

---

**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
```

**AUTHOR**

Manish Sud <msud@san.rr.com>

**COPYRIGHT**

Copyright (C) 2024 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.