### NAME

MiscUtil

### **SYNOPSIS**

import MiscUtil

#### **DESCRIPTION**

MiscUtil module provides the following functions:

CheckFileExt, CheckTextValue, DoesSMILESFileContainTitleLine, ExpandFileNames, GetExamplesTextFromDocOptText, GetExcelStyleColumnLabel, GetFormattedElapsedTime, GetFormattedFileSize, GetMayaChemToolsLibDataPath, GetTextLines, GetTextLinesWords, GetWallClockAndProcessorTime, IsEmpty, IsFloat, IsInteger, IsNumber, JoinWords, ObjectFromBase64EncodedString, ObjectToBase64EncodedString, ParseFileName, PrintError, PrintInfo, PrintWarning, ProcessOptionInfileParameters,

ProcessOptionMultiprocessingParameters, ProcessOptionOutfileParameters, ProcessOptionSeabornPlotParameters, ReplaceHTMLEntitiesInText, TruncateText, ValidateOptionFileExt, ValidateOptionFilePath, ValidateOptionFloatValue, ValidateOptionIntegerValue, ValidateOptionNumberValue, ValidateOptionNumberValues, ValidateOptionSutputFileOverwrite, WrapText

#### **FUNCTIONS**

### CheckFileExt

```
CheckFileExt(FileName, FileExts)
```

Check file type based on the specified file extensions delimited by spaces.

### Arguments:

```
FileName (str): Name of a file.
FileExts (str): Space delimited string containing valid file extensions.
```

### Returns:

bool : True, FileName contains a valid file extension; Otherwise, False.

### CheckTextValue

```
CheckTextValue(Value, ValidValues)
```

Check text value based on the specified valid values delimited by spaces.

### Arguments:

```
Value (str): Text value ValidValues (str): Space delimited string containing valid values.
```

### Returns:

```
bool : True, Value is valid; Otherwise, False.
```

### DoesSMILESFileContainTitleLine

```
DoesSMILESFileContainTitleLine(FileName)
```

Determine whether the SMILES file contain a title line based on the presence of a string SMILES, Name or ID in the first line.

### Arguments:

```
FileName (str): Name of a file.
```

### Returns:

```
bool : True, File contains title line; Otherwise, False.
```

# ExpandFileNames

```
ExpandFileNames(FilesSpec, Delimiter = ",")
```

Expand files specification using glob module to process any \* or ? wild cards in file names and return a list of expanded file names.

### Arguments:

```
FilesSpec (str): Files specifications
Delimiter (str): Delimiter for file specifications
```

### Returns:

```
list : List of expanded file names
```

### ${\sf GetExamplesTextFromDocOptText}$

```
GetExamplesTextFromDocOptText(DocOptText)
```

Get script usage example lines from a docopt doc string. The example text line start from a line containing `Examples:` keyword at the beginning of the line.

#### Arguments:

```
DocOptText (str): Doc string containing script usage examples lines starting with a line marked by 'Examples:' keyword at the beginning of a line.
```

#### Returns:

```
\operatorname{str} : A string containing text lines retrieved from the examples section of \operatorname{DocOptText} parameter.
```

### GetExcelStyleColumnLabel

```
GetExcelStyleColumnLabel(ColNum)
```

Return Excel style column label for a colum number.

### Arguments:

```
ColNum (int): Column number
```

### Returns:

```
str : Excel style column label.
```

### GetFormattedElapsedTime

```
{\tt GetFormattedElapsedTime} (Starting {\tt WallClockTime}\,,\,\, Starting {\tt ProcessorTime}\,)
```

Get elapsed wallclock and processor times as a string in the following format: %d wallclock secs ( %.2f process secs).

# Arguments:

```
StartingWallClockTime (float): Starting wallclock time in seconds. StartingProcessorTime (float): Starting processor time in seconds.
```

### Returns:

```
str : Elapsed time formatted as: %d wallclock secs ( %.2f process secs)
```

## ${\sf GetFormattedFileSize}$

```
GetFormattedFileSize(FileName, Precision = 1)
```

Get file size as a string in the following format: %.\*f <bytes, KB, MB, GB>

### Arguments:

```
FileName (str): File path.
Precision (int): File size precision.
```

### Returns:

```
str : File size formatted as: %.2f <bytes, KB, MB, GB>
```

### GetMayaChemToolsLibDataPath

```
GetMayaChemToolsLibDataPath()
```

Get location of MayaChemTools lib data directory.

#### Returns:

```
str : Location of MayaChemTools lib data directory.
```

The location of MayaChemTools lib data directory is determined relative to MayaChemTools python lib directory name available through sys.path.

#### GetTextLines

```
GetTextLines(TextFilePath)
```

Read text lines from input file, remove new line characters and return a list containing stripped lines.

## Arguments:

```
TextFilePath (str): Text file name including file path.
```

#### Returns

```
list : A list lines.
```

#### GetTextLinesWords

```
GetTextLinesWords(TextFilePath, Delimiter, QuoteChar, IgnoreHeaderLine)
```

Parse lines in the specified text file into words in a line and return a list containing list of parsed line words.

### Arguments:

```
TextFilePath (str): Text file name including file path.

Delimiter (str): Delimiter for parsing text lines.

QuoteChar (str): Quote character for line words.

IgnoreHeaderLine (bool): A flag indicating whether to ignore first valid data line corresponding to header line.
```

## Returns:

```
list: A list of lists containing parsed words for lines.
```

The lines starting with # or // are considered comment lines and are ignored during parsing along with any empty lines.

### GetWallClockAndProcessorTime

```
GetWallClockAndProcessorTime()
```

Get wallclock and processor times in seconds.

### Returns:

```
float : Wallclock time.
float : Processor time.
```

### IsEmpty

```
IsEmpty(Value)
```

Determine whether the specified value is empty after converting it in to a string and removing all leading and trailing white spaces. A value of type None is considered empty.

## Arguments:

```
Value (str, int or float): Text or a value
```

### Returns:

```
bool : True, Text string is empty; Otherwsie, False.
```

#### **IsFloat**

```
IsFloat(Value)
```

Determine whether the specified value is a float by converting it into a float.

### Arguments:

```
Value (str, int or float): Text
```

#### Returns:

```
bool : True, Value is a float; Otherwsie, False.
```

#### IsInteger

```
IsInteger(Value)
```

Determine whether the specified value is an integer by converting it into an int.

### Arguments:

```
Value (str, int or float): Text
```

#### Returns:

bool: True, Value is an integer; Otherwsie, False.

### IsNumber

```
IsNumber(Value)
```

Determine whether the specified value is a number by converting it into a float.

## Arguments:

```
Value (str, int or float): Text
```

### Returns:

```
bool : True, Value is a number; Otherwsie, False.
```

### JoinWords

```
JoinWords(Words, Delimiter, Quote = False)
```

Join words in a list using specified delimiter with optional quotes around words.

## Arguments:

```
Words (list): List containing words to join. Delimiter (string): Delimiter for joining words. Quote (boolean): Put quotes around words.
```

### Returns:

```
str : String containing joined words.
```

## ObjectFromBase64EncodedString

```
ObjectFromBase64EncodedString(EncodedObject)
```

Generate Python object from a bas64 encoded and pickled object string.

### Arguments:

```
str: Base64 encoded and pickled object string.
```

### Returns:

```
object : Python object or None.
```

### ObjectToBase64EncodedString

```
ObjectToBase64EncodedString(Object)
```

Encode Python object into base64 encoded string. The object is pickled before encoding.

### Arguments:

```
object: Python object.
```

#### Returns:

str : Base64 encode object string or None.

#### ParseFileName

```
ParseFileName(FilePath)
```

Parse specified file path and return file dir, file name, and file extension.

#### Arguments:

```
FilePath (str): Name of a file with complete file path.
```

#### Returns:

```
str : File directory.
str : File name without file extension.
str : File extension.
```

### PrintError

```
PrintError(Msg, Status=1)
```

Print message to stderr along with flushing stderr and exit with a specified status. An `Error` prefix is placed before the message.

### Arguments:

```
Msg (str): Text message.
Status (int): Exit status.
```

### Printl nfo

```
PrintInfo(Msg='')
```

Print message to stderr along with flushing stderr.

### Arguments:

```
Msg (str): Text message.
```

# PrintWarning

```
PrintWarning(msg)
```

Print message to stderr along with flushing stderr. An `Warning` prefix is placed before the message.

### Arguments:

```
Msg (str): Text message.
```

### ProcessOptionInfileParameters

```
\label{eq:processOptionInfileParameters(ParamsOptionName, ParamsOptionValue, InfileName = None, OutfileName = None)
```

Process parameters for reading input files and return a map containing processed parameter names and values.

### Arguments:

```
ParamsOptionName (str): Command line input parameters option name.

ParamsOptionValues (str): Comma delimited list of parameter name and value pairs.

InfileName (str): Name of input file.
```

```
OutfileName (str): Name of output file.
```

#### Returns:

dictionary: Processed parameter name and value pairs.

The parameter name and values specified in ParamsOptionValues are validated before returning them in a dictionary.

#### ProcessOptionMultiprocessingParameters

ProcessOptionMultiprocessingParameters(ParamsOptionName, ParamsOptionValue)

Process parameters for multiprocessing and return a map containing processed parameter names and values.

### Arguments:

```
ParamsOptionName (str): Command line multiprocessing parameters option name. ParamsOptionValues (str): Comma delimited list of parameter name and value pairs.
```

#### Returns:

dictionary: Processed parameter name and value pairs.

The parameter name and values specified in ParamsOptionValues are validated before returning them in a dictionary.

### ProcessOptionOutfileParameters

ProcessOptionOutfileParameters(ParamsOptionName, ParamsOptionValue, InfileName = None,
OutfileName = None)

Process parameters for writing output files and return a map containing processed parameter names and values.

## Arguments:

```
ParamsOptionName (str): Command line input parameters option name.

ParamsOptionValues (str): Command delimited list of parameter name and value pairs.

InfileName (str): Name of input file.

OutfileName (str): Name of output file.
```

### Returns:

dictionary: Processed parameter name and value pairs.

The parameter name and values specified in ParamsOptionValues are validated before returning them in a dictionary.

The default value of some parameters may depend on type of input file. Consequently, the input file name is also needed.

### ${\tt ProcessOptionSeabornPlotParameters}$

```
ProcessOptionSeabornPlotParameters(ParamsOptionName, ParamsOptionValue,
ParamsDefaultInfo = None)
```

Process parameters for generating Seaborn plots and return a map containing processed parameter names and values.

### Arguments:

```
ParamsOptionName (str): Command line seaborn parameters option name. ParamsOptionValues (str): Comma delimited list of parameter name and value pairs. ParamsDefaultValues (dict): Default values for selected parameters.
```

### Returns:

dictionary: Processed parameter name and value pairs.

The parameter name and values specified in ParamsOptionValues are validated before returning them in a dictionary.

### ReplaceHTMLEntitiesInText

```
ReplaceHTMLEntitiesInText(Text)
```

Check and replace the followng HTML entities to their respective code for display in a browser: < (less than), > (greater than), & (ampersand), " (double quote), and ' (single quote).

## Arguments:

```
Text (str): Text value.
```

#### Returns:

```
str : Modifed text value.
```

### TruncateText

```
TruncateText(Text, Width, TrailingChars = "...")
```

Truncate text using specified width along with appending any trailing characters.

### Arguments:

```
Text (string): Input text.
Width (int): Max number of characters before truncating text.
Delimiter (string): Trailing characters to append or None.
```

#### Returns:

```
str : Truncated text
```

### ValidateOptionFileExt

```
ValidateOptionFileExt(OptionName, FileName, FileExts)
```

Validate file type based on the specified file extensions delimited by spaces.

### Arguments:

```
OptionName (str): Command line option name.
FileName (str): Name of a file.
FileExts (str): Space delimited string containing valid file extensions.
```

The function exits with an error message for a file name containing invalid file extension.

### ValidateOptionFilePath

```
ValidateOptionFilePath(OptionName, FilePath)
```

Validate presence of the file.

### Arguments:

```
OptionName (str): Command line option name. FilePath (str): Name of a file with complete path.
```

The function exits with an error message for a file path that doesn't exist.

## ValidateOptionFloatValue

```
ValidateOptionFloatValue(OptionName, OptionValue, CmpOpValueMap)
```

Validate option value using comparison operater and value pairs in specified in a map.

### Arguments:

```
OptionName (str): Command line option name.

OptionValue (float or str): Command line option value.

CmpOpValueMap (dictionary): Comparison operator key and value pairs to validate values specified in OptionValue.
```

The function exits with an error message for an invalid option values specified in OptionValue.

### Example(s):

```
ValidateOptionNumberValue("-b, --butinaSimilarityCutoff",
    Options["--butinaSimilarityCutoff"],
    {">": 0.0, "<=" : 1.0})</pre>
```

#### ValidateOptionIntegerValue

```
ValidateOptionIntegerValue(OptionName, OptionValue, CmpOpValueMap)
```

Validate option value using comparison operater and value pairs in specified in a map.

#### Arguments:

```
OptionName (str): Command line option name.

OptionValue (int or str): Command line option value.

CmpOpValueMap (dictionary): Comparison operator key and value pairs to validate values specified in OptionValue.
```

The function exits with an error message for an invalid option values specified in OptionValue.

#### Example(s):

### ValidateOptionNumberValue

```
ValidateOptionNumberValue(OptionName, OptionValue, CmpOpValueMap)
```

Validate option value using comparison operater and value pairs in specified in a map.

### Arguments:

```
OptionName (str): Command line option name.

OptionValue (int or float): Command line option value.

CmpOpValueMap (dictionary): Comparison operator key and value pairs to validate values specified in OptionValue.
```

The function exits with an error message for an invalid option values specified in OptionValue.

### Example(s):

### ValidateOptionNumberValues

```
Validate Option Number Values (Option Name, Option Value String, Option Value Count, Option Value Delimiter, Option Value Type, Cmp Op Value Map)\\
```

Validate numerical option values using option value string, delimiter, value type, and a specified map containing comparison operator and value pairs.

### Arguments:

```
OptionName (str): Command line option name.
OptionValueString (str): Command line option value.
OptionValueCount (int): Number of values in OptionValueString.
OptionValueDelimiter (str): Delimiter used for values in OptionValueString.
OptionValueType (str): Valid number types (integer or float)
CmpOpValueMap (dictionary): Comparison operator key and value pairs to validate values specified in OptionValueString.
```

The function exits with an error message for invalid option values specified in OptionValueString

# Example(s):

```
ValidateOptionNumberValues("-m, --molImageSize",
    Options["--molImageSize"], 2, ",", "integer", {">": 0})
```

#### ValidateOptionTextValue

```
ValidateOptionTextValue(OptionName, OptionValue, ValidValues)
```

Validate option value based on the valid specified values separated by spaces.

#### Arguments:

```
OptionName (str): Command line option name.

OptionValue (str): Command line option value.

ValidValues (str): Space delimited string containing valid values.
```

The function exits with an error message for an invalid option value.

## ValidateOptionsDistinctFileNames

```
ValidateOptionsDistinctFileNames(OptionName1, FilePath1, OptionName2, FilePath2)
```

Validate two distinct file names.

### Arguments:

```
OptionNamel (str): Command line option name.
FilePathl (str): Name of a file with complete file path.
OptionName2 (str): Command line option name.
FilePath2 (str): Name of a file with complete file path.
```

The function exits with an error message for two non distinct file names.

### ValidateOptionsOutputFileOverwrite

```
ValidateOptionsOutputFileOverwrite(OptionName, FilePath, OverwriteOptionName, OverwriteStatus)
```

Validate overwriting of output file.

### Arguments:

```
OptionName (str): Command line option name.
FilePath (str): Name of a file with complete file path.
OverwriteOptionName (str): Overwrite command line option name.
OverwriteStatus (bool): True, overwrite
```

The function exits with an error message for a file that is present and is not allowed to be written as indicated by value of OverwriteStatus.

### WrapText

```
WrapText(Text, Delimiter, Width)
```

Wrap text using specified delimiter and width.

## Arguments:

```
Text (string): Input text
Delimiter (string): Delimiter for wrapping text
Width (int): Max number of characters before wrapping text
```

### Returns:

```
str : Wrapped text
```

### **AUTHOR**

Manish Sud <msud@san.rr.com>

### **COPYRIGHT**

Copyright (C) 2020 Manish Sud. All rights reserved.

This file is part of MayaChemTools.

MayaChemTools is free software; you can redistribute it and/or modify it under the terms of the GNU Lesser

General Public License as published by the Free Software Foundation; either version 3 of the License, or (at your option) any later version.