
NAME

RDKitUtil

SYNOPSIS

import RDKitUtil

DESCRIPTION

RDKitUtil module provides the following functions:

AreAtomIndicesSequentiallyConnected, FilterSubstructureMatchByAtomMapNumbers, FilterSubstructureMatchesByAtomMapNumbers, GenerateBase64EncodedMolStrings, GetInlineSVGForMolecule, GetInlineSVGForMolecules, GetMolName, GetSVGForMolecule, GetSVGForMolecules, IsMolEmpty, MolFromBase64EncodedMolString, MolFromSubstructureMatch, MolToBase64EncodedMolString, MoleculesWriter, MolsFromSubstructureMatches, ReadAndValidateMolecules, ReadMolecules, ReadMoleculesFromMol2File, ReadMoleculesFromMolFile, ReadMoleculesFromPDBFile, ReadMoleculesFromSDFFile, ReadMoleculesFromSMILESFile, SetWriterMolProps, WriteMolecules

FUNCTIONS

AreAtomIndicesSequentiallyConnected

```
AreAtomIndicesSequentiallyConnected(Mol, AtomIndices)
```

Check for the presence bonds between sequential pairs of atoms in a molecule.

Arguments:

Mol (object): RDKit molecule object.
AtomIndices (list): List of atom indices.

Returns:

bool : True - Sequentially connected; Otherwise, false.

FilterSubstructureMatchByAtomMapNumbers

```
FilterSubstructureMatchByAtomMapNumbers(Mol, PatternMol, AtomIndices)
```

Filter a list of matched atom indices by map atom numbers present in a pattern molecule. The list of atom indices correspond to a list retrieved by RDKit function GetSubstructureMatches using SMILES/SMARTS pattern. The atom map numbers are mapped to appropriate atom indices during the generation of molecules. For example: [O:1]=[S:2](=[O])[C:3][C:4].

Arguments:

Mol (object): RDKit molecule object.
PatternMol (object): RDKit molecule object for a SMILES/SMARTS pattern.
AtomIndices (list): Atom indices.

Returns:

list : A list of filtered atom indices.

FilterSubstructureMatchesByAtomMapNumbers

```
FilterSubstructureMatchesByAtomMapNumbers(Mol, PatternMol, AtomIndicesList)
```

Filter a list of lists containing matched atom indices by map atom numbers present in a pattern molecule. The list of atom indices correspond to a list retrieved by RDKit function GetSubstructureMatches using SMILES/SMARTS pattern. The atom map numbers are mapped to appropriate atom indices during the generation of molecules. For example: [O:1]=[S:2](=[O])[C:3][C:4].

Arguments:

Mol (object): RDKit molecule object.
PatternMol (object): RDKit molecule object for a SMILES/SMARTS pattern.
AtomIndicesList (list): A list of lists containing atom indices.

Returns:

list : A list of lists containing filtered atom indices.

GenerateBase64EncodedMolStrings

```
GenerateBase64EncodedMolStrings(Mols, PropertyPickleFlags =
Chem.PropertyPickleOptions.AllProps)
```

Setup an iterator for generating base64 encoded molecule string from a RDKit molecule iterator. The iterator returns a list containing a molecule index and encoded molecule string or None.

The molecules are pickled using RDKit Mol.ToBinary() function before their encoding.

Arguments:

```
iterator: RDKit molecules iterator.
PropertyFlags: RDKit property pickle options.
```

Returns:

```
object : Base64 encoded molecules iterator. The iterator returns a
list containing a molecule index and an encoded molecule string
or None.
```

The following property pickle flags are currently available in RDKit:

```
Chem.PropertyPickleOptions.NoProps
Chem.PropertyPickleOptions.MolProps
Chem.PropertyPickleOptions.AtomProps
Chem.PropertyPickleOptions.BondProps
Chem.PropertyPickleOptions.PrivateProps
Chem.PropertyPickleOptions.AllProps
```

Example(s):

```
EncodedMolsInfo = GenerateBase64EncodedMolStrings(Mols)
for MolIndex, EncodedMol in EncodedMolsInfo:
    if EncodedMol is not None:
        Mol = MolFromBase64EncodedMolString(EncodedMol)
```

GetInlineSVGForMolecule

```
GetInlineSVGForMolecule(Mol, Width, Height, Legend = None, AtomListToHighlight =
None, BondListToHighlight = None, BoldText = True, Base64Encoded = True)
```

Get SVG image text for a molecule suitable for inline embedding into a HTML page.

Arguments:

```
Mol (object): RDKit molecule object.
Width (int): Width of a molecule image in pixels.
Height (int): Height of a molecule image in pixels.
Legend (str): Text to display under the image.
AtomListToHighlight (list): List of atoms to highlight.
BondListToHighlight (list): List of bonds to highlight.
BoldText (bool): Flag to make text bold in the image of molecule.
Base64Encoded (bool): Flag to return base64 encoded string.
```

Returns:

```
str : SVG image text for inline embedding into a HTML page using "img"
tag:  or
tag: 
```

GetInlineSVGForMolecules

```
GetInlineSVGForMolecules(Mols, MolsPerRow, MolWidth, MolHeight, Legends = None,
AtomListsToHighlight = None, BondListsToHighLight = None, BoldText = True,
Base64Encoded = True)
```

Get SVG image text for molecules suitable for inline embedding into a HTML page.

Arguments:

```
Mols (list): List of RDKit molecule objects.
MolsPerRow (int): Number of molecules per row.
Width (int): Width of a molecule image in pixels.
Height (int): Height of a molecule image in pixels.
Legends (list): List containing strings to display under images.
AtomListsToHighlight (list): List of lists containing atoms to highlight
for molecules.
```

BondListsToHighlight (list): List of lists containing bonds to highlight for molecules
BoldText (bool): Flag to make text bold in the image of molecules.
Base64Encoded (bool): Flag to return base64 encoded string.

Returns:

str : SVG image text for inline embedding into a HTML page using "img"
tag: or
tag:

GetMolName

GetMolName(Mol, MolNum = None)

Get molecule name.

Arguments:

Mol (object): RDKit molecule object.
MolNum (int or None): Molecule number in input file.

Returns:

str : Molname corresponding to _Name property of a molecule, generated from specieid MolNum using the format "Mol%d" % MolNum, or an empty string.

GetSVGForMolecule

GetSVGForMolecule(Mol, Width, Height, Legend = None, AtomListToHighlight = None, BondListToHighlight = None, BoldText = True)

Get SVG image text for a molecule suitable for viewing in a browser.

Arguments:

Mol (object): RDKit molecule object.
Width (int): Width of a molecule image in pixels.
Height (int): Height of a molecule image in pixels.
Legend (str): Text to display under the image.
AtomListToHighlight (list): List of atoms to highlight.
BondListToHighlight (list): List of bonds to highlight.
BoldText (bool): Flag to make text bold in the image of molecule.

Returns:

str : SVG image text for writing to a SVG file for viewing in a browser.

GetSVGForMolecules

GetSVGForMolecules(Mols, MolsPerRow, MolWidth, MolHeight, Legends = None, AtomListsToHighlight = None, BondListsToHighlight = None, BoldText = True)

Get SVG image text for molecules suitable for viewing in a browser.

Arguments:

Mols (list): List of RDKit molecule objects.
MolsPerRow (int): Number of molecules per row.
Width (int): Width of a molecule image in pixels.
Height (int): Height of a molecule image in pixels.
Legends (list): List containing strings to display under images.
AtomListsToHighlight (list): List of lists containing atoms to highlight for molecules.
BondListsToHighlight (list): List of lists containing bonds to highlight for molecules.
BoldText (bool): Flag to make text bold in the image of molecules.

Returns:

str : SVG image text for writing to a SVG file for viewing in a browser.

IsMolEmpty

```
IsMolEmpty(Mol)
```

Check for the presence of atoms in a molecule.

Arguments:

Mol (object): RDKit molecule object.

Returns:

bool : True - No atoms in molecule; Otherwise, false.

MolFromBase64EncodedMolString

```
MolFromBase64EncodedMolString(EncodedMol)
```

Generate a RDKit molecule object from a base64 encoded string.

Arguments:

str: Base64 encoded molecule string.

Returns:

object : RDKit molecule object or None.

MolFromSubstructureMatch

```
MolFromSubstructureMatch(Mol, PatternMol, AtomIndices, FilterByAtomMapNums = False)
```

Generate a RDKit molecule object for a list of matched atom indices present in a pattern molecule. The list of atom indices correspond to a list retrieved by RDKit function GetSubstructureMatch using SMILES/SMARTS pattern. The atom indices are optionally filtered by mapping atom numbers to appropriate atom indices during the generation of the molecule. For *Example(s)*:

Arguments:

Mol (object): RDKit molecule object.

PatternMol (object): RDKit molecule object for a SMILES/SMARTS pattern.

AtomIndices (list): Atom indices.

FilterByAtomMapNums (bool): Filter matches by atom map numbers.

Returns:

object : RDKit molecule object or None.

MolToBase64EncodedMolString

```
MolToBase64EncodedMolString(Mol, PropertyPickleFlags =  
Chem.PropertyPickleOptions.AllProps)
```

Encode RDKit molecule object into a base64 encoded string. The properties can be optionally excluded. The molecule is pickled using RDKit Mol.ToBinary() function before their encoding.

Arguments:

Mol (object): RDKit molecule object.

PropertyPickleFlags: RDKit property pickle options.

Returns:

str : Base64 encode molecule string or None.

The following property pickle flags are currently available in RDKit:

```
Chem.PropertyPickleOptions.NoProps  
Chem.PropertyPickleOptions.MolProps  
Chem.PropertyPickleOptions.AtomProps  
Chem.PropertyPickleOptions.BondProps  
Chem.PropertyPickleOptions.PrivateProps  
Chem.PropertyPickleOptions.AllProps
```

MoleculesWriter

```
MoleculesWriter(FileName, **KeyWordArgs)
```

Set up a molecule writer.

Arguments:

FileName (str): Name of a file with complete path.
**KeywordArgs (dictionary) : Parameter name and value pairs for writing and processing molecules.

Returns:

RDKit object : Molecule writer.

The file extension is used to determine type of the file and set up an appropriate file writer.

MolsFromSubstructureMatches

```
MolsFromSubstructureMatches(Mol, PatternMol, AtomIndicesList, FilterByAtomMapNums = False)
```

Generate a list of RDKit molecule objects for a list containing lists of matched atom indices present in a pattern molecule. The list of atom indices correspond to a list retrieved by RDKit function GetSubstructureMatches using SMILES/SMARTS pattern. The atom indices are optionally filtered by mapping atom numbers to appropriate atom indices during the generation of the molecule. For

Example(s):

Arguments:

Mol (object): RDKit molecule object.
PatternMol (object): RDKit molecule object for a SMILES/SMARTS pattern.
AtomIndicesList (list): A list of lists containing atom indices.
FilterByAtomMapNums (bool): Filter matches by atom map numbers.

Returns:

list : A list of lists containing RDKit molecule objects or None.

ReadAndValidateMolecules

```
ReadAndValidateMolecules(FileName, **KeywordArgs)
```

Read molecules from an input file, validate all molecule objects, and return a list of valid and non-valid molecule objects along with their counts.

Arguments:

FileName (str): Name of a file with complete path.
**KeywordArgs (dictionary) : Parameter name and value pairs for reading and processing molecules.

Returns:

list : List of valid RDKit molecule objects.
int : Number of total molecules in input file.
int : Number of valid molecules in input file.

The file extension is used to determine type of the file and set up an appropriate file reader.

ReadMolecules

```
ReadMolecules(FileName, **KeywordArgs)
```

Read molecules from an input file without performing any validation and creation of molecule objects.

Arguments:

FileName (str): Name of a file with complete path.
**KeywordArgs (dictionary) : Parameter name and value pairs for reading and processing molecules.

Returns:

list : List of RDKit molecule objects.

The file extension is used to determine type of the file and set up an appropriate file reader.

ReadMoleculesFromMol2File

```
ReadMoleculesFromMol2File(FileName, Sanitize = True, RemoveHydrogens = True)
```

Read molecule from a Tripos Mol2 file.

Arguments:

FileName (str): Name of a file with complete path.
Sanitize (bool): Sanitize molecules.
RemoveHydrogens (bool): Remove hydrogens from molecules.

Returns:

list : List of RDKit molecule objects.

ReadMoleculesFromMolFile

```
ReadMoleculesFromMolFile(FileName, Sanitize = True, RemoveHydrogens = True,  
StrictParsing = True)
```

Read molecule from a MDL Mol file.

Arguments:

FileName (str): Name of a file with complete path.
Sanitize (bool): Sanitize molecules.
RemoveHydrogens (bool): Remove hydrogens from molecules.
StrictParsing (bool): Perform strict parsing.

Returns:

list : List of RDKit molecule objects.

ReadMoleculesFromPDBFile

```
ReadMoleculesFromPDBFile(FileName, Sanitize = True, RemoveHydrogens = True)
```

Read molecule from a PDB file.

Arguments:

FileName (str): Name of a file with complete path.
Sanitize (bool): Sanitize molecules.
RemoveHydrogens (bool): Remove hydrogens from molecules.

Returns:

list : List of RDKit molecule objects.

ReadMoleculesFromSDFile

```
ReadMoleculesFromSDFile(FileName, Sanitize = True, RemoveHydrogens = True,  
StrictParsing = True)
```

Read molecules from a SD file.

Arguments:

FileName (str): Name of a file with complete path.
Sanitize (bool): Sanitize molecules.
RemoveHydrogens (bool): Remove hydrogens from molecules.
StrictParsing (bool): Perform strict parsing.

Returns:

list : List of RDKit molecule objects.

ReadMoleculesFromSMILESFile

```
ReadMoleculesFromSMILESFile(FileName, SMILESDelimiter = ' ', SMILESColIndex = 0,  
SMILESNameColIndex = 1, SMILESTitleLine = 1, Sanitize = 1)
```

Read molecules from a SMILES file.

Arguments:

SMILESDelimiter (str): Delimiter for parsing SMILES line
SMILESColIndex (int): Column index containing SMILES string.
SMILESNameColIndex (int): Column index containing molecule name.

```
SMILESTitleLine (int): Flag to indicate presence of title line.  
Sanitize (int): Sanitize molecules.
```

Returns:

```
list : List of RDKit molecule objects.
```

SetWriterMolProps

```
SetWriterMolProps(Writer, Mol)
```

Setup molecule properties for a writer to output.

Arguments:

```
Writer (object): RDKit writer object.  
Mol (object): RDKit molecule object.
```

Returns:

```
object : Writer object.
```

WriteMolecules

```
WriteMolecules(FileName, Mols, **KeyWordArgs)
```

Write molecules to an output file.

Arguments:

```
FileName (str): Name of a file with complete path.  
Mols (list): List of RDKit molecule objects.  
**KeyWordArgs (dictionary) : Parameter name and value pairs for writing and  
processing molecules.
```

Returns:

```
int : Number of total molecules.  
int : Number of processed molecules written to output file.
```

The file extension is used to determine type of the file and set up an appropriate file writer.

AUTHOR

Manish Sud <msud@san.rr.com>

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