQLite database
conn = initDb("test7.db")

data(sdfsampl)

#just load the data with no features or descriptors
ids=loadSdf(conn,sdfsampl,fct=function(sdfset) cbind(mw=MW(sdfset)))
listFeatures(conn) # produces c("mw")
unlink("test7.db")
```

loadSdf

*Load SDF and SMILES Data***Description**

Load an SDF or SMILES formatted file or SDFSet objects into the database. This will also load arbitrary features from the data as well as descriptor data. The `fct` parameter can be used to specify a function which will compute features which will then be indexed and stored in the database. These features can later be used to quickly search for compounds. Descriptors can also be computed and stored in another table.

**Usage**

```
loadSdf(conn, sdfFile, fct = function(x) data.frame()), descriptors=function(x) data.frame(descriptor=
Nlines = 50000, startline = 1, restartNlines = 1e+05,updateByName=FALSE)
loadSmiles(conn, smileFile, ...)
```

**Arguments**

|                            |   |
|----------------------------|---|
| <code>conn</code>          | A database connection object, such as is returned by <a href="#">initDb</a> .   |
| <code>sdfFile</code>       | Either the filename of an SDF formatted file, or and SDFSet object.   |
| <code>smileFile</code>     | The filename of an SMILES formatted file.   |
| <code>...</code>           | When calling <code>loadSmiles</code> , any of the arguments for <code>loadSdf</code> can be used and will be passed to <code>loadSdf</code> internally.   |
| <code>fct</code>           | A function to extract features from the data. It will be handed an SDFSet generated from the data being loaded. This may be done in batches, so there is no guarantee that the given SDFSet will contain the whole dataset. This function should return a data frame with a column for each feature and a row for each compound given, and in the same order. Each of these features will become a new, indexed, table in the database which can be used later to search for compounds. The column name will become the feature name. If not given, no features are computed. |
| <code>descriptors</code>   | This function will also be given an SDFSet object, which may be done in batches. It should return a data frame with the following two columns: "descriptor" and "descriptor_type". The "descriptor" column should contain a string representation of the descriptor, and "descriptor_type" is the type of the descriptor. Our convention for atom pair is "ap" and "fp" for finger print. The order should be maintained. If not given no descriptors are computed.   |
| <code>Nlines</code>        | When reading data from a file, the number of lines to read at a time. See also <a href="#">sdfStream</a> .  |
| <code>startline</code>     | When reading data from a file, the line number to start reading from. See also <a href="#">sdfStream</a>  |
| <code>restartNlines</code> | When reading data from a file and <code>startline &gt; 1</code> , the number of lines to look forward to find the start of the next compound. See also <a href="#">sdfStream</a>  |



**updateByName** If true we make the assumption that all compounds, both in the existing database and the given dataset, have unique names. This function will then avoid re-adding existing, identical compounds, and will update existing compounds with a new definition if a new compound definition with an existing name is given. If false, we allow duplicate compound names to exist in the database, though not duplicate definitions. So identical compounds will not be re-added, but if a new version of an existing compound is added it will not update the existing one, it will add the modified one as a completely new compound with a new compound id.

## Details

Arguments to loadSmiles are the same as those to loadSdf. LoadSmiles will convert its input into an SDFSet and then call loadSdf.

New features can also be added using this function. However, all compounds must have all features so if new features are added to a new set of compounds, all existing features must be computable by the fct function given. If new features are detected, all existing compounds will be run through fct in order to compute the new features for them as well.

For example, if dataset X is loaded with features F1 and F2, and then at a later time we load dataset Y with new feature F3, the fct function used to load dataset Y must compute and return features F1, F2, and F3. loadSdf will call fct with both datasets X and Y so that all features are available for all compounds. If any features are missing an error will be raised.

If just new features are being added, but no new compounds, use the [addNewFeatures](#) function.

## Value

Returns the compound id numbers of each compound loaded. These can be used to retrieve compounds later. These are id numbers computed by the database and are not extracted from the compound data itself.

## Author(s)

Kevin Horan

## See Also

[sdfStream](#)

## Examples

```
#create and initialize a new SQLite database
conn = initDb("test6.db")

data(sdfsample)

#just load the data with no features or descriptors
ids=loadSdf(conn,sdfsample)
unlink("test6.db")
```

```
conn = initDb("test5.db")
#load data and compute 3 features: molecular weight, with the MW function,
# and counts for RINGS and AROMATIC, as computed by rings, which returns a data frame itself.
ids=loadSdf(conn,sdfsampl,
  function(sdfset)
data.frame(MW = MW(sdfset), rings(sdfset,type="count",upper=6, arom=TRUE))
)
unlink("test5.db")
```

---

makeUnique

*Uniquify CMP names*

---

### Description

Creates unique CMP names by appending a counter to each duplication set. The function can be used for any character vector.

### Usage

```
makeUnique(x, silent = FALSE)
```

### Arguments

|        |  |
|--------|--|
| x      | character vector                                       |
| silent | silent = TRUE suppresses message about duplicate count |

### Details

The function is important to maintain unique compound names in the ID slot of SDFset containers.

### Value

|           |  |
|-----------|--|
| character | of same length as x but without duplications |
|-----------|--|

### Author(s)

Thomas Girke

### References

...

### See Also

Functions: cid, sdfid

**Examples**

```
## SDFset instance
data(sdfsamples)
sdfset <- sdfsamples

## Create unique compound IDs
unique_ids <- makeUnique(sdfid(sdfset))
cid(sdfset) <- unique_ids
cid(sdfset[1:4])
```

---

maximallyDissimilar    *Maximally Dissimilar*

---

**Description**

Find a set of compounds that are far away from each other.

**Usage**

```
maximallyDissimilar(compounds, n, similarity = cmp.similarity)
```

**Arguments**

|            |  |
|------------|--|
| compounds  | The set of items from which to pick n dissimilar items. This can be a list of anything that the similarity function will accept. By default this will be an APset.   |
| n          | The number of dissimilar items to return.  |
| similarity | The similarity function to use. By default Tanimoto will be used on APset objects. Internally, this will be converted to a distance function using $1 - \text{similarity}(a,b)$ , so whatever similarity function you use should return a value between 0 and 1. |

**Details**

This will run in  $O(\text{length}(\text{compounds})n)$  time. Based on the algorithm described in (Higgs,1997).

**Value**

A vector of indexes of the dissimilar items.

**Author(s)**

Kevin Horan

**References**

Higgs, R.E., Bemis, K.G., Watson, I.A., and Wikel, J.H. 1997. Experimental designs for selecting molecules from large chemical databases. *J. Chem. Inf. Comput. Sci.* 37, 861-870

**Examples**

```
data(apset)
maximallyDissimilar(apset,10)
```

---

|                  |                          |
|------------------|--------------------------|
| nearestNeighbors | <i>Nearest Neighbors</i> |
|------------------|--------------------------|

---

**Description**

Computes the nearest neighbors of descriptors in an FPset or APset object for use with the [jarvisPatrick](#) clustering function. Only one of numNbrs or cutoff should be given, cutoff will take precedence if both are given. If numNbrs is given, then that many neighbors will be returned for each item in the set. If cutoff is given, then, for each item X, every neighbor that has a similarity value greater than or equal to the cutoff will be returned in the neighbor list for X.

**Usage**

```
nearestNeighbors(x, numNbrs = NULL, cutoff = NULL, ...)
```

**Arguments**

|         |   |
|---------|---|
| x       | Either an FPset or an APset.  |
| numNbrs | Number of neighbors to find for each item. If not enough neighbors can be found the matrix will be padded with NA.  |
| cutoff  | The minimum similarity value an item must have to another item in order to be included in that items neighbor list. This parameter takes precedence over numNbrs. This parameter allows to obtain tighter clustering results. |
| ...     | These parameters will be passed into the distance function used, either <code>cmp.similarity</code> or <code>fpSim</code> , for APset and FPset, respectively.  |

**Value**

The return value is a list with the following components:

|              |   |
|--------------|---|
| indexes      | index values of nearest neighbors, for each item. If cutoff is used, this will be a list of lists, otherwise it will be a matrix  |
| names        | The names of each item in the set, as returned by cid   |
| similarities | The similarity values of each neighbor to the item for that row. This will also be either a list of lists or a matrix, depending on whether or not cutoff was used. Each similarity values corresponds to the id number in the same position in the indexes entry |

**Author(s)**

Kevin Horan

**See Also**

[jarvisPatrick](#) [trimNeighbors](#)

**Examples**

```
data(sdfsampl)
ap = sdf2ap(sdfsampl)
nnm = nearestNeighbors(ap,cutoff=0.5)
clustering = jarvisPatrick(nnm,k=2,mode="a1b")
```

---

numBits

*numBits*

---

**Description**

Returns the number of bits in a fingerprint.

**Usage**

```
numBits(x)
```

**Arguments**

x                    Either an FP or an FPset object.

**Value**

The number of bits in this fingerprint object.

**Author(s)**

Kevin Horan

**Examples**

```
fp = new("FP",fp=c(1,0,1,1, 0,0,1,0))
n = numBits(fp) # == 8
```

---

|       |              |
|-------|--------------|
| obmol | <i>obmol</i> |
|-------|--------------|

---

**Description**

Return reference to an OBMol from OpenBabel, if available. Operates on SDF or SDFset objects.

**Usage**

```
obmol(x)
```

**Arguments**

x                    object of class SDF or SDFset

**Value**

A pointer to an OBMol object, or a vector of pointers for an SDFset.

**Author(s)**

Kevin Horan

**See Also**

header, atomcount, bondblock, datablock, cid, sdfid

**Examples**

```
## SDF/SDFset instances
if(ChemmineR:::haveOB()){
  data(sdfsamples)
  sdfset <- sdfsamples
  sdf <- sdfset[[1]]

  obmolRef = obmol(sdf)
}
```

---

openBabelPlot                      *Plot compound structures*

---

### Description

Plots compound structure(s) for molecules stored in SDF and SDFset containers.

### Usage

```
openBabelPlot(sdfset, height=600, noHbonds = TRUE, regenCoords=FALSE)
```

### Arguments

|             |  |
|-------------|--|
| sdfset      | Object of class SDFset   |
| height      | The height of the image in pixels. The generated image is always square, so this will also be the width.   |
| noHbonds    | If TRUE, then the C-hydrogens and their bonds - explicitly defined in an SDF - are excluded from the plot.   |
| regenCoords | If ChemmineOB is installed and this option is TRUE, then Open Babel will be used to re-generate the 2D coords for each compound before plotting it. This often results in a nicer layout. If you want to save the results of the coord re-generation, call the <a href="#">regenerateCoords</a> function first yourself and save the result. |

### Details

The function openBabelPlot depicts a 2D compound structure based on the XY-coordinates specified in the atom block of an SDF. If more than one compound is given in the SDFset, they will be arranged in a grid layout.

### Author(s)

Kevin Horan

### See Also

`sdf.visualize`

### Examples

```
## Not run:  
## Import SDFset sample set  
data(sdfsamples)  
(sdfset <- sdfsamples)  
  
## Plot single compound structure  
openBabelPlot(sdfset[1])
```

```
## Plot several compounds structures
openBabelPlot(sdfset[1:4])

## End(Not run)
```

---

parBatchByIndex      *Parallel Batch By Index*

---

### Description

Takes an index set, breaks it into batches and runs the given function on each batch in parallel using the given cluster. See [batchByIndex](#) for the non-parallel version.

When doing a select where the condition is a large number of ids it is not always possible to include them in a single SQL statement. This function will break the list of ids into chunks and allow the indexProcessor to deal with just a small number of ids.

### Usage

```
parBatchByIndex(allIndices, indexProcessor, reduce, cl, batchSize = 1e+05)
```

### Arguments

|                |  |
|----------------|--|
| allIndices     | A vector of values that will be broken into batches and passed as an argument to the indexProcessor function.  |
| indexProcessor | A function that takes one batch of indices. It is called once for each batch, possibly in parallel. The return value of this function is collected into a list and passed to the reduce function after all jobs have finished.   |
| reduce         | This function is run after all jobs have finished. It is called with a list of return values from the indexProcessor function runs. The order of batches is maintained. The return value of the reduce function is then returned.<br>The idea is that this function merges all the results together into one result. |
| cl             | A SNOW cluster to run jobs on.   |
| batchSize      | The size of each batch. The last batch may be smaller than this value.   |

### Value

The return value of the reduce function is returned.

### Author(s)

Kevin Horan

### See Also

[batchByIndex](#)



**Examples**

```
## Not run:

cl = makeCluster(2) # create a SNOW cluster

#function to run a query for each batch of indexes
job = function(indexBatch)
dbGetQuery(dbConnection, paste("SELECT weight FROM table WHERE id IN (",paste(indexBatch,collapse=","),")"))

# function to combine all the results, in this case by summing them up
reduce = function(results) sum(unlist(results))

indices = 1:10000

#run queries in parallel and then sum the results
totalWeight = parBatchByIndex(indices,job,reduce,cl, 1000)

## End(Not run)
```

---

plotStruc

*Plot compound structures*


---

**Description**

Plots compound structure(s) for molecules stored in SDF and SDFset containers.

**Usage**

```
## Convenience plot method
# plot(x, griddim, print_cid=cid(x), print=TRUE, ...)

## Less important for user
plotStruc(sdf, atomcex = 1.2, atomnum = FALSE, no_print_atoms = c("C"),
          noHbonds = TRUE, bondspacer = 0.12, colbonds=NULL, bondcol="red",
          regenCoords=FALSE, ...)
```

**Arguments**

|                |  |
|----------------|--|
| sdf            | Object of class SDF  |
| atomcex        | Font size for atom labels  |
| atomnum        | If TRUE, then the atom numbers are included in the plot. They are the position numbers of each atom in the atom block of an SDF. |
| no_print_atoms | Excludes specified atoms from being plotted.   |
| noHbonds       | If TRUE, then the C-hydrogens and their bonds - explicitly defined in an SDF - are excluded from the plot.                       |
| bondspacer     | Numeric value specifying the plotting distance for double/triple bonds.  |

|             |   |
|-------------|---|
| colbonds    | Highlighting of subgraphs in main structure by providing a numeric vector of atom numbers, here position index in atom block. The bonds of connected atoms will be plotted in the color provided under bondcol.   |
| bondcol     | A character or numeric vector of length one to specify the color to use for sub-structure highlighting under colbonds.  |
| regenCoords | If ChemmineOB is installed and this option is TRUE, then Open Babel will be used to re-generate the 2D coords for each compound before plotting it. This often results in a nicer layout. If you want to save the results of the coord re-generation, call the <code>regenerateCoords</code> function first yourself and save the result. |
| ...         | Arguments to be passed to/from other methods.   |

### Details

The function `plotStruc` depicts a single 2D compound structure based on the XY-coordinates specified in the atom block of an SDF. The generic method `plot` can be used as a convenient shorthand to plot one or many structures at once. Both functions depend on the availability of the XY-coordinates in the source SD file and only 2D (not 3D) representations are plotted correctly.

Additional arguments that can only be passed on to the `plot` function when supplied with an SDFset object:

`griddim`: numeric vector of length two to define the dimensions for arranging several structures in one plot.

`print_cid`: character vector for printing custom compound labels. Default is `print_cid=cid(sdfset)`.

`print`: if `print=TRUE`, then a summary of the SDF content for each supplied compound is printed to the screen. This behavior is turned off with `print=FALSE`.

### Value

Prints summary of SDF/SDFset to screen and plots their structures to graphics device.

### Note

The compound depictions created by this function are not as pretty as the structure representations generated with the `sdf.visualize` function. This will be improved in the future.

### Author(s)

Thomas Girke

### References

...

### See Also

`sdf.visualize`

## Examples

```
## Import SDFset sample set
data(sdfsamples)
(sdfset <- sdfsamples)

## Plot single compound structure
plotStruc(sdfset[[1]])

## Plot several compounds structures
plot(sdfset[1:4])

## Highlighting substructures (here all rings)
myrings <- as.numeric(gsub(".*_", "", unique(unlist(rings(sdfset[1])))))
plot(sdfset[1], colbonds=myrings)

## Customize plot
plot(sdfset[1:4], gridDim=c(2,2), print_cid=letters[1:4], print=FALSE, noHbonds=FALSE)
```

---

propOB

*Properties from OpenBabel*

---

## Description

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

## Usage

```
propOB(sdfSet)
```

## Arguments

sdfSet            An SDFset object.

## Value

A data frame with a row for each compound in the given data frame and a named column for each property.

## Author(s)

Kevin Horan

**Examples**

```
## Not run:  
library(ChemmineR)  
data(sdfsamplE)  
propOB(sdfsamplE)  
  
## End(Not run)
```

---

pubchemCidToSDF

*Import Compounds from PubChem*

---

**Description**

Accepts one or more PubChem compound ids and downloads the corresponding compounds from PubChem Power User Gateway (PUG) returning results in an SDFset container.

**Usage**

```
pubchemCidToSDF(cids)
```

**Arguments**

**cids**            A numeric object which contains one or more PubChem cids

**Value**

SDFset            for details see ?"SDFset-class"

**Author(s)**

Kevin Horan

**References**

PubChem PUG REST: [https://pubchem.ncbi.nlm.nih.gov/pug\\_rest/PUG\\_REST\\_Tutorial.html](https://pubchem.ncbi.nlm.nih.gov/pug_rest/PUG_REST_Tutorial.html)

**Examples**

```
## Not run:  
## fetch 2 compounds from PubChem  
compounds <- pubchemCidToSDF(c(111,123))  
## End(Not run)
```

---

|                   |   |
|-------------------|---|
| pubchemFPencoding | <i>Encoding of PubChem Fingerprints</i> |
|-------------------|---|

---

**Description**

Data frame with bit positions and substructure specifications.

**Usage**

```
data(pubchemFPencoding)
```

**Format**

The format is a data frame with 881 rows and 2 columns.

**Source**

From: [ftp://ftp.ncbi.nih.gov/pubchem/specifications/pubchem\\_fingerprints.txt](ftp://ftp.ncbi.nih.gov/pubchem/specifications/pubchem_fingerprints.txt)

**References**

See: [ftp://ftp.ncbi.nih.gov/pubchem/specifications/pubchem\\_fingerprints.txt](ftp://ftp.ncbi.nih.gov/pubchem/specifications/pubchem_fingerprints.txt)

**Examples**

```
data(pubchemFPencoding)  
pubchemFPencoding[1:4,]
```

---

|                  |   |
|------------------|---|
| pubchemInchi2cid | <i>Query pubchem by InChI strings and return CIDs</i> |
|------------------|---|

---

**Description**

Use PubChem API to get CIDs by InChI strings. This function sends one request per InChI. For courtesy, it is not recommended to parallelize this function.

**Usage**

```
pubchemInchi2cid(inchis, verbose = TRUE)
```

**Arguments**

|         |                                    |
|---------|------------------------------------|
| inchis  | Character vector of InChI strings  |
| verbose | Logical, show verbose information? |

**Value**

a numeric vector of CIDs with names. Successful requests will have empty names, requests with invalid InChI strings will have name "invalid" and requests with valid InChI but not found in PubChem will have name "not\_found"

**Author(s)**

Le Zhang

**References**

PubChem PUG REST: [https://pubchem.ncbi.nlm.nih.gov/pug\\_rest/PUG\\_REST\\_Tutorial.html](https://pubchem.ncbi.nlm.nih.gov/pug_rest/PUG_REST_Tutorial.html)

**Examples**

```
## Not run:
inchis <- c(
  "InChI=1S/C15H26O/c1-9(2)11-6-5-10(3)15-8-7-14(4,16)13(15)12(11)15/h9-13,16H,5-8H2,1-4H3/t10-,11+,12-,13",
  "InChI=1S/C3H8/c1-3-2/h3H2,1-2H3",
  "InChI=1S/C15H20Br2O2/c1-2-12(17)13-7-3-4-8-14-15(19-13)10-11(18-14)6-5-9-16/h3-4,6,9,11-15H,2,7-8,10H2,
  "InChI=abc"
)
pubchemInchi2cid(inchis)

## End(Not run)
```

---

pubchemInchikey2sdf     *Query pubchem by InChIKeys strings and get SDF back*

---

**Description**

Use PubChem API to get CIDs by InChIKeys

**Usage**

```
pubchemInchikey2sdf(inchikeys)
```

**Arguments**

inchikeys     Character vector, InChIKey strings.

**Value**

a list of 2 items. the first item "sdf\_set" is a 'SDFset' object. It contains all queried and successful SDF information. The second item "sdf\_index" is a named numeric vector. It records whether all input InChIKeys have successful returns in the 'SDFset' object. If so, a non-zero value is returned as the index of where it exists in the 'SDFset' object, if not, 0 is returned.

**Author(s)**

Le Zhang

**References**PubChem PUG REST: [https://pubchem.ncbi.nlm.nih.gov/pug\\_rest/PUG\\_REST\\_Tutorial.html](https://pubchem.ncbi.nlm.nih.gov/pug_rest/PUG_REST_Tutorial.html)**Examples**

```
## Not run:
## fetch 2 compounds from PubChem
inchikeys <- c(
  "ZFUYSOHVJVQNB-FZERPYLPSA-N",
  "KONGRWVLXLWGDV-BYGOPZEFSA-N",
  "AANKDJLVHZQCFG-WLIQWNBFA-N",
  "SNFRINMTRPQLE-JQWAAABSSA-N"
)
pubchemInchikey2sdf(inchikeys)

## End(Not run)
```

---

`pubchemName2CID`*Translate compound name to pubchem compound id*

---

**Description**

Takes any compound name and queries pubchem to find its pubchem id (CID).

**Usage**`pubchemName2CID(name)`**Arguments**`name` Any compound name, used to query pubchem to find the compound.**Value**

The result is the pubchem compound id. If the name is not found, NA will be returned.

**Author(s)**

Kevin Horan

**References**PubChem PUG REST: [https://pubchem.ncbi.nlm.nih.gov/pug\\_rest/PUG\\_REST\\_Tutorial.html](https://pubchem.ncbi.nlm.nih.gov/pug_rest/PUG_REST_Tutorial.html)

**Examples**

```
## Not run:  
## fetch 2 compounds from PubChem  
cid <- pubchemName2CID("CHEMBL460363")  
  
## End(Not run)
```

---

pubchemSDFSearch

*PubChem Similarity (Fingerprint) Search*

---

**Description**

Accepts one SDFset container and performs a similarity PubChem fingerprint search, returning hits in an SDFset container. If the input object contains multiple items, only the first is used as a query.

**Usage**

```
pubchemSDFSearch(sdf)
```

**Arguments**

sdf                    A SDFset object which contains one compound

**Value**

SDFset                for details see ?"SDFset-class"

**Author(s)**

Kevin Horan

**References**

PubChem PUG REST: [https://pubchem.ncbi.nlm.nih.gov/pug\\_rest/PUG\\_REST\\_Tutorial.html](https://pubchem.ncbi.nlm.nih.gov/pug_rest/PUG_REST_Tutorial.html)

SMILES Format: [http://en.wikipedia.org/wiki/Chemical\\_file\\_format#SMILES](http://en.wikipedia.org/wiki/Chemical_file_format#SMILES)

**Examples**

```
## Not run:  
## get a sample compound  
data(sdfsamples); sdfset <- sdfsamples[2]  
## search a compound on PubChem  
compounds <- pubchemSDFSearch(sdfset)  
## End(Not run)
```



---

pubchemSmilesSearch    *PubChem Similarity (Fingerprint) SMILES Search*

---

### Description

Accepts one SMILE string or SMIset container and performs a PubChem fingerprint search, returning hits in an SDFset container. If the input object contains multiple items, only the first is used as a query.

### Usage

```
pubchemSmilesSearch(smiles)
```

### Arguments

smiles            A SMIset object which contains one compound, or a SMILES string

### Value

SDFset            for details see ?"SDFset-class"

### Author(s)

Kevin Horan

### References

PubChem PUG REST: [https://pubchem.ncbi.nlm.nih.gov/pug\\_rest/PUG\\_REST\\_Tutorial.html](https://pubchem.ncbi.nlm.nih.gov/pug_rest/PUG_REST_Tutorial.html)

SMILES Format: [http://en.wikipedia.org/wiki/Chemical\\_file\\_format#SMILES](http://en.wikipedia.org/wiki/Chemical_file_format#SMILES)

### Examples

```
## Not run:  
## get a sample compound  
data(sdfsampl); sdfset <- sdfsampl[2]  
## search a compound on PubChem  
compounds <- pubchemSmilesSearch(sdfset)  
## End(Not run)
```

---

`read.AP`*Read Atom Pair/Fingerprint Strings*

---

**Description**

Function to convert atom pairs (AP) or fingerprints (e.g. AP fingerprints) stored as character strings to APset or FPset objects (e.g. generated by sdfStream). Alternatively, one can provide the AP or fingerprint strings in a named character vector.

**Usage**

```
read.AP(x, type, colid, isFile = class(x) == "character" & length(x) == 1)
```

**Arguments**

|                     |   |
|---------------------|---|
| <code>x</code>      | name of file from where to read the AP/APFP character strings; or named character vector containing the AP/APFP strings |
| <code>type</code>   | <code>type="ap"</code> for AP character string input, and <code>type="fp"</code> for fingerprint character string input |
| <code>colid</code>  | column containing AP/FP character strings if <code>x</code> is a file   |
| <code>isFile</code> | Is <code>x</code> a file name or not?   |

**Details**

...

**Value**

object of class APset or FPset

**Author(s)**

Thomas Girke

**References**

...

**See Also**

sdf2ap, sdfStream

**Examples**

```

## Load sample data
library(ChemmineR)
data(sdfsample); sdfset <- sdfsample
## Not run: write.SDF(sdfset, "test.sdf")

## Define descriptor set in a simple function
desc <- function(sdfset) {
  cbind(SDFID=sdfid(sdfset),
        # datablock2ma(datablocklist=datablock(sdfset)),
        MW=MW(sdfset),
        groups(sdfset),
        APFP=desc2fp(x=sdf2ap(sdfset), descnames=1024, type="character"),
        AP=sdf2ap(sdfset, type="character"),
        rings(sdfset, type="count", upper=6, arom=TRUE)
  )
}

## Run sdfStream with desc function and write results to a file called 'matrix.xls'
sdfStream(input="test.sdf", output="matrix.xls", fct=desc, Nlines=1000)

## Select molecules from SD File using line index from sdfStream
indexDF <- read.delim("matrix.xls", row.names=1)[,1:4]
indexDFsub <- indexDF[indexDF$MW < 400, ] # Selects molecules with MW < 400
sdfset <- read.SDFindex(file="test.sdf", index=indexDFsub, type="SDFset")

## Write result directly to SD file without storing larger numbers of molecules in memory
read.SDFindex(file="test.sdf", index=indexDFsub, type="file", outfile="sub.sdf")

## Read AP/APFP strings from file into APset or FP object
apset <- read.AP(x="matrix.xls", type="ap", colid="AP")
apfp <- read.AP(x="matrix.xls", type="apfp", colid="APFP")

## Alternatively, one can provide the AP/APFP strings in a named character vector
apset <- read.AP(x=sdf2ap(sdfset[1:20]), type="character"), type="ap")
apfp <- read.AP(x=desc2fp(x=sdf2ap(sdfset[1:20]), descnames=1024, type="character"), type="apfp")

## End(Not run)

```

---

read.SDFindex

*Extract Molecules from SD File by Line Index*


---

**Description**

Extracts specific molecules from SD File based on a line position index computed by the sdfStream function.

**Usage**

```
read.SDFindex(file, index, type = "SDFset", outfile)
```

**Arguments**

|         |   |
|---------|---|
| file    | file name of source SD file used to generate index  |
| index   | data frame containing in the first two columns the start and end positions (index) of molecules in an SD File, respectively. Typically, this index would be imported with read.table/read.delim from a tabular descriptor file generated by the sdfStream function. |
| type    | if type="file", the SDF output will be written to a file named as specified under outfile; if type="SDFset", the SDF data is collected will be a SDFset container.  |
| outfile | name of output file when type="file"  |

**Details**

...

**Value**

Writes molecules in SDF format to file or collects them in SDFset container.

**Author(s)**

Thomas Girke

**References**

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

**See Also**

Import/export functions: read.SDFset, read.SDFstr, read.SDFstr, read.SDFset, write.SDFsplit

**Examples**

```
## Load sample data
library(Cheminer)
data(sdfsampl); sdfset <- sdfsampl
## Not run: write.SDF(sdfset, "test.sdf")

## Define descriptor set in a simple function
desc <- function(sdfset) {
  cbind(SDFID=sdfid(sdfset),
        # datablock2ma(datablocklist=datablock(sdfset)),
        MW=MW(sdfset),
        groups(sdfset),
        # AP=sdf2ap(sdfset, type="character"),
        rings(sdfset, type="count", upper=6, arom=TRUE)
  )
}

## Run sdfStream with desc function and write results to a file called 'matrix.xls'
```

```
sdfStream(input="test.sdf", output="matrix.xls", fct=desc, Nlines=1000)

## Select molecules from SD File using line index from sdfStream
indexDF <- read.delim("matrix.xls", row.names=1)[,1:4]
indexDFsub <- indexDF[indexDF$MW < 400, ] # Selects molecules with MW < 400
sdfset <- read.SDFindex(file="test.sdf", index=indexDFsub, type="SDFset")

## Write result directly to SD file without storing larger numbers of molecules in memory
read.SDFindex(file="test.sdf", index=indexDFsub, type="file", outfile="sub.sdf")

## End(Not run)
```

---

|             |                          |
|-------------|--------------------------|
| read.SDFset | <i>SD file to SDFset</i> |
|-------------|--------------------------|

---

### Description

Imports one or many molecules from an SD/MOL file and stores it in an SDFset container. Supports both the V2000 and V3000 formats.

### Usage

```
read.SDFset(sdfstr = sdfstr, skipErrors=FALSE, ...)
```

### Arguments

|            |   |
|------------|---|
| sdfstr     | path/name to an SD file; alternatively an SDFstr object can be provided   |
| skipErrors | If true, molecules which fail to parse will be removed from the output. Otherwise an error will be thrown and processing of the input will stop.  |
| ...        | option to pass on additional arguments. Possible arguments are:<br>datablock: true or false, whether to include the data fields or not. Defaults to TRUE.<br>tail2vec: true or false, whether to return data fields as a vector or not. Defaults to TRUE.<br>extendedAttributes: true or false, whether to parse the extended attributes available on the V3000 format. Defaults to FALSE. When set to TRUE, the resulting objects will be of type ExtSDF, which is a sub-class of SDF. However, some functions, such as plot, may not work with this type right now. |

### Details

...

### Value

|        |  |
|--------|--|
| SDFset | for details see <code>?SDFset-class</code> |
|--------|--|

**Author(s)**

Thomas Girke

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

Functions: read.SDFstr

**Examples**

```
## Write instance of SDFset class to SD file
data(sdfsampl); sdfset <- sdfsampl
# write.SDF(sdfset[1:4], file="sub.sdf")

## Import SD file
# read.SDFset("sub.sdf")

## Pass on SDFstr object
sdfstr <- as(sdfset, "SDFstr")
read.SDFset(sdfstr)
```

---

|             |                          |
|-------------|--------------------------|
| read.SDFstr | <i>SD file to SDFstr</i> |
|-------------|--------------------------|

---

**Description**

Imports one or many molecules from an SD/MOL file and stores it in an SDFstr container.

**Usage**

read.SDFstr(sdfstr)

**Arguments**

|        |  |
|--------|--|
| sdfstr | path/name to an SD file; alternatively one can pass on a character vector containing lines of an SD file |
|--------|--|

**Details**

...

**Value**

SDFstr for details see ?"SDFstr-class"

**Author(s)**

Thomas Girke

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

Functions: read.SDFset

**Examples**

```
## Write instance of SDFstr class to SD file
data(sdfsampl); sdfset <- sdfsampl
sdfstr <- as(sdfset, "SDFstr")
# write.SDF(sdfset[1:4], file="sub.sdf")

## Import SD file
# read.SDFstr("sub.sdf")

## Pass on SDFstr object
sdfstr <- as(sdfset, "SDFstr")
read.SDFset(sdfstr)
```

---

`read.SMIset`*SMILES file to SMIset*

---

**Description**

Imports one or many molecules from a SMILES file and stores content in a SMIset container. The input file is expected to contain one SMILES string per row with tab-separated compound identifiers at the end of each line. The compound identifiers are optional.

**Usage**

```
read.SMIset(file, removespaces = TRUE, ...)
```

**Arguments**

|              |  |
|--------------|--|
| file         | path/name to a SMILES file             |
| removespaces | if set to TRUE spaces will be removed  |
| ...          | option to pass on additional arguments |

**Details**

...

**Value**

SMIset            for details see ?"SMIset-class"

**Author(s)**

Thomas Girke

**References**

SMILES (Simplified molecular-input line-entry system) format definition: [http://en.wikipedia.org/wiki/Simplified\\_molecular\\_input\\_line-entry\\_system](http://en.wikipedia.org/wiki/Simplified_molecular_input_line-entry_system)

**See Also**

Functions: read.SDFset

**Examples**

```
## Write instance of SMIset class to SMILES file
data(smisample); smiset <- smisample
# write.SMI(smiset[1:4], file="sub.smi")

## Import SMILES file
# read.SMIset("sub.smi")
```

---

regenerateCoords            *Re-generate 2D Coordinates*

---

**Description**

This uses Open Babel (requires ChemmineOB package) to re-generate the 2D coordinates of compounds. This often results in a nicer layout of the compound when plotting.

**Usage**

```
regenerateCoords(sdf)
```

**Arguments**

sdf            A SDF or SDFset object whose coordinates will be re-generated.

**Value**

Either an SDF object if given an SDF, or else an SDFset.

**Author(s)**

Kevin Horan



**See Also**[plotStruc](#)**Examples**

```
## Not run:  
data(sdfsamplE)  
prettySdfset = regenerateCoords(sdfsamplE[1:4])  
  
## End(Not run)
```

---

**result***Obtain the resulting output data from a ChemMine Tools Job*

---

**Description**

Accepts a jobToken job as returned by the function launchCMTool and returns the final result. If the job is still running, the function will loop until the job is ready.

**Usage**

```
result(object)
```

**Arguments**

object            A jobToken job as returned by the function launchCMTool

**Value**

Output will be in the format specified for this tool, as listed with the listCMTools function.

**Author(s)**

Tyler William H Backman

**References**

See ChemMine Tools at <http://chemmine.ucr.edu>.

**See Also**

Functions: toolDetails, listCMTools, launchCMTool, browseJob, status

## Examples

```
## Not run:
## list available tools
listCMTools()

## get detailed instructions on using a tool
toolDetails("Fingerprint Search")

## download compound 2244 from PubChem
job1 <- launchCMTool("pubchemID2SDF", 2244)

## check job status and download result
status(job1)
result1 <- result(job1)

## End(Not run)
```

---

rings

*Ring and Aromaticity Perception*

---

## Description

Identifies all possible rings in molecules using the exhaustive ring perception algorithm from Hanser et al (1996). In addition, the function can return all smallest possible rings as well as aromaticity information for each ring.

Note that large molecules can cause this function to run for an extremely long amount of time. Use the upper parameter to limit the ring size if run time is a problem.

## Usage

```
rings(x, upper = Inf, type = "all", arom = FALSE, inner = FALSE)
```

## Arguments

|       |   |
|-------|---|
| x     | SDF or SDFset containers  |
| upper | allows to specify an upper length limit for ring predictions. The default setting upper=Inf will return all possible rings. Smaller length limits will reduce the search space resulting in shortened compute times.  |
| type  | if type="all", the function returns each ring of a compound as character vector of atom symbols that are numbered by their position in the atom block of an SDF/SDFset object. Note: the example below shows how to plot structures with the same numbering information for visual inspection. If type="arom", only aromatic rings are returned, while type="count" returns the ring and/or aromaticity counts for each compound in a matrix. |

|       |   |
|-------|---|
| arom  | <p>if arom="TRUE", ring aromaticity information will be computed. If type="all", the output is a logical vector where 'TRUE' values indicate aromatic rings in the associated ring list. If type="arom", then the function returns only aromatic rings. A ring is considered aromatic if it meets the following requirements: (i) all atoms in the ring need to be sp<sup>2</sup> hybridized. This means each atom has to have a double bond or at least one lone electron pair and it needs to be attached to an sp<sup>2</sup> hybridized atom. (ii) In addition, Hueckel's rule '4n + 2' needs to be true, where 'n' is either zero or any positive integer.</p> <p>Note that setting arom="TRUE" will also set upper=Inf.</p> |
| inner | <p>if inner="TRUE", only inner (smallest possible) rings will be returned. They are identified by first computing all possible rings and then selecting only the inner rings. Note: this requires the setting upper=Inf. If only rings below a certain size limit (e.g. 6) are of interest, then it will be more time efficient to set this limit under the upper argument than identifying all smallest rings.</p>   |

### Details

...

### Value

The settings type="all" and type="arom" return lists, and type="count" returns a matrix.

### Author(s)

Thomas Girke

### References

Hanser, Jauffret and Kaufmann (1996) A New Algorithm for Exhaustive Ring Perception in a Molecular Graph. *Journal of Chemical Information and Computer Sciences*, 36: 1146-1152. URL: <http://pubs.acs.org/doi/abs/10.1021/ci960322f>

### See Also

...

### Examples

```
## Instances of SDFset class
data(sdfsampl)
sdfset <- sdfsampl

## Return all possible rings for a single compound
rings(sdfset[1], upper=Inf, type="all", arom=FALSE, inner=FALSE)
plot(sdfset[1], print=FALSE, atomnum=TRUE, no_print_atoms="H")

## Return all possible rings for several compounds plus their
## aromaticity information
rings(sdfset[1:4], upper=Inf, type="all", arom=TRUE, inner=FALSE)
```

```

## Return rings with no more than 6 atoms
rings(sdfset[1:4], upper=6, type="all", arom=TRUE, inner=FALSE)

## Return rings with no more than 6 atoms that are also aromatic
rings(sdfset[1:4], upper=6, type="arom", arom=TRUE, inner=FALSE)

## Return shortest possible rings (no complex rings)
rings(sdfset[1:4], upper=Inf, type="all", arom=TRUE, inner=TRUE)

## Count shortest possible rings
rings(sdfset[1:4], upper=Inf, type="count", arom=TRUE, inner=TRUE)

```

---

SDF-class

*Class "SDF"*


---

### Description

Container for storing every element of a single molecule defined in an SD/MOL file without information loss in a list-like container. The import occurs via the `SDFstr` container class. The header block is stored as named character vector, the atom/bond blocks as matrices and the data block as named character vector.

### Objects from the Class

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

### Slots

**header:** Object of class "character"  
**atomblock:** Object of class "matrix"  
**bondblock:** Object of class "matrix"  
**datablock:** Object of class "character"  
**obmolRef:** Object of class "ExternalReferenceOrNULL"  
**version:** Object of class "character"

### Methods

**[** signature(x = "SDF"): subsetting of class with bracket operator  
**[[** signature(x = "SDF"): returns one of the four object components  
**[[<-** signature(x = "SDF"): replacement method for the four sub-components  
**[<-** signature(x = "SDF"): replacement method for the four sub-components  
**atomblock** signature(x = "SDF"): returns atom block as matrix  
**atomcount** signature(x = "SDF"): returns atom frequency  
**bondblock** signature(x = "SDF"): returns bond block as matrix

**obmol** signature(x = "SDF"): returns an OBMol pointer  
**coerce** signature(from = "character", to = "SDF"): as(character, "SDF")  
**coerce** signature(from = "list", to = "SDF"): as(list, "SDF")  
**coerce** signature(from = "SDF", to = "character"): as(sdf, "character")  
**coerce** signature(from = "SDF", to = "list"): as(sdf, "list")  
**coerce** signature(from = "SDF", to = "SDFset"): as(sdf, "SDFset")  
**coerce** signature(from = "SDF", to = "SDFstr"): as(SDF, "SDFstr")  
**coerce** signature(from = "SDFset", to = "SDF"): as(sdfset, "SDF")  
**datablock** signature(x = "SDF"): returns data block as named character vector  
**datablocktag** signature(x = "SDF"): returns data block as named character vector with subsetting support  
**header** signature(x = "SDF"): returns header block as named character vector  
**plot** signature(x = "SDF"): plots molecule structure for SDF object  
**sdf2list** signature(x = "SDF"): returns SDF object as list  
**sdf2str** signature(sdf = "SDF"): returns SDF object as character vector  
**sdfid** signature(x = "SDF"): returns molecule ID field from header block  
**show** signature(object = "SDF"): prints summary of SDF

### Author(s)

Thomas Girke

### References

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

### See Also

Related classes: SDFset, SDFstr, AP, APset

### Examples

```
showClass("SDF")

## Instances of SDF class
data(sdfsamples); sdfset <- sdfsamples
(sdf <- sdfset[[1]]) # returns first molecule in sdfset as SDF object

## Accessing SDF components
header(sdf); atomblock(sdf); bondblock(sdf); datablock(sdf)
sdfid(sdf)

## Plot molecule structure of SDF
plot(sdf) # plots to R graphics device
# sdf.visualize(sdf) # viewing in browser
```

---

`sdf.subset`*Subset a SDF and return SDF segments for selected compounds*

---

### Description

'sdf.subset' will take a descriptor database generated by 'cmp.parse' and an array of indices, and return an SDF string consisting of SDFs for compounds corresponding to that list of indices. The returned value is a character string.

### Usage

```
sdf.subset(db, cmps)
```

### Arguments

|      |  |
|------|--|
| db   | The database generated by 'cmp.parse'  |
| cmps | An array of indices that correspond to a set of selected compounds from the database |

### Details

'sdf.subset' depends on information embedded in the descriptor database returned by 'cmp.parse'. It also relies on the availability of the original SDF where the database has been generated from. Basically, when 'cmp.parse' parses the original SDF file, it will store the path of that SDF file as well as offset information for SDF segment in that file. Therefore, if the SDF file has been changed or deleted, 'sdf.subset' cannot function properly.

The result SDF will also have names added to compounds if they are not present in the original SDF.

### Value

Return a character string whose content is the concatenation of SDFs for the selected compounds.

### See Also

[cmp.parse](#), [sdf.visualize](#)

### Examples

```
## Note: this functionality has become obsolete since the introduction of the
## 'SDFset' and 'apset' S4 classes.

# load sample database from web
# db <- cmp.parse("http://bioweb.ucr.edu/ChemMineV2/static/example_db.sdf")
# select SDF for 1st and 2nd compound in that SDF
# sdf_segments <- sdf.subset(db, c(1, 2))
# now sdf_segments contain the 2 SDFs for those 2 compounds
```

---

|               |  |
|---------------|--|
| sdf.visualize | <i>Visualize an SDFset online using ChemMine Tools</i> |
|---------------|--|

---

**Description**

'sdf.visualize' will take an SDFset object and send the compounds to the ChemMine Tools website, for visualization and further analysis. The results are launched in the users web browser.

**Usage**

```
sdf.visualize(sdf)
```

**Arguments**

sdf                    A SDFset object which containing the given compounds

**Value**

Returns the URL of the webpage containing all the SDFs and 2D images corresponding to the selected compounds.

**Author(s)**

Tyler Backman

**References**

ChemMine Tools web service: <http://chemmine.ucr.edu>

**See Also**

[cmp.parse](#), [sdf.subset](#), [plotStruc](#)

**Examples**

```
## Load sample SD file
data(sdfsamples)
sdfset <- sdfsamples

## Not run:
## Plot structures using web service ChemMine Tools
sdf.visualize(sdfset[1:4])

## End(Not run)
```

---

`sdf2ap`*Atom pair library*

---

**Description**

Creates from a SDFset a searchable atom pair library that is stored in a container of class APset.

**Usage**

```
sdf2ap(sdfset, type = "AP",uniquePairs=TRUE)
```

**Arguments**

|                          |   |
|--------------------------|---|
| <code>sdfset</code>      | Objects of classes SDFset or SDF  |
| <code>type</code>        | if type="AP", the function returns APset/AP objects; if type="character", it returns the result as a character vector of length one. The latter is useful for storing AP data in tabular files. |
| <code>uniquePairs</code> | When the same atom pair occurs more than once in a single compound, should the names be unique or not? Setting this to true will take slightly longer to compute.                               |

**Details**

...

**Value**

|       |                    |
|-------|--------------------|
| APset | if input is SDFset |
| AP    | if input is SDF    |

**Author(s)**

Thomas Girke

**References**

Chen X and Reynolds CH (2002). "Performance of similarity measures in 2D fragment-based similarity searching: comparison of structural descriptors and similarity coefficients", J Chem Inf Comput Sci.

**See Also**

Functions: desc2fp, SDF2apcmp, apset2descdb, cmp.search, cmp.similarity

Related classes: SDF, SDFset, SDFstr, APset.



**Examples**

```
## Instance of SDFset class
data(sdfsampl)
sdfset <- sdfsampl[1:50]
sdf <- sdfsampl[[1]]

## Compute atom pair library
ap <- sdf2ap(sdf)
(apset <- sdf2ap(sdfset))
view(apset[1:4])

## Return main components of APset object
cid(apset[1:4]) # compound IDs
ap(apset[1:4]) # atom pair descriptors

## Return atom pairs in human readable format
db.explain(apset[1])

## Coerce APset to other objects
apset2descdb(apset) # returns old list-style AP database
tmp <- as(apset, "list") # returns list
as(tmp, "APset") # convert list back to APset

## Compound similarity searching with APset
cmp.search(apset, apset[1], type=3, cutoff=0.2)
plot(sdfset[names(cmp.search(apset, apset[6], type=2, cutoff=0.4))])

## Identify compounds with identical AP sets
cmp.duplicated(apset, type=2)

## Structure similarity clustering
cmp.cluster(db=apset, cutoff = c(0.65, 0.5))[1:20,]
```

---

SDF2apcmp

*SDF to list for AP generation*

---

**Description**

Returns SDF class as list containing the components for generating atom pair descriptors.

**Usage**

```
SDF2apcmp(SDF)
```

**Arguments**

SDF                    SDF

**Details**

...

**Value**

list with atom and bond components

**Author(s)**

Thomas Girke

**References**

Chen X and Reynolds CH (2002). "Performance of similarity measures in 2D fragment-based similarity searching: comparison of structural descriptors and similarity coefficients", J Chem Inf Comput Sci.

**See Also**

Functions: sdf2ap, apset2descdb, cmp.search, cmp.similarity

**Examples**

```
## Instances of SDFset class
data(sdfsampl)
sdf <- sdfsampl[[1]]

## Return list
cmp <- SDF2apcmp(sdf)
```

---

sdf2list

SDF to list

---

**Description**

Returns objects of class SDF as list.

**Usage**

```
sdf2list(x)
```

**Arguments**

x object of class SDF

**Details**

...

**Value**

|           |                            |
|-----------|----------------------------|
| list      | with following components: |
| character | SDF header block           |
| matrix    | SDF bond block             |
| matrix    | SDF atom block             |
| character | SDF data block             |

**Author(s)**

Thomas Girke

**References**

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

**See Also**

Functions: sdfstr2list, sdf2str, SDFset2list, SDFset2SDF

**Examples**

```
## Instance of SDF class
data(sdfsampl); sdfset <- sdfsampl
sdf <- sdfset[[1]]

## Return as list
sdf2list(sdf)
as(sdf, "list") # similar result
```

---

|            |   |
|------------|---|
| sdf2smiles | SDFset to character <i>Convert SDFset to SMILES</i> (character) |
|------------|---|

---

**Description**

Accepts compounds in an SDFset container and returns the corresponding SMILES (Simplified Molecular Input Line Entry Specification) strings as SMIset object. If ChemineOB is available then OpenBabel for the format conversion. Otherwise the compound is submitted to the ChemMine Tools web service for conversion with the Open Babel Open Source Chemistry Toolbox. If the input object contains multiple items, only the first is converted.

**Usage**

```
sdf2smiles(sdf)
```

**Arguments**

sdf                    A SDFset object which containing the given compounds

**Value**

character for details see ?"character"

**Author(s)**

Tyler Backman, Kevin Horan

**References**

Chemmine web service: <http://chemmine.ucr.edu>

Open Babel: <http://openbabel.org>

SMILES Format: [http://en.wikipedia.org/wiki/Chemical\\_file\\_format#SMILES](http://en.wikipedia.org/wiki/Chemical_file_format#SMILES)

**Examples**

```
## Not run:
## get a sample compound
data(sdfsamples); sdfset <- sdfsamples[1]
## convert to smiles
(smiles <- sdf2smiles(sdfset))
as.character(smiles)

## End(Not run)
```

---

sdf2str

SDF to SDFstr

---

**Description**

Converts SDF to SDFstr. Its main use is to facilitate the export to SD files. It contains optional arguments to generate custom SDF output.

**Usage**

```
sdf2str(sdf, head, ab, bb, db, cid = NULL, sig = FALSE, ...)
```

**Arguments**

|      |   |
|------|---|
| sdf  | object of class SDF   |
| head | optional character vector to supply custom header block   |
| ab   | optional matrix to supply custom atom block   |
| bb   | optional matrix to supply custom bond block   |
| db   | optional character vector to supply custom data block   |
| cid  | character can be provided to inject custom compound ID into header block                            |
| sig  | if = TRUE then the ChemmineR signature will be injected into the header block for tracking purposes |
| ...  | option to pass on additional arguments  |

**Details**

If the export function `write.SDF` is supplied with an `SDFset` object, then `sdf2str` is used internally to customize the export of many molecules to a single SD file using the same optional arguments.

**Value**

`sdfstr`                    SDF data of one molecule collapsed to character vector

**Author(s)**

Thomas Girke

**References**

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

**See Also**

Coerce functions: `sdfstr2list`, `sdf2str`, `SDFset2list`, `SDFset2SDF`

Export function: `write.SDF`

**Examples**

```
## Instance of SDF class
data(sdfsamples); sdfset <- sdfsamples
sdf <- sdfset[[1]]

## Customize SDF blocks for export to SD file
sdf2str(sdf=sdf, sig=TRUE, cid=TRUE) # uses default SDF components
sdf2str(sdf=sdf, head=letters[1:4], db=NULL) # uses custom components for header and datablock

## The same arguments can be supplied to the write.SDF function for
## batch export of custom SDFs
# write.SDF(sdfset[1:4], file="sub.sdf", sig=TRUE, cid=TRUE, db=NULL)
```

---

SDFDataTable

*SDF Data Table*

---

**Description**

Creates an HTML DataTable showing the compound image along with the fields in the compound data block. Using a browser, this table can be filtered and paged, among other things.

This uses the DT library to create the DataTable.

**Usage**

```
SDFDataTable(sdfset)
```

**Arguments**

sdfset            An SDFSet object

**Value**

Returns the result of the datatable function from the DT library. An HTML file can be created from this value by calling the saveWidget function on it.

**Author(s)**

Kevin Horan

**References**

DT library: <https://rstudio.github.io/DT/> DataTables javascript library: <https://datatables.net/>

**Examples**

```
## Not run: #depends on ChemmineOB
library(ChemmineR)
library(DT)
data(sdfsamples)

# this will open a browser to display the result
x=SDFDataTable(sdfsamples[1:3])

# if no GUI is available or you want to save the HTML result:
saveWidget(x,"output.html")

## End(Not run)
```

---

sdfid                            *Return SDF compound IDs*

---

**Description**

Returns the compound identifiers from the header block of SDF or SDFset objects.

**Usage**

```
sdfid(x, tag = 1)
```

**Arguments**

x                            object of class SDFset or SDF  
tag                          values from 1-4 to extract different header block fields; SDF ID is in first one (default)

**Details**

...

**Value**

character vector

**Author(s)**

Thomas Girke

**References**

...

**See Also**

atomblock, atomcount, bondblock, datablock, header, cid

**Examples**

```
## SDF/SDFset instances
data(sdfsampl)
sdfset <- sdfsampl
sdf <- sdfset[[1]]

## Extract IDs from header block
sdfid(sdf, tag=1)
sdfid(sdfset[1:4])

## Extract compound IDs from ID slot in SDFset container
cid(sdfset[1:4])

## Assigning compound IDs and keeping them unique
unique_ids <- makeUnique(sdfid(sdfset))
cid(sdfset) <- unique_ids
cid(sdfset[1:4])
```

---

sdfsampl

*SD file in SDFset object*

---

**Description**

First 100 compounds from PubChem SD file: Compound\_00650001\_00675000.sdf.gz

**Usage**

```
data(sdfsampl)
```

**Format**

Object of class sdfset

**Details**

Object stores 100 molecules from a sample SD file.

**Source**

[ftp://ftp.ncbi.nih.gov/pubchem/Compound/CURRENT-Full/SDF/Compound\\_00650001\\_00675000.sdf.gz](ftp://ftp.ncbi.nih.gov/pubchem/Compound/CURRENT-Full/SDF/Compound_00650001_00675000.sdf.gz)

**References**

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

**Examples**

```
data(sdfsampl)  
sdfset <- sdfsampl  
view(sdfset[1:4])
```

---

SDFset-class

*Class "SDFset"*

---

**Description**

List-like container for storing one or many objects of class SDF each containing the structure definition information of molecules provided by an SD/MOL file. The SDFset is the most important class in the ChemmineR package for accessing and manipulating information stored in SD files.

**Objects from the Class**

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

**Slots**

SDF: Object of class "list" storing SDF components

ID: Object of class "character" storing compound identifiers

**Methods**

[ signature(x = "SDFset"): subsetting of class with bracket operator

[[ signature(x = "SDFset"): returns single component as SDF object

[[<- signature(x = "SDFset"): replacement method for single SDF component

[<- signature(x = "SDFset"): replacement method for several SDF components

**atomblock** signature(x = "SDFset"): returns all atom blocks as list



**atomcount** signature(x = "SDFset"): returns all atom frequencies as list  
**bondblock** signature(x = "SDFset"): returns all bond blocks as list  
**obmol** signature(x = "SDFset"): returns pointers to OBMol objects as a vector  
**c** signature(x = "SDFset"): concatenates two SDFset containers  
**cid** signature(x = "SDFset"): returns all compound identifiers from ID slot  
**header<-** signature(x = "SDFset"): replacement method for header block  
**atomblock<-** signature(x = "SDFset"): replacement method for atom block  
**bondblock<-** signature(x = "SDFset"): replacement method for bond block  
**datablock<-** signature(x = "SDFset"): replacement method for data block  
**coerce** signature(from = "list", to = "SDFset"): as(list, "SDFset")  
**coerce** signature(from = "SDF", to = "SDFset"): as(sdf, "SDFset")  
**coerce** signature(from = "SDFset", to = "list"): as(sdfset, "list")  
**coerce** signature(from = "SDFset", to = "SDF"): as(sdfset, "SDF")  
**coerce** signature(from = "SDFset", to = "SDFstr"): as(sdfset, "SDFstr")  
**coerce** signature(from = "SDFstr", to = "SDFset"): as(sdfstr, "SDFset")  
**datablock** signature(x = "SDFset"): returns all data blocks as list  
**datablocktag** signature(x = "SDFset"): returns all data blocks as named as list with subsetting support  
**header** signature(x = "SDFset"): returns all header blocks as list  
**length** signature(x = "SDFset"): returns number of entries stored in object  
**plot** signature(x = "SDFset"): plots one or many molecule structures from SDFset object  
**sdfid** signature(x = "SDFset"): returns molecule ID field from header block  
**SDFset2list** signature(x = "SDFset"): returns SDFset object as list  
**SDFset2SDF** signature(x = "SDFset"): returns SDFset object as list with SDF components  
**SDFset2SDF<-** signature(x = "SDFset"): replacement method for SDFset component in SDFset using accessor method  
**show** signature(object = "SDFset"): prints summary of SDFset  
**view** signature(x = "SDFset"): prints extended summary of SDFset  
**SDFset** SDFset(SDF, ID): interface to SDFset constructor

**Author(s)**

Thomas Girke

**References**

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

**See Also**

Related classes: SDF, SDFstr, AP, APset

Import function: read.SDFset("some\_SDF\_file")

Export function: write.SDF(sdfset, "some\_file.sdf")

## Examples

```
showClass("SDFset")

## Instances of SDFset class
data(sdfsample); sdfset <- sdfsample
sdfset; view(sdfset[1:4])
sdfset[[1]]

## Import and store SD File in SDFset container
# sdfset <- read.SDFset("some_SDF_file")

## Miscellaneous accessor methods
header(sdfset[1:4])
atomblock(sdfset[1:4])
atomcount(sdfset[1:4])
bondblock(sdfset[1:4])
datablock(sdfset[1:4])

## Assigning compound IDs and keeping them unique
cid(sdfset); sdfid(sdfset)
unique_ids <- makeUnique(sdfid(sdfset))
cid(sdfset) <- unique_ids

## Convert data block to matrix
blockmatrix <- datablock2ma(datablocklist=datablock(sdfset)) # Converts data block to matrix
numchar <- splitNumChar(blockmatrix=blockmatrix) # Splits to numeric and character matrix
numchar[[1]][1:4,]; numchar[[2]][1:4,]

## Compute atom frequency matrix, molecular weight and formula
propma <- data.frame(MF=MF(sdfset), MW=MW(sdfset), atomcountMA(sdfset))
propma[1:4, ]

## Assign matrix data to data block
datablock(sdfset) <- propma
view(sdfset[1:4])

## String Searching in SDFset
grepSDFset("650001", sdfset, field="datablock", mode="subset") # To return index, set mode="index")

## Export SDFset to SD file
# write.SDF(sdfset[1:4], file="sub.sdf", sig=TRUE)

## Plot molecule structure of SDF
plot(sdfset[1:4]) # plots to R graphics device
# sdf.visualize(sdfset[1:4]) # viewing in browser
```

**Description**

Returns object of class SDFset as list where each component consists of a list of the four SDF sub-components: header block, atom block, bond block and data block.

**Usage**

```
SDFset2list(x)
```

**Arguments**

x                    object of class SDFset

**Details**

...

**Value**

|           |  |
|-----------|--|
| list      | containing one or many lists each with following components: |
| character | SDF header block   |
| matrix    | SDF bond block   |
| matrix    | SDF atom block   |
| character | SDF data block   |

**Author(s)**

Thomas Girke

**References**

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

**See Also**

Functions: sdfstr2list, sdf2str, sdf2list, SDFset2SDF

**Examples**

```
## Instance of SDFset class
data(sdfsampl); sdfset <- sdfsampl
sdfset

## Returns sdfset as list
SDFset2list(sdfset[1:4])
as(sdfset, "list")[1:4] # similar result
```

---

**SDFset2SDF***SDFset to list with many SDF*

---

**Description**

Returns object of class SDFset as list where each component consists of an SDF object.

**Usage**

```
SDFset2SDF(x)
```

**Arguments**

x                    object of class SDFset

**Details**

...

**Value**

list                containing one or many SDF objects

**Author(s)**

Thomas Girke

**References**

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

**See Also**

Functions: sdfstr2list, sdf2str, sdf2list, SDFset2list

**Examples**

```
## Instance of SDFset class
data(sdfsampl); sdfset <- sdfsampl
sdfset

## Returns sdfset as list
SDFset2SDF(sdfset[1:4])
as(sdfset, "SDF")[1:4] # similar result
view(sdfset[1:4]) # same result
```

---

SDFstr-class

Class "SDFstr"

---

### Description

List-like container for storing one or many molecules from an SD (or MOL) file. Each component of an SDFstr object stores the SD data line by line from a single molecule in a character vector. The SDFstr class is an intermediate container to import SD files into the more important SDFset object or to export the data back from an SDFset container to a valid SD file.

### Objects from the Class

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

### Slots

a: Object of class "list" with character components

### Methods

[ signature(x = "SDFstr"): subsetting of class with bracket operator  
[[ signature(x = "SDFstr"): returns single component as character vector  
[[<- signature(x = "SDFstr"): replacement method for single SDFstr component  
[<- signature(x = "SDFstr"): replacement method for several SDFstr components  
**coerce** signature(from = "character", to = "SDFstr"): as(character, "SDFstr")  
**coerce** signature(from = "list", to = "SDFstr"): as(list, "SDFstr")  
**coerce** signature(from = "SDF", to = "SDFstr"): as(sdf, "SDFstr")  
**coerce** signature(from = "SDFset", to = "SDFstr"): as(sdfset, "SDFstr")  
**coerce** signature(from = "SDFstr", to = "list"): as(sdfstr, "list")  
**coerce** signature(from = "SDFstr", to = "SDFset"): as(sdfstr, "SDFset")  
**length** signature(x = "SDFstr"): returns length of SDFstr  
**sdfstr2list** signature(x = "SDFstr"): accessor method to return SDFstr as list  
**sdfstr2list<-** signature(x = "SDFstr"): replacement method for several SDFstr components  
**show** signature(object = "SDFstr"): prints summary of SDFstr

### Author(s)

Thomas Girke

### References

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

**See Also**

Related classes: SDFset, AP, APset

Import function: read.SDFstr("some\_SDF\_file")

**Examples**

```
showClass("SDFstr")

## Instances of SDFstr class
data(sdfsampl); sdfset <- sdfsampl
sdfstr <- as(sdfset, "SDFstr")
sdfstr[1:4] # print summary of container content
sdfstr[[1]] # returns character vector

## Import: sdfstr <- read.SDFstr("some_SDF_file")
## Export: write.SDF(sdfstr, "some_file.sdf")
```

---

sdfstr2list

SDFstr to list

---

**Description**

Returns objects of class SDFstr as list.

**Usage**

```
sdfstr2list(x)
```

**Arguments**

x                    object of class SDFstr

**Details**

...

**Value**

list                with many of the following components:  
character          SDF content of one molecule vectorized line by line

**Author(s)**

Thomas Girke

**References**

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

**See Also**

Functions: sdf2list, sdf2str, SDFset2list, SDFset2SDF

**Examples**

```
## Instance of SDFstr class
data(sdfsampl); sdfset <- sdfsampl
sdfstr <- as(sdfset, "SDFstr")

## Return as list
sdfstr2list(sdfstr)
as(sdfstr, "list") # similar result
```

---

sdfStream

*Streaming through large SD files*


---

**Description**

Streaming function to compute descriptors for large SD Files without consuming much memory. In addition to descriptor values, it returns a line index that defines the positions of each molecule in the source SD File. This line index can be used by the read.SDFindex function to retrieve specific compounds of interest from large SD Files without reading the entire file into memory.

**Usage**

```
sdfStream(input, output, append=FALSE, fct, Nlines = 10000, startline=1, restartNlines=10000, silent =
```

**Arguments**

|               |   |
|---------------|---|
| input         | file name of input SD file  |
| output        | file name of tabular descriptor file  |
| append        | if append=FALSE, a new output file will be created, if one with the same name exists it will be overwritten; whereas append=TRUE will be appended to this file.   |
| fct           | Function to select descriptor sets; any combination of descriptors, supported by ChemmineR, can be chosen here, as long as they can be represented in tabular format.   |
| Nlines        | Number of lines to read from input SD File at a time; the memory consumption will be proportional to this value.  |
| startline     | For restarting sdfStream at specific line assigned to startline argument. If assigned startline value does not match the first line of a molecule in the SD file then it will be reset to the start position of the next molecule in the SD file. |
| restartNlines | Number of lines to parse when startline > 1 in order to identify proper molecule start position. The default value of 10,000 is usually a good choice.  |
| silent        | if silent=FALSE, the processing status will be printed to the screen, while silent=TRUE suppresses this output.   |
| ...           | Arguments to be passed to/from other methods.   |

**Details**

...

**Value**

Writes a descriptor matrix to a tabular file. The first and last line number (position index) of each molecule is specified in the first two columns of the tabular output file, respectively.

**Author(s)**

Thomas Girke

**References**

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

**See Also**

Import/export functions: read.AP, read.SDFset, read.SDFstr, read.SDFstr, read.SDFset, write.SDFsplit

**Examples**

```
## Load sample data
library(ChemmineR)
data(sdfsamples); sdfset <- sdfsamples
## Not run: write.SDF(sdfset, "test.sdf")

## Define descriptor set in a simple function
desc <- function(sdfset) {
  cbind(SDFID=sdfid(sdfset),
        # datablock2ma(datablocklist=datablock(sdfset)),
        MW=MW(sdfset),
        groups(sdfset),
        # AP=sdf2ap(sdfset, type="character"),
        rings(sdfset, type="count", upper=6, arom=TRUE)
  )
}

## Run sdfStream with desc function and write results to a file called 'matrix.xls'
sdfStream(input="test.sdf", output="matrix.xls", append=FALSE, fct=desc, Nlines=1000)

## Same as before but starting in SD file at line number 950
sdfStream(input="test.sdf", output="matrix.xls", append=FALSE, fct=desc, Nlines=1000, startline=950)

## Select molecules from SD File using line index from sdfStream
indexDF <- read.delim("matrix.xls", row.names=1)[,1:4]
indexDFsub <- indexDF[indexDF$MW < 400, ] # Selects molecules with MW < 400
sdfset <- read.SDFindex(file="test.sdf", index=indexDFsub, type="SDFset")

## Write result directly to SD file without storing larger numbers of molecules in memory
read.SDFindex(file="test.sdf", index=indexDFsub, type="file", outfile="sub.sdf")
```



```
## Read atom pair string representation from file into APset
apset <- read.AP(file="matrix.xls", colid="AP")
cid(apsdf) <- as.character(indexDF$SDFID)

## End(Not run)
```

---

searchSim-deprecated    *PubChem Similarity (Fingerprint) Search*

---

### Description

Accepts one SDFset container and performs a >0.9 similarity PubChem fingerprint search, returning up to 200 hits in an SDFset container. The ChemMine Tools web service is used as an intermediate, to translate queries from plain HTTP POST to a PubChem Power User Gateway (PUG) query. If the input object contains multiple items, only the first is used as a query.

### Usage

```
searchSim(sdf)
```

### Arguments

sdf                    A SDFset object which contains one compound

### Value

SDFset                for details see ?"SDFset-class"

### Author(s)

Tyler Backman

### References

PubChem PUG SOAP: [http://pubchem.ncbi.nlm.nih.gov/pug\\_soap/pug\\_soap\\_help.html](http://pubchem.ncbi.nlm.nih.gov/pug_soap/pug_soap_help.html)

Chemmine web service: <http://chemmine.ucr.edu>

PubChem help: [http://pubchem.ncbi.nlm.nih.gov/search/help\\_search.html](http://pubchem.ncbi.nlm.nih.gov/search/help_search.html)

SMILES Format: [http://en.wikipedia.org/wiki/Chemical\\_file\\_format#SMILES](http://en.wikipedia.org/wiki/Chemical_file_format#SMILES)

### Examples

```
## Not run:
## get a sample compound
data(sdfsamples); sdfset <- sdfsamples[2]
## search a compound on PubChem
compounds <- searchSim(sdfset)
## End(Not run)
```

---

searchString-deprecated

*PubChem Similarity (Fingerprint) SMILES Search*

---

### Description

Accepts one SMILES string (Simplified Molecular Input Line Entry Specification) and performs a >0.95 similarity PubChem fingerprint search, returning the hits in an SDFset container. The ChemMine Tools web service is used as an intermediate, to translate queries from plain HTTP POST to a PubChem Power User Gateway (PUG) query.

### Usage

```
searchString(smiles)
```

### Arguments

smiles            A character object which contains one SMILES string

### Value

SDFset            for details see ?"SDFset-class"

### Author(s)

Tyler Backman

### References

PubChem PUG SOAP: [http://pubchem.ncbi.nlm.nih.gov/pug\\_soap/pug\\_soap\\_help.html](http://pubchem.ncbi.nlm.nih.gov/pug_soap/pug_soap_help.html)

Chemmine web service: <http://chemmine.ucr.edu>

PubChem help: [http://pubchem.ncbi.nlm.nih.gov/search/help\\_search.html](http://pubchem.ncbi.nlm.nih.gov/search/help_search.html)

SMILES Format: [http://en.wikipedia.org/wiki/Chemical\\_file\\_format#SMILES](http://en.wikipedia.org/wiki/Chemical_file_format#SMILES)

### Examples

```
## Not run:  
## search a compound on PubChem  
compounds <- searchString("CC(=O)OC1=CC=CC=C1C(=O)O")  
## End(Not run)
```

---

|                 |                          |
|-----------------|--------------------------|
| selectInBatches | <i>Select in Batches</i> |
|-----------------|--------------------------|

---

### Description

When doing a select where the condition is a large number of ids it is not always possible to include them in a single SQL statement. This function will break the list of ids into chunks and send the query for each batch. The results are appended and returned as one data frame.

### Usage

```
selectInBatches(conn, allIndices, genQuery, batchSize = 1e+05)
```

### Arguments

|            |  |
|------------|--|
| conn       | Database connection object   |
| allIndices | A vector of indices to pass to the genQuery function in batches.   |
| genQuery   | A function which takes a vector of indices and constructs an SQL SELECT statement returning records for the given indices. |
| batchSize  | How many indices to put in each batch.   |

### Value

A data frame with the results of the query as if all indices had been included in a single SELECT statement.

### Author(s)

Kevin Horan

### Examples

```
##---- Should be DIRECTLY executable !! ----
##-- ==> Define data, use random,
##--or do help(data=index) for the standard data sets.

## The function is currently defined as
function (conn, allIndices, genQuery, batchSize = 1e+05)
{
  batchByIndex(allIndices, function(indexBatch) {
    df = dbGetQuery(conn, genQuery(indexBatch))
    result = rbind(result, df)
  }, batchSize)
  result
}
```

---

 setPriorities

*Set Priorities*


---

### Description

This function should be run after loading a complete set of data. It will find each group of compounds which share the same descriptor and call the given function, `priorityFn`, with the `compound_id` numbers of the group. This function should then assign priorities to each compound-descriptor pair, however it wishes. Priorities are integer values with lower values being used in preference of higher values.

It is important that this function be called after all data is loaded. It may be that a compound loaded at the beginning of a data set shares a descriptor with a compound loaded near the end of the data set. If the priorities were set at some point in between these then it would not see all the compounds for that one descriptor.

If a SNOW cluster and connection source function are given, it will run in parallel.

Some pre-defined functions that can be use for `priorityFn` are:

`randomPriorities`: Set the priorities of compounds within a descriptor group randomly.

`forestSizePriorities`: Set the priority based on the number of disconnected components (trees) within the compound. Compounds with fewer trees will have a higher priority (lower numerical value) than compounds with more trees.

### Usage

```
setPriorities(conn,priorityFn,descriptorIds=c(),cl=NULL,connSource=NULL)
forestSizePriorities(conn,compIds)
randomPriorities(conn,compIds)
```

### Arguments

|                            |   |
|----------------------------|---|
| <code>conn</code>          | A database connection object.   |
| <code>priorityFn</code>    | This function will be called with the <code>compound_id</code> numbers associated with the same descriptor. It should use the id numbers to lookup whatever data it wants to assign a priority to each compound. These priority values will be used to pick a compound to represent the group in cases where only one compound is needed for each descriptor.<br>The function should return a <code>data.frame</code> with the fields " <code>compound_id</code> " and " <code>priority</code> ". The order of the rows is not important. |
| <code>descriptorIds</code> | If given then only re-compute priorities for groups involving descriptors in this list. This is useful for updating priorities after adding new compounds to an existing database.  |
| <code>cl</code>            | A SNOW cluster on which to run jobs on.   |
| <code>connSource</code>    | A function to create a new database connection with. This will be run once for each new job created. It must return a newly created connection, not a reference to an existing connection.  |
| <code>compIds</code>       | The <code>compound_id</code> values for each group.   |

**Value**

For `setPriorities`, no value is returned. `randomPriorities` and `forestSizePriorities` return a `data.frame` with columns "compound\_id" and "priority".

**Author(s)**

Kevin Horan

**Examples**

```
## Not run:  
data(sdfsamples)  
conn = initDb("sample.db")  
sdfLoad(conn, sdfsamples)  
setPriorities(conn, forestSizePriorities)  
  
## End(Not run)
```

---

smartsSearchOB

*SMARTS Search OB*

---

**Description**

Perform searches for SMARTS patterns using Open Babel (requires ChemmineOB package to be installed).

**Usage**

```
smartsSearchOB(sdfset, smartsPattern, uniqueMatches = TRUE)
```

**Arguments**

|                            |  |
|----------------------------|--|
| <code>sdfset</code>        | An SDFset of the compounds you want to search  |
| <code>smartsPattern</code> | The SMARTS pattern as a string.  |
| <code>uniqueMatches</code> | If true, only return the number of distinct matches, otherwise return the number of all matches. |

**Value**

Returns a vector of counts, one for each input compound.

**Author(s)**

Kevin Horan

## Examples

```
## Not run:  
library(ChemmineOB)  
data(sdfsamples)  
#look for rotatable bonds  
rotatableBonds = smartsSearchOB(sdfsamples[1:5], "[!$(***)&!D1]-@[!$(***)&!D1]", uniqueMatches=FALSE)  
  
## End(Not run)
```

---

SMI-class

Class "SMI"

---

## Description

Container for storing the SMILES string of a single molecule.

## Objects from the Class

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

## Slots

`smiles`: Object of class "character" of length one

## Methods

**as.character** signature(`x` = "SMI"): returns content as character vector

**coerce** signature(`from` = "character", `to` = "SMI"): `as(smi, "SMI")`

**coerce** signature(`from` = "SMIset", `to` = "SMI"): `as(smiset, "SMI")`

**show** signature(`object` = "SMI"): prints summary of SMI

## Author(s)

Thomas Girke

## References

SMILES (Simplified molecular-input line-entry system) format definition: [http://en.wikipedia.org/wiki/Simplified\\_molecular\\_input\\_line-entry\\_system](http://en.wikipedia.org/wiki/Simplified_molecular_input_line-entry_system)

## See Also

Related classes: SMIset, SDF, SDFset

## Examples

```
showClass("SMI")

## Instances of SMI class
data(smisample); smiset <- smisample
(smi <- smiset[[1]]) # returns first molecule in smiset as SMI object
```

---

|            |   |
|------------|---|
| smiles2sdf | <i>Convert SMILES (character) to SDFset</i> |
|------------|---|

---

## Description

Accepts a named vector or SMIset of SMILES (Simplified Molecular Input Line Entry Specification) strings and returns its equivalent as an SDFset container.

This function runs in two modes. If ChemmineOB is available then it will use OpenBabel to convert all the given smiles into an SDFset with 2D coordinates. Otherwise the compound is submitted to the ChemMine Tools web service for conversion with the Open Babel Open Source Chemistry Toolbox. In this case only the first element will be used since this is a very slow operation.

## Usage

```
smiles2sdf(smiles)
```

## Arguments

|        |   |
|--------|---|
| smiles | A named vector of SMILES strings. The names will be used to name the SDF objects. |
|--------|---|

## Value

|        |                                 |
|--------|---------------------------------|
| SDFset | for details see ?"SDFset-class" |
|--------|---------------------------------|

## Author(s)

Tyler Backman, Kevin Horan

## References

Chemmine web service: <http://chemmine.ucr.edu>

Open Babel: <http://openbabel.org>

SMILES Format: [http://en.wikipedia.org/wiki/Chemical\\_file\\_format#SMILES](http://en.wikipedia.org/wiki/Chemical_file_format#SMILES)

**Examples**

```
## Not run:  
## convert to sdf  
data(smisample)  
(sdf <- smiles2sdf(smisample[1:4]))  
  
## End(Not run)
```

---

smisample

*SMILES file in SMIset object*

---

**Description**

First 100 compounds from PubChem SD file (Compound\_00650001\_00675000.sdf.gz) converted to SMILES format

**Usage**

```
data(smisample)
```

**Format**

Object of class smiset

**Details**

Object stores 100 molecules from a sample SMILES file.

**Source**

[ftp://ftp.ncbi.nih.gov/pubchem/Compound/CURRENT-Full/SDF/Compound\\_00650001\\_00675000.sdf.gz](ftp://ftp.ncbi.nih.gov/pubchem/Compound/CURRENT-Full/SDF/Compound_00650001_00675000.sdf.gz)

**References**

SMILES (Simplified molecular-input line-entry system) format definition: [http://en.wikipedia.org/wiki/Simplified\\_molecular\\_input\\_line-entry\\_system](http://en.wikipedia.org/wiki/Simplified_molecular_input_line-entry_system)

**Examples**

```
data(smisample)  
smiset <- smisample  
view(smiset[1:4])
```



---

|              |                |
|--------------|----------------|
| SMIset-class | Class "SMIset" |
|--------------|----------------|

---

### Description

List-like container for storing SMILES strings of many compounds.

### Objects from the Class

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

### Slots

**smilist**: Object of class "list" with compound identifiers stored in name slots

### Methods

**[** signature(x = "SMIset"): subsetting of class with bracket operator  
**[[** signature(x = "SMIset"): returns single component as SMI object  
**[<-** signature(x = "SMIset"): replacement method for one or many entries  
**as.character** signature(x = "SMIset"): returns content as named character vector  
**c** signature(x = "SMIset"): concatenates two SMIset containers  
**cid** signature(x = "SMIset"): returns compound identifiers  
**cid<-** signature(x = "SMIset"): replacement method for compound identifiers  
**coerce** signature(from = "character", to = "SMIset"): `as(character, "SMIset")`  
**coerce** signature(from = "list", to = "SMIset"): `as(list, "SMIset")`  
**coerce** signature(from = "SMIset", to = "SMI"): `as(smiset, "SMI")`  
**length** signature(x = "SMIset"): returns number of entries stored in object  
**show** signature(object = "SMIset"): prints summary of SMIset  
**view** signature(x = "SMIset"): prints extended summary of SMIset

### Author(s)

Thomas Girke

### References

SMILES (Simplified molecular-input line-entry system) format definition: [http://en.wikipedia.org/wiki/Simplified\\_molecular\\_input\\_line-entry\\_system](http://en.wikipedia.org/wiki/Simplified_molecular_input_line-entry_system)

### See Also

Related classes: SMI, SDF, SDFset  
Import function: `read.SMIset("some_SMILES_file")`  
Export function: `write.SMI(smiset, "some_file.smi")`

## Examples

```
showClass("SMIset")

## Instances of SMIset class
data(smisample); smiset <- smisample
smiset; view(smiset[1:4])
smiset[[1]]

## Import and store SMILES file in SMIset container
# smiset <- read.SMIset("some_SMILES_file")

## Miscellaneous accessor methods
cid(smiset[1:4])
(smivec <- as.character(smiset[1:4]))

## Construct SMIset from named vector
as(smivec, "SMIset")

## Assigning compound IDs and keeping them unique
unique_ids <- makeUnique(cid(smiset))
cid(smiset) <- unique_ids

## Export SMIset to SMILES file
# write.SMI(smiset[1:4], file="sub.smi", cid=TRUE)
```

---

status

*Get Status of a ChemMine Tools Job*

---

## Description

Returns the status of a launched ChemMine Tools job as represented by a jobToken object.

## Usage

```
status(object)
```

## Arguments

object            A jobToken job as returned by the function launchCMTool

## Value

The status of the specified job is returned as a string. Possible values include "RUNNING", "FINISHED", or "FAILED".

## Author(s)

Tyler William H Backman

## References

See ChemMine Tools at <http://chemmine.ucr.edu>.

## See Also

Functions: toolDetails, listCMTools, launchCMTool, browseJob, result

## Examples

```
## Not run:
## list available tools
listCMTools()

## get detailed instructions on using a tool
toolDetails("Fingerprint Search")

## download compound 2244 from PubChem
job1 <- launchCMTool("pubchemID2SDF", 2244)

## check job status and download result
status(job1)
result1 <- result(job1)

## End(Not run)
```

---

toolDetails

*Detailed instructions for each ChemMine Tools web tool*

---

## Description

Connects to the ChemMine Tools web service, and provides detailed instructions and example function calls for any tool.

## Usage

```
toolDetails(tool_name)
```

## Arguments

tool\_name      A tool name matching verbatim an existing tool name as listed by listCMTools.

## Details

Prints instructions to console.

## Author(s)

Tyler William H Backman

## References

See ChemMine Tools at <http://chemmine.ucr.edu>.

## See Also

Functions: launchCMTool, listCMTools, result, browseJob, status

## Examples

```
## Not run:
## list available tools
listCMTools()

## get detailed instructions on using a tool
toolDetails("Fingerprint Search")

## download compound 2244 from PubChem
job1 <- launchCMTool("pubchemID2SDF", 2244)

## check job status and download result
status(job1)
result1 <- result(job1)

## End(Not run)
```

---

trimNeighbors

*Trim Neighbors*

---

## Description

Further reduce the cutoff value of a nearest neighbor (NN) table, as produced by [nearestNeighbors](#). This allows one to compute a very relaxed NN table initially, and then quickly restrict it later without having to re-compute all the similarities.

## Usage

```
trimNeighbors(nnm, cutoff)
```

## Arguments

|        |   |
|--------|---|
| nnm    | A nearest neighbor table, as produced by <a href="#">nearestNeighbors</a> .   |
| cutoff | The new similarities cutoff value. All pairs with a similarity less than this value will be removed from the table. |

## Value

The return value has the same structure as `nnm`, with some neighbors removed from the indexes and similarities entries.

**Author(s)**

Kevin Horan

**See Also**[jarvisPatrick nearestNeighbors](#)**Examples**

```
data(sdfsamplE)
ap = sdf2ap(sdfsamplE)
nnm = nearestNeighbors(ap,numNbrs=20)
nnm = trimNeighbors(nnm,cutoff=0.5)
clustering = jarvisPatrick(nnm,k=2,mode="a1b")
```

---

**validSDF***Validity check of SDFset*

---

**Description**

Performs validity check of SDFs stored in SDFset objects. Currently, the function tests whether the atom block and the bond block in each SDF component of an SDFset have at least Nabcol and Nbbcol columns (default is 3 for both). In additions, it tests for the presence of NA values in the atom and bond blocks. The function returns a logical vector with TRUE values for valid compounds and FALSE values for invalid ones.

**Usage**

```
validSDF(x, Nabcol = 3, Nbbcol = 3, logic = "&", checkNA=TRUE)
```

**Arguments**

|         |   |
|---------|---|
| x       | x object of class SDFset                                    |
| Nabcol  | minimum number of columns in atom block                     |
| Nbbcol  | minimum number of columns in bond block                     |
| logic   | logical connection (& or  ) among Nabcol and Nbbcol cutoffs |
| checkNA | checks for NA values in atom and bond blocks                |

**Details**

The function is important to remove invalid compounds from SDFset containers.

**Value**

logical vector of length x with TRUE for valid compounds and FALSE for invalid compounds.

**Author(s)**

Thomas Girke

**References**

...

**See Also**

Functions: read.SDFset

**Examples**

```
## SDFset instance
data(sdfsampl)
sdfset <- sdfsampl

## Detect and remove invalid SDFs in SDFset.
valid <- validSDF(sdfset)
which(!valid) # Returns index for invalid SDFs
sdfset <- sdfset[valid] # Returns only valid SDFs.
```

---

view

*Viewing of complex objects*

---

**Description**

Convenience function for viewing the content of complex objects like SDFset and APset containers. The function is a shorthand wrapper for `as(sdfset, "SDF")` and `as(apset, "AP")`.

**Usage**

```
view(x)
```

**Arguments**

x                    object of class SDFset or APset

**Details**

...

**Value**

List populated with SDF and AP components.

**Author(s)**

Thomas Girke

## References

...

## See Also

Classes: SDF, SDFset, AP, APset

## Examples

```
## Viewing content of SDFset
data(sdfsamples); sdfset <- sdfsamples
view(sdfset[1:4])
```

```
## Viewing content of APset
apset <- sdf2ap(sdfset[1:10])
view(apset)
```

---

write.SDF

*SDF export function*

---

## Description

Writes one or many molecules stored in a SDFset, SDFstr or SDF object to SD file.

## Usage

```
write.SDF(sdf, file, cid = FALSE, ...)
```

## Arguments

|      |   |
|------|---|
| sdf  | object of class SDFset, SDFstr or SDF   |
| file | name of SD file to write to   |
| cid  | if cid = TRUE and an SDFset object is provide as input, then the compound IDs in the ID slot of the SDFset are used for compound naming                         |
| ...  | the optional arguments of the sdf2str function can be provided here, including head, ab, bb, db; details are provided in the help page for the sdf2str function |

## Details

If the write.SDF function is supplied with an SDFset object, then it uses internally the sdf2str function to allow customizing the resulting SD file. For this all optional arguments of the sdf2str function can be passed on to write.SDF.

## Author(s)

Thomas Girke

## References

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

## See Also

Import function: read.SDFset, read.SDFstr

## Examples

```
## Instance of SDFset class
data(sdfsample); sdfset <- sdfsample

## Write objects of classes SDFset/SDFstr/SDF to file
# write.SDF(sdfset[1:4], file="sub.sdf")

## Example for writing customized SDFset to file containing
## ChemmineR signature, IDs from SDFset and no data block
# write.SDF(sdfset[1:4], file="sub.sdf", sig=TRUE, cid=TRUE, db=NULL)

## Example for injecting a custom matrix/data frame into the data block of an
## SDFset and then writing it to an SD file
props <- data.frame(MF=MF(sdfset), MW=MW(sdfset), atomcountMA(sdfset))
datablock(sdfset) <- props
view(sdfset[1:4])
# write.SDF(sdfset[1:4], file="sub.sdf", sig=TRUE, cid=TRUE)
```

---

|                |                           |
|----------------|---------------------------|
| write.SDFsplit | <i>SDF split function</i> |
|----------------|---------------------------|

---

## Description

Splits SD Files into any number of smaller SD Files

## Usage

```
write.SDFsplit(x, filetag, nmol)
```

## Arguments

|         |  |
|---------|--|
| x       | object of class SDFset, SDFstr                           |
| filetag | string to prepend to file names                          |
| nmol    | integer specifying number of molecules in split SD files |

## Details

To split an SD File into smaller ones, one can read the source file into R with read.SDFstr and write out smaller ones with write.SDFsplit. Note: when importing big SD Files, read.SDFstr will be much faster than read.SDFset, and there is no need to go through an SDFset object instance in this case.



**Author(s)**

Thomas Girke

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

Import/export functions: read.SDFset, read.SDFstr, read.SDFstr, read.SDFset

**Examples**

```
## Load sample data
library(ChemmineR)
data(sdfsampl)

## Not run: ## Create sample SD File with 100 molecules
write.SDF(sdfsampl, "test.sdf")

## Read in sample SD File
sdfstr <- read.SDFstr("test.sdf")

## Run export on SDFstr object
write.SDFsplit(x=sdfstr, filetag="myfile", nmol=10)

## Run export on SDFset object
write.SDFsplit(x=sdfsampl, filetag="myfile", nmol=10)

## End(Not run)
```

---

`write.SMI`*SMI export function*

---

**Description**

Writes one or many molecules stored in a SMISet object to a SMILES file.

**Usage**`write.SMI(smi, file, cid = TRUE, ...)`**Arguments**

|                   |  |
|-------------------|--|
| <code>smi</code>  | object of class SMISet   |
| <code>file</code> | name of SMILES file to write to  |
| <code>cid</code>  | if <code>cid = TRUE</code> the compound identifiers will be exported by appending them in tab-separated format to each SMILES string |
| <code>...</code>  | option to pass on additional arguments   |

**Details**

...

**Author(s)**

Thomas Girke

**References**

SMILES (Simplified molecular-input line-entry system) format definition: [http://en.wikipedia.org/wiki/Simplified\\_molecular\\_input\\_line-entry\\_system](http://en.wikipedia.org/wiki/Simplified_molecular_input_line-entry_system)

**See Also**

Functions: write.SDF

**Examples**

```
## Instance of SMIsset class
data(smisample); smisset <- smisample

## Write objects of classes SMIsset to file with and
## without compound identifiers
# write.SMI(smisset[1:4], file="sub.smi", cid=TRUE)
# write.SMI(smisset[1:4], file="sub.smi", cid=FALSE)
```

# Index

- \* **aplot**
  - openBabelPlot, 95
  - plotStruc, 97
- \* **canonical**
  - canonicalize, 26
  - canonicalNumbering, 27
- \* **classes**
  - AP-class, 8
  - APset-class, 11
  - ExtSDF-class, 53
  - FP-class, 58
  - FPset-class, 61
  - jobToken-class, 83
  - SDF-class, 116
  - SDFset-class, 128
  - SDFstr-class, 133
  - SMI-class, 142
  - SMIset-class, 145
- \* **datasets**
  - apfp, 9
  - apset, 10
  - atomprop, 17
  - pubchemFPencoding, 101
  - sdfsamples, 127
  - smisamples, 144
- \* **datatable,sdfset,compounds,display**
  - SDFDataTable, 125
- \* **dissimilar**
  - maximallyDissimilar, 91
- \* **evaluate**
  - genParameters, 68
- \* **exact**
  - exactMassOB, 52
- \* **fingerprint**
  - genParameters, 68
- \* **mass**
  - exactMassOB, 52
- \* **monoisotopic**
  - exactMassOB, 52
- \* **morgan**
  - canonicalize, 26
  - canonicalNumbering, 27
- \* **pvalue**
  - genParameters, 68
- \* **similarity**
  - genParameters, 68
- \* **utilities**
  - ap, 6
  - apset2descdb, 12
  - atomblock, 14
  - atomcount, 15
  - atomssubset, 17
  - bondblock, 20
  - bonds, 21
  - browseJob, 22
  - cid, 28
  - cluster.sizestat, 29
  - cluster.visualize, 30
  - cmp.cluster, 32
  - cmp.duplicated, 34
  - cmp.parse, 36
  - cmp.parse1, 37
  - cmp.search, 38
  - cmp.similarity, 40
  - conMA, 42
  - datablock, 44
  - datablock2ma, 45
  - db.explain, 46
  - db.subset, 47
  - desc2fp, 49
  - fp2bit, 59
  - fpSim, 62
  - getIds-deprecated, 75
  - grepSDFset, 76
  - groups, 77
  - header, 78
  - jarvisPatrick, 80
  - launchCMTool, 84

- listCMTools, 86
- makeUnique, 90
- obmol, 94
- openBabelPlot, 95
- plotStruc, 97
- pubchemCidToSDF, 100
- pubchemInchi2cid, 101
- pubchemInchikey2sdf, 102
- pubchemName2CID, 103
- pubchemSDFSearch, 104
- pubchemSmilesSearch, 105
- read.AP, 106
- read.SDFindex, 107
- read.SDFset, 109
- read.SDFstr, 110
- read.SMIset, 111
- result, 113
- rings, 114
- sdf.subset, 118
- sdf.visualize, 119
- sdf2ap, 120
- SDF2apcmp, 121
- sdf2list, 122
- sdf2smiles, 123
- sdf2str, 124
- sdfid, 126
- SDFset2list, 130
- SDFset2SDF, 132
- sdfstr2list, 134
- sdfStream, 135
- searchSim-deprecated, 137
- searchString-deprecated, 138
- smiles2sdf, 143
- status, 146
- toolDetails, 147
- validSDF, 149
- view, 150
- write.SDF, 151
- write.SDFsplit, 152
- write.SMI, 153
- [, APset-method (APset-class), 11
- [, FPset-method (FPset-class), 61
- [, SDF-method (SDF-class), 116
- [, SDFset-method (SDFset-class), 128
- [, SDFstr-method (SDFstr-class), 133
- [, SMIset-method (SMIset-class), 145
- [<-, APset-method (APset-class), 11
- [<-, FPset-method (FPset-class), 61
- [<-, SDF-method (SDF-class), 116
- [<-, SDFset-method (SDFset-class), 128
- [<-, SDFstr-method (SDFstr-class), 133
- [<-, SMIset-method (SMIset-class), 145
- [[, APset-method (APset-class), 11
- [[, FPset-method (FPset-class), 61
- [[, SDF-method (SDF-class), 116
- [[, SDFset-method (SDFset-class), 128
- [[, SDFstr-method (SDFstr-class), 133
- [[, SMIset-method (SMIset-class), 145
- [[<-, APset-method (APset-class), 11
- [[<-, SDF-method (SDF-class), 116
- [[<-, SDFset-method (SDFset-class), 128
- [[<-, SDFstr-method (SDFstr-class), 133
- addDescriptorType, 5
- addNewFeatures, 5, 89
- ap, 6
- ap, AP-method (AP-class), 8
- ap, APset-method (APset-class), 11
- AP-class, 8
- ap-methods (ap), 6
- apfp, 9
- apset, 10
- APset-class, 11
- apset2descdb, 12
- as.character, FP-method (FP-class), 58
- as.character, FPset-method (FPset-class), 61
- as.character, SMI-method (SMI-class), 142
- as.character, SMIset-method (SMIset-class), 145
- as.matrix, FPset-method (FPset-class), 61
- as.numeric, FP-method (FP-class), 58
- as.vector, FP-method (FP-class), 58
- atomblock, 14
- atomblock, SDF-method (SDF-class), 116
- atomblock, SDFset-method (SDFset-class), 128
- atomblock-methods (atomblock), 14
- atomblock<- (atomblock), 14
- atomblock<-, SDFset-method (SDFset-class), 128
- atomcount, 15
- atomcount, SDF-method (SDF-class), 116
- atomcount, SDFset-method (SDFset-class), 128
- atomcountMA (atomcount), 15
- atomprop, 17

- atomssubset, 17
- batchByIndex, 19, 96
- bondblock, 20
- bondblock, SDF-method (SDF-class), 116
- bondblock, SDFset-method (SDFset-class), 128
- bondblock-methods (bondblock), 20
- bondblock<- (bondblock), 20
- bondblock<- , SDFset-method (SDFset-class), 128
- bonds, 21
- browseJob, 22
- bufferLines, 23
- bufferResultSet, 24
- byCluster, 25
- c, APset-method (APset-class), 11
- c, FP-method (FP-class), 58
- c, FPset-method (FPset-class), 61
- c, SDFset-method (SDFset-class), 128
- c, SMiset-method (SMiset-class), 145
- canonicalize, 26, 27
- canonicalNumbering, 26, 27
- cid, 28
- cid, APset-method (APset-class), 11
- cid, FPset-method (FPset-class), 61
- cid, SDFset-method (SDFset-class), 128
- cid, SMiset-method (SMiset-class), 145
- cid<- (cid), 28
- cid<- , APset-method (APset-class), 11
- cid<- , FPset-method (FPset-class), 61
- cid<- , SDFset-method (SDFset-class), 128
- cid<- , SMiset-method (SMiset-class), 145
- cluster.sizestat, 29, 32
- cluster.visualize, 30, 30
- cmp.cluster, 30, 32, 32, 37–39, 41
- cmp.duplicated, 34
- cmp.parse, 32, 34, 35, 36, 38, 39, 41, 47, 48, 118, 119
- cmp.parse1, 34, 37, 37, 39, 41
- cmp.search, 34, 35, 37, 38, 38, 39, 41
- cmp.similarity, 34, 37–39, 40
- coerce, APset, AP-method (APset-class), 11
- coerce, APset, list-method (APset-class), 11
- coerce, character, FPset-method (FPset-class), 61
- coerce, character, SDF-method (SDF-class), 116
- coerce, character, SDFstr-method (SDFstr-class), 133
- coerce, character, SMI-method (SMI-class), 142
- coerce, character, SMiset-method (SMiset-class), 145
- coerce, FPset, FP-method (FPset-class), 61
- coerce, list, APset-method (APset-class), 11
- coerce, list, SDF-method (SDF-class), 116
- coerce, list, SDFset-method (SDFset-class), 128
- coerce, list, SDFstr-method (SDFstr-class), 133
- coerce, list, SMiset-method (SMiset-class), 145
- coerce, matrix, FPset-method (FPset-class), 61
- coerce, numeric, FP-method (FP-class), 58
- coerce, SDF, character-method (SDF-class), 116
- coerce, SDF, list-method (SDF-class), 116
- coerce, SDF, SDFset-method (SDF-class), 116
- coerce, SDF, SDFstr-method (SDF-class), 116
- coerce, SDFset, list-method (SDFset-class), 128
- coerce, SDFset, SDF-method (SDFset-class), 128
- coerce, SDFset, SDFstr-method (SDFset-class), 128
- coerce, SDFstr, list-method (SDFstr-class), 133
- coerce, SDFstr, SDFset-method (SDFstr-class), 133
- coerce, SMiset, SMI-method (SMiset-class), 145
- conMA, 42
- connections, 43
- datablock, 44
- datablock, SDF-method (SDF-class), 116
- datablock, SDFset-method (SDFset-class), 128
- datablock-methods (datablock), 44
- datablock2ma, 45

- datablock<- (datablock), 44
- datablock<- , SDFset-method (SDFset-class), 128
- datablocktag (datablock), 44
- datablocktag, SDF-method (SDF-class), 116
- datablocktag, SDFset-method (SDFset-class), 128
- db.explain, 46
- db.subset, 47
- dbTransaction, 48
- desc2fp, 49
- draw\_sdf, 50
- DrugBank (connections), 43
- DUD (connections), 43
  
- exactMassOB, 52
- ExtSDF-class, 53
  
- findCompounds, 54, 74, 87
- findCompoundsByName, 55
- fingerprintOB, 56
- fold, 57
- fold, FP-method (FP-class), 58
- fold, FPset-method (FPset-class), 61
- foldCount, 57
- foldCount, FP-method (FP-class), 58
- foldCount, FPset-method (FPset-class), 61
- forestSizePriorities (setPriorities), 140
- FP-class, 58
- fp2bit, 59
- FPset-class, 61
- fpSim, 62, 69
- fptype, 65
- fptype, FP-method (FP-class), 58
- fptype, FPset-method (FPset-class), 61
- fromNNMatrix, 65
  
- genAPDescriptors, 66
- generate3DCoords, 67
- genParameters, 63, 68
- getAllCompoundIds, 69
- getAtomAttr, 70
- getAtomAttr, ExtSDF-method (ExtSDF-class), 53
- getBondAttr, 71
- getBondAttr, ExtSDF-method (ExtSDF-class), 53
- getCompoundFeatures, 71
  
- getCompoundNames, 73
- getCompounds, 54, 74
- getIds (getIds-deprecated), 75
- getIds-deprecated, 75
- grepSDFset, 76
- groups, 77
  
- header, 78
- header, SDF-method (SDF-class), 116
- header, SDFset-method (SDFset-class), 128
- header-methods (header), 78
- header<- (header), 78
- header<- , SDFset-method (SDFset-class), 128
  
- initDb, 6, 48, 54, 55, 69, 72–74, 79, 88
  
- jarvisPatrick, 25, 66, 80, 82, 92, 93, 149
- jarvisPatrick\_c, 82
- jobToken-class, 83
  
- largestComponent, 84
- launchCMTTool, 84
- length, APset-method (APset-class), 11
- length, FPset-method (FPset-class), 61
- length, SDFset-method (SDFset-class), 128
- length, SDFstr-method (SDFstr-class), 133
- length, SMIsset-method (SMIsset-class), 145
- listCMTTools, 86
- listFeatures, 87
- loadSdf, 6, 74, 88
- loadSmiles (loadSdf), 88
  
- makeUnique, 90
- maximallyDissimilar, 91
- MF (atomcount), 15
- MW (atomcount), 15
  
- nearestNeighbors, 80, 81, 92, 148, 149
- numBits, 93
- numBits, FP-method (FP-class), 58
- numBits, FPset-method (FPset-class), 61
  
- obmol, 94
- obmol, SDF-method (SDF-class), 116
- obmol, SDFset-method (SDFset-class), 128
- obmol-methods (obmol), 94
- openBabelPlot, 95
  
- parBatchByIndex, 19, 96

- plot (plotStruc), 97
- plot, SDF-method (SDF-class), 116
- plot, SDFset-method (SDFset-class), 128
- plotStruc, 97, 113, 119
- propOB, 99
- pubchemCidToSDF, 100
- pubchemFPencoding, 101
- pubchemInchi2cid, 101
- pubchemInchikey2sdf, 102
- pubchemName2CID, 103
- pubchemSDFSearch, 104
- pubchemSmilesSearch, 105
  
- randomPriorities (setPriorities), 140
- read.AP, 106
- read.SDFindex, 107
- read.SDFset, 53, 109
- read.SDFstr, 110
- read.SMIset, 111
- regenerateCoords, 95, 98, 112
- result, 113
- rings, 114
  
- SDF-class, 116
- sdf.subset, 48, 118, 119
- sdf.visualize, 39, 118, 119
- sdf2ap, 120
- SDF2apcmp, 121
- sdf2list, 122
- sdf2list, SDF-method (SDF-class), 116
- sdf2smiles, 123
- sdf2smilesOB (sdf2smiles), 123
- sdf2str, 124
- sdf2str, SDF-method (SDF-class), 116
- sdf2str-methods (sdf2str), 124
- SDFDataTable, 125
- sdfid, 55, 126
- sdfid, SDF-method (SDF-class), 116
- sdfid, SDFset-method (SDFset-class), 128
- sdfsamples, 127
- SDFset (SDFset-class), 128
- SDFset-class, 128
- SDFset2list, 130
- SDFset2list, SDFset-method (SDFset-class), 128
- SDFset2list-methods (SDFset2list), 130
- SDFset2SDF, 132
- SDFset2SDF, SDFset-method (SDFset-class), 128
- SDFset2SDF-methods (SDFset2SDF), 132
- SDFset2SDF<- (SDFset2SDF), 132
- SDFset2SDF<-, SDFset-method (SDFset-class), 128
- SDFstr-class, 133
- sdfstr2list, 134
- sdfstr2list, SDFstr-method (SDFstr-class), 133
- sdfstr2list-methods (sdfstr2list), 134
- sdfstr2list<- (sdfstr2list), 134
- sdfstr2list<-, SDFstr-method (SDFstr-class), 133
- sdfStream, 88, 89, 135
- searchSim (searchSim-deprecated), 137
- searchSim-deprecated, 137
- searchString (searchString-deprecated), 138
- searchString-deprecated, 138
- selectInBatches, 139
- setPriorities, 140
- show, AP-method (AP-class), 8
- show, APset-method (APset-class), 11
- show, ExtSDF-method (ExtSDF-class), 53
- show, FP-method (FP-class), 58
- show, FPset-method (FPset-class), 61
- show, jobToken-method (jobToken-class), 83
- show, SDF-method (SDF-class), 116
- show, SDFset-method (SDFset-class), 128
- show, SDFstr-method (SDFstr-class), 133
- show, SMI-method (SMI-class), 142
- show, SMIset-method (SMIset-class), 145
- smartsSearchOB, 141
- SMI-class, 142
- smiles2sdf, 143
- smiles2sdfOB (smiles2sdf), 143
- smisample, 144
- SMIset-class, 145
- splitNumChar (datablock2ma), 45
- status, 146
  
- toolDetails, 147
- trimNeighbors, 81, 93, 148
  
- validSDF, 149
- view, 150
- view, APset-method (APset-class), 11
- view, FPset-method (FPset-class), 61
- view, SDFset-method (SDFset-class), 128

view, SMiset-method (SMiset-class), [145](#)

view-methods (view), [150](#)

write.SDF, [151](#)

write.SDFsplit, [152](#)

write.SMI, [153](#)