

NAME

RDKitUtil

SYNOPSIS

```
import RDKitUtil
```

DESCRIPTION

RDKitUtil module provides the following functions:

GetMolName, IsMolEmpty, MoleculesWriter, ReadAndValidateMolecules, ReadMolecules, ReadMoleculesFromMol2File, ReadMoleculesFromMolFile, ReadMoleculesFromPDBFile, ReadMoleculesFromSDFFile, ReadMoleculesFromSMILESFile, WriteMolecules

FUNCTIONS

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.

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.

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.

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.

ReadMoleculesFromSDFFile

```
ReadMoleculesFromSDFFile(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.
```

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.

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The functionality available in the script is implemented using RDKit, an open source toolkit for cheminformatics developed by Greg Landrum.

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