
NAME

MiscUtil

SYNOPSIS

import MiscUtil

DESCRIPTION

MiscUtil module provides the following functions:

CheckFileExt, CheckTextValue, DoesSMILESFileContainTitleLine, ExpandFileNames, GetExamplesTextFromDocOptText, GetExcelStyleColumnLabel, GetFormattedElapsedTime, GetFormattedFileSize, GetMayaChemToolsLibDataPath, GetMayaChemToolsVersion, GetTextLines, GetTextLinesWords, GetWallClockAndProcessorTime, IsEmpty, IsFloat, IsInteger, IsNumber, JoinWords, ObjectFromBase64EncodedString, ObjectToBase64EncodedString, ParseFileName, PrintError, PrintInfo, PrintWarning, ProcessOptionConformerGenerator, ProcessOptionConformerParameters, ProcessOptionInfileParameters, ProcessOptionMultiprocessingParameters, ProcessOptionNameValuePairParameters, ProcessOptionOutfileParameters, ProcessOptionPyMOLCubeFileViewParameters, ProcessOptionSeabornPlotParameters, ReplaceHTMLEntitiesInText, TruncateText, ValidateOptionFileExt, ValidateOptionFilePath, ValidateOptionFloatValue, ValidateOptionIntegerValue, ValidateOptionNumberValue, ValidateOptionNumberValues, ValidateOptionTextValue, ValidateOptionsDistinctFileNames, ValidateOptionsOutputFileOverwrite, 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(FileSpec, 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:

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

Returns:

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

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:

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

GetExcelStyleColumnLabel

```
GetExcelStyleColumnLabel(ColNum)
```

Return Excel style column label for a column number.

Arguments:

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

Returns:

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

GetFormattedElapsedTime

```
GetFormattedElapsedTime(StartingWallClockTime, StartingProcessorTime)
```

Get elapsed wallclock and processor times as a string in the following format: Wallclock: %s days, %d hrs, %d mins, %d secs (Process: %d days, %d hrs, %d mins, %.2f secs).

Arguments:

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

Returns:

```
str : Elapsed time formatted as:  
Wallclock: %s days, %d hrs, %d mins, %d secs (Process: %d days,  
%d hrs, %d mins, %.2f secs)
```

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.

GetMayaChemToolsVersion

GetMayaChemToolsVersion()

Get version number for MayaChemTools from PackageInfo.csv file in MayaChemTool lib data directory.

Returns:

str : Version number

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 (bool): 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.

PrintInfo

```
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.

ProcessOptionConformerGenerator

ProcessOptionConformerGenerator(OptionName, OptionValue)

Process conformer generator option and return a map containing parameter name and values for generating conformers.

Arguments:

ParamOptionName (str): Command line conformer generator option name
 ParamOptionValue (str): Command line conformer generator option value

Returns:

dictionary: Conformer generation parameter name and value pairs.

ProcessOptionConformerParameters

ProcessOptionConformerParameters(ParamsOptionName, ParamsOptionValue, ParamsDefaultInfo = None)

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

Arguments:

ParamsOptionName (str): Command line conformer generation parameters option name.
 ParamsOptionValue (str): Comma delimited list of parameter name and value pairs.
 ParamsDefaultInfo (dict): Default values to override 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.

ProcessOptionInfileParameters

ProcessOptionInfileParameters(ParamsOptionName, ParamsOptionValue, InfileName = None, OutfileName = None, ParamsDefaultInfo = 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.
 ParamsOptionValue (str): Comma delimited list of parameter name and value pairs.
 InfileName (str): Name of input file.
 OutfileName (str): Name of output file.
 ParamsDefaultInfo (dict): Default values to override for selected parameters.

Returns:

dictionary: Processed parameter name and value pairs.

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

ProcessOptionNameValuePairParameters

```
ProcessOptionNameValuePairParameters(ParamsOptionName, ParamsOptionValue,
ParamsDefaultInfo)
```

Process name and value parameter pairs for an option and return a map containing processed parameter names and values.

Arguments:

ParamsOptionName (str): Command line option name for name and value parameter pairs.
 ParamsOptionValue (str): Comma delimited list of parameter name and value parameter pairs.
 ParamsDefaultInfo (dict): A dictionary containing a list of parameter type and default value pairs keyed by parameter name. Supported parameter types: bool, int, float, file, and str.

Returns:

dictionary: Processed parameter name and value pairs.

The parameter names and values specified in ParamsOptionValue are validated before returning them in a dictionary.

Example(s):

```
ParamsDefaultInfo = {"Cleanup": ["bool", True], "RemoveFragments":
["bool", True], "Neutralize": ["bool", True],
"CanonicalizeTautomer": ["bool", True]}
ProcessOptionNameValuePairParameters("--methodologyParams",
Options["--methodologyParams"], ParamsDefaultInfo)
```

ProcessOptionOutfileParameters

```
ProcessOptionOutfileParameters(ParamsOptionName, ParamsOptionValue, InfileName = None,
OutfileName = None, ParamsDefaultInfo = 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.
 ParamsOptionValue (str): Comma delimited list of parameter name and value pairs.
 InfileName (str): Name of input file.
 OutfileName (str): Name of output file.
 ParamsDefaultInfo (dict): Default values to override for selected parameters.

Returns:

dictionary: Processed parameter name and value pairs.

The parameter name and values specified in ParamsOptionValue 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.

ProcessOptionPyMOLCubeFileViewParameters

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

Process PyMOL parameters for cube file views and return a map containing processed parameter names and values.

ParamsOptionValue is a comma delimited list of parameter name and value pairs for setting up PyMOL views.

The supported parameter names along with their default and possible values are shown below:

```
ContourColor1, red, ContourColor2, blue,
ContourLevel1, -0.02, ContourLevel2, 0.02,
ContourLevel, 0.02,
ContourLevelAutoAt, 0.5,
ESPRampValues, -1.0 0 1.0,
ESPRampColors, red white blue,
HideHydrogens, yes, DisplayESP, OnSurface,
DisplayMolecule, BallAndStick,
DisplaySphereScale, 0.3, DisplayStickRadius, 0.2,
MeshQuality, 2, MeshWidth, 0.5,
SurfaceQuality, 2, SurfaceTransparency, 0.25,
VolumeColorRamp, auto, VolumeColorRampOpacity, 0.2,
VolumeContourWindowFactor, 0.05
```

Arguments:

```
ParamsOptionName (str): Command line PyMOL view option name.
ParamsOptionValues (str): Comma delimited list of parameter name and value pairs.
ParamsDefaultInfo (dict): Default values to override for selected parameters.
```

Returns:

```
dictionary: Processed parameter name and value pairs.
```

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.
ParamsOptionValue (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 ParamsOptionValue are validated before returning them in a dictionary.

ReplaceHTMLEntitiesInText

```
ReplaceHTMLEntitiesInText(Text)
```

Check and replace the following 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 : Modified 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 operator 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})
```

ValidateOptionIntegerValue

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

Validate option value using comparison operator 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):

```
ValidateOptionIntegerValue("--maxConfs", Options["--maxConfs"],
    {">": 0})
```

ValidateOptionNumberValue

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

Validate option value using comparison operator 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):

```
ValidateOptionNumberValue("--maxConfs", int(Options["--maxConfs"]),
    {">": 0})
ValidateOptionNumberValue("-b, --butinaSimilarityCutoff",
    float(Options["--butinaSimilarityCutoff"]),
    {">": 0.0, "<=" : 1.0})
```

ValidateOptionNumberValues

```
ValidateOptionNumberValues(OptionName, OptionValueString, OptionValueCount,
    OptionValueDelimiter, OptionValueType, CmpOpValueMap)
```

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:

```
OptionName1 (str): Command line option name.  
FilePath1 (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
```

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