

NAME

MDLMolFileIO

SYNOPSIS

```
use FileIO::MDLMolFileIO;

use FileIO::MDLMolFileIO qw(:all);
```

DESCRIPTION

MDLMolFileIO class provides the following methods:

new, GenerateMoleculeString, IsMDLMolFile, ParseMoleculeString, ReadMolecule, ReadMoleculeString, WriteMolecule

The following methods can also be used as functions:

GenerateMoleculeString, IsMDLMolFile, ParseMoleculeString

Data specific to MDLMolFileIO class not directly used by Molecule, Atom and Bond objects - data label/value pairs, atom StereoParity and so on - is associated to and retrieved from appropriate objects using following methods:

```
SetMDL<PropertyName>
GetMDL<PropertyName>.
```

MDLMolFileIO class is derived from *FileIO* class and uses its methods to support generic file related functionality.

METHODS

new

```
$NewMDLMolFileIO = new FileIO::MDLMolFileIO(%NamesAndValues);
```

Using specified *MDLMolFileIO* property names and values hash, new method creates a new object and returns a reference to newly created MDLMolFileIO object.

GenerateMoleculeString

```
$MoleculeString = $MDLMolFileIO->GenerateMoleculeString($Molecule);
$MoleculeString = FileIO::MDLMolFileIO::GenerateMoleculeString($Molecule);
```

Returns a MoleculeString in MDLMol format corresponding to *Molecule*.

IsMDLMolFile

```
$Status = $MDLMolFileIO->IsMDLMolFile($FileName);
$Status = FileIO::MDLMolFileIO::IsMDLMolFile($FileName);
```

Returns 1 or 0 based on whether *FileName* is a MDLMol file.

ParseMoleculeString

```
$Molecule = $MDLMolFileIO->ParseMoleculeString($MoleculeString);
$Molecule = FileIO::MDLMolFileIO::ParseMoleculeString($MoleculeString);
```

Parses *MoleculeString* and returns a Molecule object.

ReadMolecule

```
$Molecule = $MDLMolFileIO->ReadMolecule($FileHandle);
```

Reads data for the compound in a file using already opened *FileHandle*, creates, and returns a Molecule object.

ReadMoleculeString

```
$MoleculeString = $MDLMolFileIO->ReadMoleculeString($FileHandle);
```

Reads data for the compound in a file using already opened *FileHandle* and returns a MoleculeString

corresponding to compound structure and other associated data.

WriteMolecule

```
$MDLMolFileIO->WriteMolecule($Molecule);
```

Writes *Molecule* data to a file in MDLMol format and returns MDLMolFileIO.

AUTHOR

Manish Sud <msud@san.rr.com>

SEE ALSO

MoleculeFileIO.pm, SDFFileIO.pm

COPYRIGHT

Copyright (C) 2017 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.